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Institut für Neutronenphysik und Reaktortechnik
Projekt Schneller Brüter

MIGRØS-3:
A Code for the Generation of Group Constants for Reactor Calculations from Neutron Nuclear Data in KEDAK Format

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Abstract:

The code MIGRØS-3 was developed from MIGRØS-2. The main advantage of MIGRØS-3 is its compatibility with the new conventions of the latest version of the Karlsruhe nuclear data library, KEDAK-3. Moreover, to some extent refined physical models were used and numerical methods were improved.

MIGRØS-3 allows the calculation of microscopic group cross sections of the ABBN type from isotopic neutron data given in KEDAK-format. All group constants, necessary for diffusion-, consistent P_l- and S_N-calculations can be generated. Anisotropy of elastic scattering can be taken into account up to P_5.

A description of the code and the underlying theory is given. The input and output description, a sample problem and the program lists are provided.

MIGRØS-3: Ein Code zur Erzeugung von Gruppenkonstanten für Reaktorrechnungen aus Neutronen-Kerndaten im KEDAK-Format

Zusammenfassung:

Der Code MIGRØS-3 ist eine Weiterentwicklung von MIGRØS-2. Der Hauptvorteil von MIGRØS-3 gegenüber MIGRØS-2 ist, daß in MIGRØS-3 die in der letzten Version der Karlsruher Kerndatenbibliothek KEDAK-3 eingeführten neuen Konventionen berücksichtigt werden. Darüber hinaus wurden teilweise verfeinerte physikalische Modelle und verbesserte numerische Methoden benutzt.

MIGRØS-3 erlaubt die Berechnung von mikroskopischen Gruppenwirkungsquerschnitten vom ABBN Typ für isotopenweise gegebene Neutronendaten im KEDAK-Format. Alle für Diffusions-, konsistente P_l- und S_N-Rechnungen benötigten Gruppenkonstanten können erzeugt werden. Dabei kann die Anisotropie der elastischen Streuung bis P_5 berücksichtigt werden.

Der Code und die zugrunde liegende Theorie werden beschrieben. Es werden die Eingabe- und Ausgabebeschreibung, ein Rechenbeispiel und die Programmlisten bereitgestellt.

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   (H. Huschke, B. Krieg)[+)]

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   (P. Vertes)[+)]

[+)] The authors given in parentheses are the authors of the original modules as described in /1/.

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INTRODUCTION

The code MIGRØS-3 has been further developed from MIGRØS-2, described in /1/. MIGRØS-3 is compatible with the latest version of the Karlsruhe nuclear data file KEDAK-3, /2/. That means the formal differences between KEDAK-2 and KEDAK-3 have been taken account of in MIGRØS-3. These main formal differences are

1. Introduction of an individual energy grid for each data type of each isotope, within which the data can be obtained by linear interpolation. (On KEDAK-2 the same energy grid was used for all data types of one isotope.)

2. Introduction of new data types.

Moreover the physical and numerical approaches have been improved in many of the modules.

A more detailed description of the changes in each module is given in the corresponding chapters (chapters 4 - 12).

MIGRØS-3 calculates microscopic group constants for isotopes given in KEDAK format. These can be used for the production of macroscopic group cross sections for diffusion-, consistent P_l- and S_n-calculations. Anisotropy of elastic scattering can be taken into account up to P_5 in S_N-P_L- or S_N-T_L-approximations (higher order transport approximations /6/). Microscopic elastic scattering transfer matrices can be calculated with fine-structure weighting functions generated for special material mixtures (specified by the input; module 6) and as basic data for the REMO-correction, where mixture-dependent fine-structure weighting is performed in GRUCAL, /5/, during the computation of macroscopic cross sections, /4/, (module 9). Resonance self shielding is treated according to the method developed by ABBN, /3/.

In the following a brief description is given of the calculation of the different types of group constants in modules 1 to 10 of MIGRØS-3.

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The calculation of weighted average group constants from pointwise data on KEDAK. (Chapter 3, module 4)

Weighted average group cross sections for infinite dilution are calculated from pointwise tabulated data for all reaction types given on KEDAK. Besides this weighted group values are provided for the average elastic scattering cosine, $\bar{\mu}$, for the number of secondary neutrons per fission, ν, for the ratio of capture to fission cross section, α, and for the number of fission neutrons per neutron absorption, η.

Integrations are carried out by a trapezoidal rule. In the case of an energy pointwise weighting spectrum the energy points of KEDAK and of the weighting function are used as integration grid. If the weighting spectrum is given as analytic function, an automatic interval subdivision is used, starting with the KEDAK points as integration grid.

The calculation of energy resonance self-shielding factors and group cross sections for infinite dilution from resolved resonance parameters and from statistical resonance parameters. (Chapters 4 and 5, modules 1 and 2)

For capture, fission and elastic scattering flux-weighted ($w(E) \sim \frac{1}{\sigma_t(E)+\sigma_o}$) resonance self-shielding factors and for elastic scattering and the total neutron reaction current-weighted ($w(E) \sim \{\frac{1}{\sigma_t(E)+\sigma_o}\}^2$) self-shielding factors dependent on temperature and on the background cross section σ_o and the average group cross sections are calculated from resonance parameters.

In the resolved-resonance region Breit-Wigner single level parameters and Doppler-broadened line shape functions are used. Interference between potential and resonance scattering and the overlapping of resonances is taken into account exactly. Integrations are carried out by a trapezoidal rule with automatic interval subdivision. The integration starts with the resonance energies and the group boundaries as interval limits.

In the unresolved resonance region an analytical model, based on average resonance parameters and χ^2-distributions for the parameters, is used. Interference between potential and resonance scattering is partly taken into account. Overlapping of resonances is considered approximately. For the calculation of the statistical averages an approximate procedure of numerical integration is used.

The calculation of average group cross sections for infinite dilution and of energy resonance self-shielding factors from energy pointwise data. (Chapter 9, module 3)

The module calculates flux weighted average group cross sections for infinite dilution and σ_o-dependant (also flux weighted) energy resonance self-shielding factors for the cross section types σ_c (capture) resp. σ_a (absorption), σ_f (fission), σ_e (elastic scattering), and the product $\sigma_e \cdot \bar{\mu}_e$. For the total reaction and the product $\sigma_e \cdot \bar{\mu}_e$ additionally current weighted quantities are produced.

Both the flux weighted and the current weighted quantities can only be calculated for the temperature for which the cross sections are stored on the KEDAK library.

The grid, which is used as integration base, is composed out of the grids of all participating cross sections (and eventually the grid of the weighting function). Within an integration interval, which is defined by two adjacent energy points of the composed grid, the numerical Romberg integration method is used to compute the various integrals. If the expression of the weighting function is known, these integrals can also be solved analytically.

The calculation of normalized elastic-scattering matrices up to the fifth Legendre-order, of total elastic flux-weighted and of total group cross sections with moment-dependent weighting. (Chapter 7, module 6)

Group-to-grop transfer elements are calculated from the Legendre-moments of the elastic scattering kernel for $\ell = 0,1,\ldots,5$. Different options for the approximation of the moments of neutron flux density to be used as weighting functions are built in. Weighting dependent on ℓ with $\psi_\ell(E) = F(E)/|\Sigma_t(E)|^{\ell+1}$ is recommended, $F(E)$ = total collision density, $\Sigma_t(E)$ = total macroscopic cross section of the reactor subzone under consideration. Required data are: tabulated elastic angular distributions in the c.m.-system with a unique angular grid for each isotope, total elastic, total reaction cross sections, and mean elastic scattering cosines in the laboratory system. For one isotope the energy grids for the elastic distributions, the cross sections and the scattering cosines may be different. Different isotopes may have different distribution cosine grids. Energy and angle interpolation of the scattering distributions (after transformation into the laboratory system) is achieved with polynomials up to degree three. Integration over the inscattering group is performed as integration over the corresponding angular interval with use of Simpson's rule, the weighted integration over the outscattering group is

done with an improved trapezoid technique. Special account is taken of strongly fluctuating integrands in case of higher ℓ-values as well as in resonance regions of Σ_t. Total flux weighted elastic and ψ_ℓ-weighted total reaction group cross sections (the latter for higher transport approximations) are computed with the modified trapezoid technique.

The calculation of the interval cross sections and the zero'th and higher moments of the normalized elastic transferelements for the REMO correction. (Chapter 8, module 9)

The REMØ correction, described in chapter 3.5 of /4/, improves the treatment of the elastic downscattering in a coarse energy group system ($\simeq$ 26 energy groups). For a material mixture the coarse group scattering matrix is calculated with the help of the mixture weighting spectrum in a narrow resonance approximation, e.g. with the program GRUCAL /5/. The coarse-group system is subdivided into a number of fine groups with intervals. (Usually 14 fine groups with 6 intervals each.)

MIGRØS calculates the following input for the REMØ correction:

- weighted scalar group constants for the KEDAK reaction types SGT, SGN and MUEL. For the integration the trapezoidal rule is applied with the energy mesh points from KEDAK.

- weighted transfer probabilities from interval to inscattering group. The required angle and energy integrations are performed with the Romberg method over the whole energy region to be calculated. If no angular distributions are available on KEDAK linear anisotropy is assumed. Generally the interpolations are linear in energy or in the cosine of the scattering angle. Only for angular distributions with a small number of angle meshpoints a cubic interpolation is applied.

The calculation of the normalized transfer matrices for inelastic scattering, (n,2n)- and (n,3n)-reactions. (Chapter 6, module 5)

The transfer matrix for inelastic scattering is calculated as a combination of transfer probabilities due to the excitation of discrete levels and of transfer probabilities due to the excitation of continuous levels of the residual nucleus. The energy loss of the inelastically scattered neutron is calculated from the excitation energies of the discrete levels and from evaporation models. For the calculation of the transfer matrices of (n,2n)- or (n,3n)-reactions evaporation models are used. The numerical integrations in connection

with the calculations of transfer probabilities due to the excitation of discrete levels are carried out by a trapezoidal rule. As integration points the combination of all energy points of the inelastic excitation cross sections and the energy points of the spectrum are used. The numerical integration in connection with the treatment of continuous excitation levels of the residual nucleus (evaporation models) are carried out by the Simpson rule.

The calculation of the fission spectra. (Chapter 12, module 7)

Fission spectra are calculated by the Watt-Cranberg formula using the fragment kinetic energy per nucleon and the Watt fragment nuclear "temperature" or by a Maxwellian distribution, using the Maxwellian fragment nuclear "temperature", depending on the information given on KEDAK.

The calculation of weighted 1/v-group values. (Chapter 11, module 8)

A trapezoidal rule with automatic interval subdivision is used for the integration.

Thermal cross sections

One thermal group with a Maxwellian spectrum is assumed.

As a consequence of its modular structure MIGRØS-3 is very flexible in its need of storage.

A standard input is provided internally for the production of a 26-group cross section set with the same group structure as the ABN-set, /3/, and with a 1/E weighting spectrum. All details of the standard input are given in the input description in chapter 2.1. If the user does not apply the standard input, he has to make sure, that his input is physically meaningful.

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1. The organization of MIGRØS-3

1.1 The logical structure of MIGRØS-3

The code MIGRØS-3 has a modular structure. It consists of a control module and of several computational modules. In the control module all the input information, except the nuclear data, is checked, the order of processing is fixed and the information for the single computational modules is prepared. A computational module is defined as a logically complete, executable computer procedure, consisting of several subroutines and functions. In a computational module a specific type of group constants is calculated. The necessary nuclear data are read from the Karlsruhe nuclear data library, KEDAK /1/, in the computational modules, which also produce an output of the group constants on paper and on an external storage unit. The available computational modules are given in table I.

Control is transferred from the control module to a computational module by a CALL statement, which calls the entry subroutine of the module. It is not possible to transfer control directly from one module to another. A computational module can be called by the control module several times.

All computational modules are written in FØRTRAN-IV. All arrays are variably dimensioned, when they are influenced by input information. the control module is written in FØRTRAN-IV, except for the routines GAREA and DDTEST, which are written in IBM/370 ASSEMBLER.

Since the input of nuclear data and the output of the results is performed in the computational modules, the only information that must be transferred between the control module and the computational modules is input information other than nuclear data and information necessary for the control of the program. The transfer of data is partly done by an unlabeled CØMMØN-array. However, most of the data transfer is accomplished by the parameter lists in the entry subroutines of the computational modules.

MIGRØS-3 is organized in an overlay structure, which is given in table II.

1.2 The control module

The control module has three tasks:

- to read all input information except the nuclear data,
- to provide a central data array and the unlabeled CØMMØN-array,
- to control the order of computation of the computational modules.

In the routines GAREA and MAIN a central data array is provided, whose length depends on the total region available for the program. All region not used by the program itself or for other system purposes as e.g. input/output buffers is taken as data array (see 1.3 and 2.).

In the subroutine INPUT, all input information except the nuclear data is read and checked. The central data array is prepared and the computational modules are called.

The input information is stored and the working arrays for the computational modules are provided in the central data array. It consists of two sections. One is permanent and the same for all computational modules. The other section depends on the particular module being considered and is allocated only when control is actually transferred to the module. All information of the central data array is transferred by parameter lists in the entry subroutines of the computational modules. A description is given in table III.

There is also an unlabeled CØMMØN-array, which is described in table IV.

1.3 The organization of the central data array XL

The ASSEMBLER routine GAREA provides a central array named XL for the subroutine MAIN. The length of XL is defined by the difference between the length given by the REGION-parameter of the JOB-card in the IBM/OS control language, the length of the MIGRØS-3 program system itself (≈ 165 K bytes) and the length of input/output buffers.

The subroutine MAIN calls the subroutine EING, which first prints an input description of the MIGRØS system. Then all the input for the first material is read and the information necessary for the variable dimensioning of the input arrays in the XL array is retained, as e.g. the number of group boundaries, the number of points of the weighting function, the number of computational modules to be used etc. The input unit is "backspaced" to the beginning and then the subroutine INPUT is called. The starting addresses of the input arrays in the XL array are arguments of INPUT. The index NFR indicates the beginning of the non-permanent section of the XL array and is also an argument of the subroutine INPUT. All input arrays are filled with the information from the input cards or the standard built-in data. The input is also checked for consistency. Then the computational modules are called in the order fixed by the input.

Before each call of a computational module the length of the non-permanent section of the XL array is checked, whether it is long enough for the working arrays of the module. The length of these working arrays depends on the input information and, in some cases, can finally be defined only in the computational module itself. In this case an iterative procedure is used to determine the proper length. As a first step, a minimum length of such a working array is assumed. If it turns out to be too small, control is given back to the control module and the size of the array is increased. When the required size of all working arrays for the computational module in question is so large that it can not be accommodated by the XL array this module is bypassed and a message to the user is given.

After all the required computational modules for one material have been called, a RETURN-statement to the subroutine MAIN is given. If there are more materials, a new arrangement of the XL-array is made etc.

1.4 Auxiliary subroutines

1.4.1 Reading program for the Karlsruhe nuclear data library KEDAK

For reading KEDAK, the subroutine NDF is necessary. A description is given in /3/.

1.4.2 Weighting functions

In case no weighting functions are specified for the group cross sections and matrices in the input, the following two FUNCTIØNs are used:

```
FUNCTIØN PHI(E)
PHI = 1./E
RETURN
END
```

respectively the double precision version used by module 3 (FSTRUK)

```
REAL FUNCTIØN DPHI*8(E)
REAL*8 E
DPHI = 1.0D+0/E
RETURN
END
```

E is the energy in eV.

This weighting function is used for all group constants except the first and higher Legendre moments for elastic scattering.

The following tables are given in chapter 1:

Table I : Computational modules of MIGRØS-3, their tasks and their subroutines and functions.

Table II : Overlay structure of MIGRØS-3.

Table III : Structure of the central data array XL.

Table IV : Structure of the unlabeled COMMON array.

Table I Computational modules of MIGRØS-3, their tasks and their subroutines and functions

number of the module	described in	content	names of the subroutine and functions	entry subroutine
1	chapter 4	average group cross sections for infinite dilution and energy resonance selfshielding factors from resolved Breit-Wigner resonance parameters	DOPW, FGEM, NDF, PHI, PSIXI(with entry EXPPX), STOSS, WIRQ, WIRQU	FGEM
2	chapter 5	average group cross sections for infinite dilution and energy resonance selfshielding factors from statistical Breit-Wigner resonance parameters	DELTA, DMIT, DØPW, EPSI, EZZ, FSTAT, GAFM, GAMG, GAMN, NDF, PHASE, PHI, PØL, QUER, SIGC, SUCH, TAB	FSTAT
3	chapter 9	average group cross sections for infinite dilution and energy resonance self-shielding factors from energy pointwise neutron cross section data	DPHI, FSANO2,FSANO3,FSANO4, FSANO5, FSANO6, FSANO7, FSANO8, FSANO9, FSEXIN, FSGRAL, FSGRA1, FSGRA2, FSGRA3, FSLOMQ, FSNUO1, FSNUO2, FSNUO3, FSNUO4, FSNUO5, FSNUO6, FSNUO7, FSNUO8, FSNUO9, FSQUER, FSROMB, FSSNGL, FSTOLE, FSTRUK, FSTRUO, FSTRU1, FSTRU2, FSTRU3, FSTRU4, FSTRU5, FSXINT, FSWRS1, FSWRS2, FSWRS3, FSWRS9, FSWROO, NDF	FSTRUK
4	chapter 3	average group cross sections, for infinite dilution (without resonance self-shielding) from point data and average group values of $\overline{\mu}$, η, α, ν	DØPW, FL, GRUP, NDF, PHI, SUND,	SUND
5	chapter 6	normalized transfer matrices for inelastic scattering (calculated from discrete level excitation cross sections and from evaporation models) and normalized transfer matrices for (n,2n)- and (n,3n)-reactions (calculated from evaporation models	AKED, CUTS, DAØRG, DNFAK, DØPW, ENØRG, EXD, FINT, FIPØLA, FIPØLD, NDF, NDREAD, ØRDNEN, ØRD1, PHI, PRØB RENUDA, REPRØB, SCAT, SCATC, SCATD, SGINT, SIMPSI, SINPØL, SIØRG, SPECT TEMP, THETA, TRA, XINPØL	SCAT

Table I, continued

number of the module	described in	content	names of the subroutines and functions	entry subroutine
6	chapter 7	normalized elastic-scattering matrices up to the fifth Legendre order, elastic and total group cross sections	ADD, FLUMMI, GRUPIN, G, INFØRM, IPØLA, IPØLIN, LECAL, LEGANS, LEGINT, LEGIST, LEGPØL, LØØKO, LØØK1, LØØK2, LØØK3, MAKRØ, MIXSGT, MUKØN, NDF, PHI, PRINT, PUNK, PUSUM, SPRAL, SUM, TRAFØ.	FLUMMI
7	chapter 12	fission spectra	CHIINM, DØPW, NDF, SPALT	SPALT
8	chapter 11	1/V-average group values	EDV, PHI	EDV
9	chapter 8	zero'th and higher moments of elastic scattering for the "REMO"-correction	AKØR, AMESH, ANG, ANINT, AUSGL, BCM, EGRENZ, ENERG, FIPØL, FXINT, HIDR, ICSØP, INTEN, IPØL, ISØFAL, IWIN, IWØ, KEDDAT, LININT, LMI, MASSIN, NDF, NØRM, ORDN1, PHI, REMØ, REMP, SEARCH, SINT, SMØRN, SUCHM, WAHRS, WINK, ZWIN	REMØ
10	chapter 10	group cross sections in the thermal group	DØPW, NDF, THERM	THERM
control module	chapter 2		DDTEST, DØPW, EING, FREEFØ, FSTAE, GAREA, INPUT, MAIN, NDF	

Table II:

Overlay Structure of MIGRØS-3

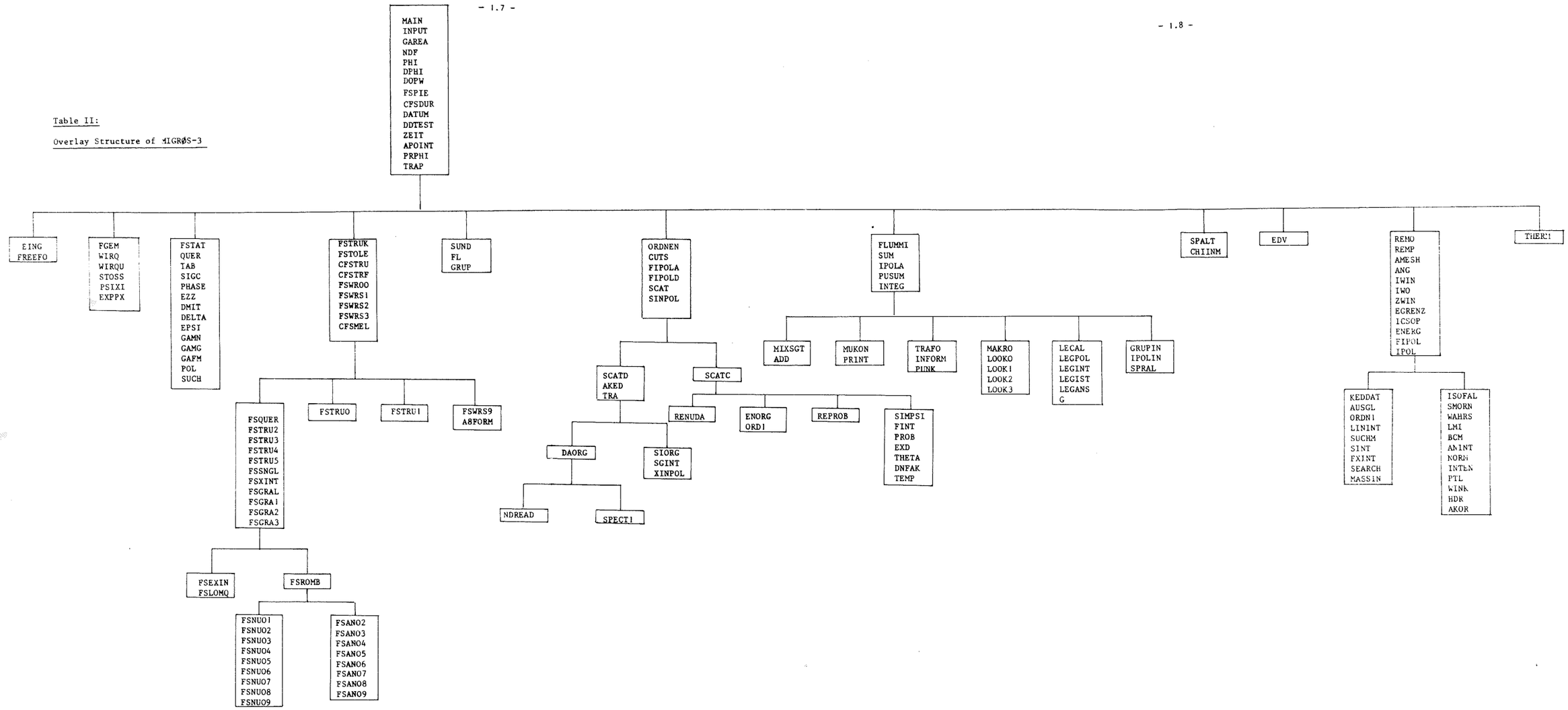

Table III

Structure of the central data array XL in the subroutine MAIN

a) The permanent section

The symbols of the input description in chapter 2 are used

length of the subarray	type	content of the subarray	see card n of the input description
NTYP	REAL*8	ITYP(I),I=1,NTYP	13
NMAT	REAL*8	NAME(I),I=1,NMAT	33
NMAT	REAL*4	TZ(I),I=1,NMAT	33
NE	REAL*4	ENG(I),I=1,NE	3
NFE+NE	REAL*4	EF(I),I=1,NFE and ENG(I),I=1,NE in increasing succession	3, 5
(NFE+NE)+ NSPEC	REAL*4	(F(I,J),I=1,(NFE+NE)), J=1,NSPEC	5
3*NA	INTEGER*4	(NR(I,J),I=1,3),J=1,NA	7
NT	REAL*4	TEMP(I),I=1,NT	9
MI+1	REAL*4	SIGO(I),I=1,MI	11
NA	INTEGER*4	NGRE(I),I=1,NA	7, 44, 41
NA*NE	INTEGER*4	(N1(I,J),I=1,NA) J=1,NE	3, 7, 44, 41
NA*NE	INTEGER*4	(N2(I,J),I=1,NA), J=1,NE	3, 7, 44, 41
NA*NE	INTEGER*4	(NFG(I,J),I=1,NA), J=1,NE	3, 7, 44, 41
NA*NE	INTEGER*4	(NFI(I,J),I=1,NA), J=1,NE	3, 7, 44, 41
2*NE	INTEGER*4	this subarray is defined, but information is actually only stored if module 9 is called	-

Table III, cont.

b) The non-permanent section

Besides the permanent section a non-permanent section is defined when a computational module is called. This non-permanent part exists only during the execution of a computational module. The non-permanent section starts with the index NFR, defined in the subroutine MAIN. The names of the auxiliary arrays are the same as those used in the formal parameters of the entry subroutines of the computational modules. All other symbols are the same as in the input description of chapter 2. (NE: see card 3 of the input description, MI: see card 11 of the input description. Some symbols used in b3) module 3 are also explained in 2.1.2.)

b1) Module 1

length of the subarray	type	name of the subarray
MI x 7	Real*4	SUM
NE x 3	Real*4	SUØ
max (300,r)	Real*4	ER
max (300,r)	Integer*4	L
max (300,r)	Real*4	GJ
max (300,r)	Real*4	GAT
max (300,r)	Real*4	GAN
max (300,r)	Real*4	GAG
max (300,r)	Real*4	GAF
5 x max (400,i)	Real*4	STE
max (400,i)	Real*4	STE1

r = number of resonances on the KEDAK-library for the isotope in question.

i = number of integration points for the integration of the effective group cross section in one energy group.

Table III, cont.

b2) Module 2

length of the subarray	type	name of the subarray
3 x 5 x MI	Real*4	SE
3 x 5 x MI	Real*4	SM
5 x MI	Real*4	XEUGZ

b3) Module 3

lenght of the subarray	type	name of the subarray
MIBER	Real*4	GIBER
MIBER	Integer*4	IIBER
MIBER	Real*4	GIBER
MI*6	Real*4	FFAKT
MABWF*4	Real*4	ABWF
MXINT	Real*4	XINT
MABQ1*4	Real*4	ABQ1
MABQ2*4	Real*4	ABQ2
MABQ3*4	Real*4	ABQ3
KMROM	Real*8	AUXROM
MI*MRF	Real*4	RF
MI*MRF	Real*4	RFL

Table III, cont.

MIBER = maximum number of ranges with different weighting functions or different integration methods. MIBER is set equal to 5 in the subroutine INPUT.

MABWF = maximum number of energy points in one group of the pointwise given weighting function.

MXINT = maximum number of energy points in one group summed over all participating cross sections (and eventually the pointwise given weighting function).

MABQ1 = maximum number of energy points in one group for the cross section types σ_t, σ_a, σ_e and - if existent - σ_f.

MABQ2 = maximum number of energy points in one group for the cross section type $\bar{\mu}_e$.

MABQ3 = maximum number of energy points in one group for the cross section type σ_t.

KMROM : KMROM-1 = maximum number of bisections in the Romberg integration routine FSROMB.

MRF = 7 for nonfissionable material
8 for fissionable material

b4) Module 4

length of the subarray	type	name of the subarray
NE	Real*4	SGC
NE	Real*4	DUE
NE	Real*4	XINTE
NE	Real*4	ZINT
NE	Real*4	XNEN
NE	Real*4	STREU
max (1500,i)	Real*4	SE
max (1500,i)	Real*4	FSE

i = number of $\bar{\mu}_e$ values or ν_f values for one isotope in the KEDAK library.

Table III, cont.

b5) Module 5

In the organizing subroutine INPUT the XL-array minus the permanent section is transferred to the entry subroutine of module 5, SCAT. In SCAT this array, X(MMAxx), is subdivided into fields of different lengths, which are described in more detail in the following tables (and in chapter 6).

1. Fields used in SCATD and its subroutines:

length of the subarray	type	name of the subarray
NE*NE	Real*4	WEIN
NE	Real*4	QUOT
NE	Real*8	WAHR
NE	Real*8	VW
NE27	Real*8	E
max(30,j)	Real*8	AE
NE	Real*4	SU
NE	Real*4	LBA
max(200,i)	Real*4	SGIT
max(30,j)	Real*4	IANF
max(6000,i*j)	Real*4	SGIP
max(200,i)	Real*4	WERT
max(400,k)	Real*8	EZ

NE27: = NE, if the energy groups given on card 3 of the input contain the thermal group,
= NE+1 otherwise

i : maximum number of energy points that are needed during the calculation for any of the outscattering energy groups, specified in the input. These energy points are the joint set of the energy points of all SGIZ on KEDAK and the energy points of the weighting function.

Table III, cont.

j : maximum number of excited levels of one isotope that contribute in any outscattering energy group specified in the input.

k : i + maximum number of energy points of any SGIZ (for one isotope) on KEDAK in any of the (outscattering) energy groups specified in the input.

b5) 2. Fields used in SCATC and its subroutines

length of the subarray	type	name of the subarray
NE*NE	Real*4	WEINC
NE	Real*4	QUOTC
NE27	Real*4	ENG
max(200,i)	Real*4	EZ
max(200,i)	Real*4	SGIZC
max(300,j)	Real*4	EI
max(30,k)	Real*4	EP
max(150,k*1)	Real*4	F1
max(150,k*1)	Real*4	F2
max(150,k*1)	Real*4	F3
max(150,k*1)	Real*4	F4

NE27: = NE, if the energy groups, given on card 3 of the input contain the thermal group

= NE+1 otherwise

i : maximum number of energy points of SGIZC (SGI,SG2N,SG3N) on KEDAK in any of the outscattering energy groups specified in the input.

j : maximum number of energy points, that are obtained by combination of the energy points on KEDAK for type SGIZC (SGI,SG2N,SG3N) and the energy points of the weighting function in any of the outscattering groups specified in the input.

Table III, cont.

k: number of incident neutron energies, given in KEDAK-type SEDIC(SED2N, SED3N).

l: number of different analytical spectra - as given in KEDAK-type SEDIC(SED2N, SED3N) - from which the total spectrum has to be combined.

b6) Module 6

length of the subarray	type	name of the subarray
max (i,400)	Real*4	A
max (i,400)	Real*4	B
max (i,400)	Real*4	EA
max (i,400)	Real*4	EB
max (i,400)	Real*4	E
max (j,1000)	Real*4	EN
max (j,1000)	Real*4	SGN
max (j,1000)	Real*4	ECØ
max (j,1000)	Real*4	SCØ
max (j,1000)	Real*4	V
max (j,1000)	Real*4	W
max (j,1000)	Real*4	F
k	Real*4	AR
k	Real*4	FU
NE + 1	Real*4	ABN
NE + 1	Integer*4	INT
NE + 1	Real*4	GR
NE + 1	Real*4	FEKØE
NE	Real*4	R
6 x NE	Real*4	RSP
k x i	Real*4	SGNC
l x i	Real*4	FEKØ
6 x l x NE	Real*4	ELSIG
2 x NE	Real*4	ELTØT
max (m,3000)	Real*4	ET
max (m,3000)	Real*4	ST
max (j,1000)	Real*4	GE
max (j,1000)	Real*4	SG
6 x NE	Real*4	SGTØT

Table III, cont.

i: 300 + maximum number of energy points for the data type SGNC on KEDAK in one energy group.

j : i + maximum number of energy points for the data types SGN or MUEL or SGT on KEDAK in one energy group.

k : number of cosine mesh points for the data type SGNC on KEDAK.

l : maximum energy degradation

m : maximum number of energy points for the data type SGT on KEDAK in one group for the given mixture of isotopes.

b7) Module 7

length of the subarray	type	name of the subarray
NE	Real*4	X

b8) Module 8

length of the subarray	type	name of the subarray
NE	Real*4	V
max (200,m)	Real*4	ST
max (200,m)	Real*4	FI

m : maximum number of integration points in one energy group.

b9) Module 9

length of the subarray	type	name of the subarray
XL-array minus the permanent section	Real*4	WØRK

Table III, cont.

b10) Module 10

This module uses only the permanent section of the XL-array.

Table IV: Structure of the unlabeled COMMON array

length of the subarray	type	content of the subarray	see card n of the input description
1	Real*8	MAT	1
1	Integer*4	ISTRUK	1
1	Integer*4	ISPA[+)]	-
1	Integer*4	unit number for print output	-
1	Integer*4	external storage number for the output of the results	-
2	Integer*4	NR(2,J), NR(3,J) J is the index of the module actually called	7
1	Integer*4	KL at the end of each module KL must be enlarged by one	7

+) In MIGRØS-3 ISPA is only used internally. ISPA = 1 for fissile isotopes, ISPA = 0 for non-fissile isotopes.

References

/1/ J.J. Schmidt
Neutron Cross Sections for Fast Reactor Materials
KFK 120, EANDC-E-35 U, 1966

/2/ B. Hinkelmann, B. Krieg, I. Langner, J.J. Schmidt, D. Woll
Status of the Karlsruhe Evaluated Nuclear Data File KEDAK
KFK 1340, EANDC(E), "U", 1971

/3/ B. Krieg
Handling and Service Programs for the Karlsruhe Nuclear Data File KEDAK
Part I: Management and Retrieval Programs
KFK 1725, 1972
see also chapter II of the KEDAK Program Compendium (KFK 2387, II 2.9)

2. Input and output of MIGRØS-3

2.1 Description of the input

On the following pages the computer output of the input description of MIGRØS-3 is given.

INPUT DESCRIPTION FOR THE PROGRAM SYSTEM MIGROS-3

****

INTRODUCTION

THE PROGRAM SYSTEM MIGROS CALCULATES MICROSCOPIC GROUP CONSTANTS FROM NUCLEAR CROSS SECTION DATA STORED IN THE NUCLEAR DATA LIBRARY KFDAK. THE SYSTEM CONSISTS OF THE FOLLOWING MODULES:

MODULE NO.	PURPOSE
1	CALCULATION OF GROUP CROSS SECTIONS FOR INFINITE DILUTION AND OF RESONANCE SELF SHIELDING FACTORS FROM RESOLVED RESONANCE PARAMETERS.
2	CALCULATION OF GROUP CROSS SECTIONS FOR INFINITE DILUTION AND OF RESONANCE SELF SHIELDING FACTORS FROM STATISTICAL RESONANCE PARAMETERS.
3	CALCULATION OF GROUP CROSS SECTIONS FOR INFINITE DILUTION AND OF RESONANCE SELF SHIELDING FACTORS FROM POINT CROSS SECTION DATA.
4	CALCULATION OF WEIGHTED GROUP AVERAGES FOR INFINITE DILUTION.
5	CALCULATION OF NORMALIZED TRANSFER MATRICES FOR INELASTIC SCATTERING, (N,2N) AND (N,3N) PROCESSES.
6	CALCULATION OF NORMALIZED ELASTIC SCATTERING MATRICES UP TO 5-TH ORDER (LEGENDRE REPRESENTATION), OF ELASTIC GROUP CROSS SECTIONS, OF THE AVERAGE ELASTIC SCATTERING COSINE AND OF TOTAL GROUP CROSS SECTIONS WITH ORDER-DEPENDENT WEIGHTING.
7	CALCULATION OF FISSION SPECTRA.
8	CALCULATION OF WEIGHTED 1/V GROUP AVERAGES.
9	CALCULATION OF NORMALIZED ELASTIC SCATTERING MATRICES UP TO 5-TH ORDER (LEGENDRE REPRESENTATION), OF WEIGHTED TOTAL AND ELASTIC SCATTERING GROUP CROSS SECTIONS AND OF GROUP-AVERAGED SCATTERING COSINES FOR THE REMO CORRECTION.
10	CALCULATION OF THERMAL CROSS SECTIONS.

THE FOLLOWING INPUT MUST BE PROVIDED. IF GROUP CONSTANTS ARE TO BE CALCULATED FOR SEVERAL MATERIALS THE COMPLETE INPUT MUST BE REPEATED FOR EACH ONE. THE INPUT IS FORMAT-FREE FOLLOWING THE FREEFC CONVENTIONS: EACH DATA RECORD STARTS IN COLUMN 1 OF A DATA CARD. IF IT IS NOT POSSIBLE TO PLACE ALL THE DATA OF ONE DATA RECORD ON ONE CARD, A SECOND, THIRD, ETC. CARD MAY BE USED, WHICH MUST HAVE A BLANK IN COLUMN 1. OR: A NON BLANK COLUMN 1 IN THE INPUT CARD IS AN INDICATION FOR A NEW INPUT RECORD. ONE HAS TO DISTINGUISH BETWEEN AN ALPHAMERIC WORD OF THE LENGTH REAL*4 AND OF THE LENGTH REAL*8. A REAL*4 WORD MUST BE ENCLOSED IN APOSTROPHIES AND IS STORED LEFT-ADJUSTED IN THE COMPUTER AND FILLED UP WITH BLANKS IF NOT ALL 4 BYTES ARE OCCUPIED. EXAMPLE: 'ARG' OR 'ABCD'. A REAL*8 WORD MAY BE ENCLOSED IN APOSTROPHIES COMPRISING AT LEAST 5 CHARACTERS AND AT MOST 8 CHARACTERS, WHICH ARE STORED LEFT-ADJUSTED IN THE COMPUTER IF NOT ALL 8 BYTES ARE OCCUPIED. A SPECIAL CASE ARE REAL*8 WORDS WITH A NUMBER OF OCCUPIED BYTES LESS THAN OR EQUAL TO 5. THESE WORDS MAY BE ALSO ENCLOSED IN @-SIGNS. THEY ARE ALSO STORED LEFT-ADJUSTED IN THE COMPUTER AND FILLED UP WITH BLANKS. EXAMPLES: 'PU239'='PU239 '=@PU239@;
'RES '=@RES@. FIXED POINT AND FLOATING POINT NUMBERS ARE WRITTEN IN THE USUAL MANNER, E. G: FIXED POINT NUMBERS: 1 10 875 AND FLOATING POINT NUMBERS: 10. 5.E3 0.7E-3 0.01 .
THE INPUT DATA ITEMS ARE SEPARATED BY ONE OR MORE BLANKS.

CARD 1

MAT		MATERIAL NAME IN KEDAK NOMENCLATURE (8-BYTE ALPHAMERIC REPRESENTATION).
ISTRUK	=0 :	DOPPLER BROADENING IS NEGLIGIBLE AS IS TYPICAL FOR S-WAVE RESONANCES OF STRUCTURAL MATERIALS,
	=1 :	DOPPLER BROADENING MUST BE ACCOUNTED FOR AS IS TYPICAL FOR HEAVY NUCLIDES.

MORE SPECIFICALLY: IF MODULES 1 AND 2 ARE UTILIZED, INFINITE DILUTION GROUP CROSS SECTIONS AND RESONANCE SELF SHIELDING FACTORS ARE CALCULATED FROM RESONANCE PARAMETERS FOR THE FOLLOWING STANDARD TEMPERATURES :
T=0 K IF ISTRUK=0,
T=300, 900, 2100 K IF ISTRUK=1.
IF MODULE 3 IS UTILIZED THE SAME QUANTITIES ARE CALCULATED FROM POINT DATA FOR THAT TEMPERATURE FOR WHICH THE POINT DATA ARE STORED (T=0 K IN THE PRESENT VERSION, KEDAK-3), REGARDLESS OF THE ISTRUK VALUE.
IF TEMPERATURES DIFFERING FROM THE STANDARD TEMPERATURES ARE TO BE USED, THIS MUST BE SPECIFIED ON CARD 9 BELOW.

IF GROUP BOUNDARIES DIFFERING FROM THOSE OF THE 26-GROUP ABBN SET ARE TO BE USED (VIZ. 0.215EV, 0.465EV, 1EV, 2.15EV, 4.65EV 10EV, 21.5EV, 46.5EV, 100EV, 215EV, 465EV, 1KEV, 2.15KEV, 4.65KEV, 10KEV, 21.5KEV, 46.5KEV, 100KEV, 200KEV, 400KEV, 800KEV, 1.4MEV, 2.5MEV, 4MEV, 6.5MEV, 10.5MEV) TWO MORE CARDS FOLLOW:

CARD 2

&BLOCK	1	INVARIANT

CARD 3

NE	NUMBER OF ENERGY GROUP BOUNDARIES (ARBITRARY),
(ENG(I),I=1,NE)	ENERGY GROUP BOUNDARIES IN UNITS OF EV IN ASCENDING ORDER.

NOTE THAT THE NUMBER OF ENERGY GROUPS THAT MIGROS CAN TREAT IS NOT RESTRICTED TO 26.

THE STANDARD WEIGHTING FUNCTION IS THE COLLISION DENSITY F(I,1)=PHI(E(I))=1./E(I). ALTERNATIVELY ONE CAN EMPLOY OTHER WEIGHTING FUNCTIONS AFTER LINKAGE OF AN APPROPRIATE FUNCTION PHI(E) WITH MIGROS. IF IN THIS CASE MODULE 3 IS USED ONE MUST LINK AN ADDITIONAL FUNCTION DPHI(E) YIELDING BASICALLY THE SAME RESULT AS PHI BUT WITH DOUBLE PRECISION. A THIRD ALTERNATIVE IS UTILIZATION OF A POINTWISE GIVEN COLLISION DENSITY FOR WHICH ONE NEEDS THE FOLLOWING CARDS:

```
CARD 4
  @BLOC@   2          INVARIANT
CARD 5
  NSPEC               NUMBER OF SPECTRA,
  NFE                 NUMBER OF ENERGY GRID POINTS,
  (EF(I),I=1,NFE),((F(I,J),I=1,NFE),J=1,NSPEC)   WITH
                      EF: ENERGY GRID POINTS IN UNITS OF EV
                          IN ASCENDING ORDER,
                       F: COLLISION DENSITY VALUES.
```

IF THE NUMBER OF SPECTRA (COLLISION DENSITY FUNCTIONS) IS GREATER THAN 1 THE SPECTRA 2, 3,... ARE INTERPRETED ONLY IN MODULE 6 WHERE THEY ARE TAKEN AS THE WEIGHTING FUNCTIONS FOR THE 1ST, 2ND,... MOMENT OF THE ELASTIC SCATTERING MATRIX (MW=1 ON CARD 35). MAKE SURE THAT THE NUMBER OF SPECTRA IS CONSISTENT WITH THE NUMBER OF MOMENTS CALCULATED. IF ONLY ONE SPECTRUM IS SPECIFIED IT WILL BE EMPLOYED FOR ALL REQUIRED MOMENTS OF THE ELASTIC SCATTERING MATRIX. A SPECIAL MODIFICATION, HOWEVER, ALLOWS AN IMPROVED TREATMENT OF FINE-STRUCTURE WEIGHTING (SEE CARDS 32-35). THE NUMBER OF GRID POINTS IS ARBITRARY BUT CARE SHOULD BE TAKEN THAT THE SPECTRA COVER THE WHOLE ENERGY RANGE OF INTEREST.

```
CARD 6
  @BLOC@   3          INVARIANT
CARD 7
  NA                  NUMBER OF MODULES UTILIZED,
  ((NR(I,J),I=1,3),J=1,NA)   WITH
                      NR(1,J)  NUMBER OF MODULE,
                      NR(2,J)  NUMBER OF ENERGY GROUP WHERE CAL-
                               CULATION WITH MODULE NR(1,J) IS
                               TO BEGIN,
                      NR(3,J)  NUMBER OF ENERGY GROUP UP TO
                               WHICH CALCULATION WITH MODULE
                               NR(1,J) IS TO BE EXTENDED.
                               THE LIMITS NR(2,J), NR(3,J) ARE
                               TO BE GIVEN IN THE USUAL SENSE OF
                               ASCENDING ENERGY. NOTE THAT THEN
                               NR(3,J)<=NR(2,J), SINCE GROUPS
                               ARE CONVENTIONALLY LABELED IN THE
                               REVERSE SENSE, I. E. GROUP NUMBER
                               1 IS ASSIGNED TO THE GROUP BE-
                               TWEEN THE HIGHEST TWO ENERGY
                               VALUES ON CARD 3.
```

COMMENT:
MODULES CAN BE CALLED MORE THAN ONCE. THIS IS NECESSARY IF SEVERAL UNCONNECTED RANGES OF ENERGY GROUPS MUST BE TREATED. FOR EACH RANGE ONE CALL MUST BE MADE.
NR(2,J) AND NR(3,J) ARE INTERPRETED AS REFERRING TO OUT-SCATTERING GROUPS IN THE CASE OF ELASTIC AND INELASTIC SCATTERING

MATRICES. THE CALCULATION IS PERFORMED FOR ALL IN-SCATTERING GROUPS, I. E. ALL GROUPS LISTED IN @BLOCK@ 1 INTO WHICH A NEUTRON CAN GET IN THE COURSE OF SCATTERING PROCESSES. THE THERMAL GROUP IS INCLUDED AS IN-SCATTERING GROUP.

*****

IF MODULE 1 AND 2 FOR CALCULATION OF SELF-SHIELDING FACTORS FROM RESOLVED AND STATISTICAL RESONANCE PARAMETERS ARE CALLED, AND TEMPERATURES OTHER THAN THE STANDARD TEMPERATURES (0KELVIN FOR STRUCTURAL MATERIALS, ISTRUK=0, 300, 900 AND 2100 KELVIN FOR HEAVY NUCLEI, ISTRUK=1) ARE NEEDED, TWO MORE CARDS MUST FOLLOW:

CARD 8

@BLOCK@ 4	INVARIANT

CARD 9

NT	NUMBER OF TEMPERATURES (ARBITRARY),
(TEMP(I),I=1,NT)	TEMPERATURES IN KELVIN.

IF SELF-SHIELDING FACTORS ARE TO BE CALCULATED (WITH MODULE 1, 2 OR 3) FOR DILUTION CROSS SECTIONS SIGMA0 (SIGC(I)) DIFFERING FROM THOSE OF THE ABBN GROUP CONSTANT SET (VIZ. 0, 10, 100, 1000, 10000, 100000 AND 1000000 BARN) THE FOLLOWING CARDS ARE NEEDED:

CARD 10

@BLOCK@ 5	INVARIANT

CARD 11

MI	NUMBER OF DILUTION CROSS SECTIONS (ARBITRARY),
(SIGC(I),I=1,MI)	DILUTION CROSS SECTION VALUES (SIGMA0-VALUES) IN BARN.

*****

IF WEIGHTED GROUP AVERAGES FOR INFINITE DILUTION ARE TO BE CALCULATED (WITH MODULES 4 AND 10) FOR DATA TYPES OTHER THAN THE 8 STANDARD TYPES NUEL, NUF, SGA, SGF, SGI, SGN, SG2N, AND SCT THE FOLLOWING CARDS ARE NEEDED:

CARD 12

@BLOCK@ 6	INVARIANT

CARD 13

NTYP	NUMBER OF DATA TYPES (ARBITRARY),
(ITYP(I),I=1,NTYP)	DATA TYPES (KEDAK NOMENCLATURE).

COMMENT:
WEIGHTED GROUP AVERAGES CAN BE CALCULATED FOR ALL DATA TYPES WHICH CAN BE REPRESENTED AS ONE-VALUED FUNCTIONS OF A SINGLE ARGUMENT (INCIDENT NEUTRON ENERGY). THE POSSIBLE TYPES ARE LISTED IN KFK 1725 OR KFK 2234. SPECIAL DEFINITIONS OF GROUP AVERAGES ARE USED FOR COMPOSITE QUANTITIES SUCH AS ALPHA, ETA, MUEL OR NUE (CF. KFK 1784). IF THE CROSS SECTION TYPES SGF AND SGA (SEE KFK 2234) ARE TREATED THE CROSS SECTION TYPE SGC=SGA-SGF IS AUTOMATICALLY TREATED, TOO.

*****

IF RESONANCE SELF-SHIELDING FACTORS ARE TO BE CALCULATED FROM INDIVIDUAL RESONANCE PARAMETERS (MODULE 1), BUT ONLY WITH A LIMITED NUMBER OF RESONANCES ON EITHER SIDE OF EACH ENERGY GRID POINT, TWO MORE CARDS FOLLOW:

CARD 14		
&BLOC&	11	INVARIANT
CARD 15		
NRES		NUMBER OF RESONANCES TO BE CONSIDERED ON EITHER SIDE OF A GIVEN ENERGY.

IF MODULE 1 IS TO BE EMPLOYED, BUT NOT WITH THE STANDARD VALUE 0.01 OF THE MAXIMUM ADMISSIBLE RELATIVE ERROR FOR THE INTEGRATION, ONE NEEDS THE FOLLOWING TWO CARDS:

CARD 16		
&BLOC&	12	INVARIANT
CARD 17		
ERROR		MAXIMUM ADMISSIBLE RELATIVE INTEGRATION ERROR.

*****

IF GROUP CROSS SECTIONS AND SELF-SHIELDING FACTORS ARE TO BE CALCULATED FROM POINT DATA (MODULE 3) BUT NOT WITH THE STANDARD VALUES EPSROM=5.0E-05, DRINWA=5.0, (EXPLAINED BELOW) ONE NEEDS THE FOLLOWING TWO CARDS:

CARD 18		
&BLOC&	31	INVARIANT
CARD 19		
EPSROM		RELATIVE ACCURACY FOR THE ROMBERG INTEGRATION. THE ITERATION STOPS IF THE RELATIVE DIFFERENCE BETWEEN TWO SUCCESSIVE APPROXIMATIONS IS NOT GREATER THAN EPSROM,

ORINWA	CONTROL OF ERROR PRINTING IN THE ROMBERG ITERATION SUBROUTINE. IF THE ITERATION IS STOPPED (E. G. BY ROUND-OFF ERRORS) BEFORE THE EPSROM CRITERION IS FULFILLED, AN ERROR MESSAGE IS PRINTED ONLY IF THE CRITERION IS NOT EVEN FULFILLED WITH ORINWA TIMES EPSROM.

IF MODULE 3 IS TO BE EMPLOYED BUT NOT WITH THE DEFAULT VALUES ITEST=0, IZPUMS=-1 AND ITUMS=0 (CF. CARD 21), THE FOLLOWING TWO CARDS ARE NEEDED:

CARD 20

@BLOC@	32	INVARIANT

CARD 21

ITEST	CONTROL OF ERROR MESSAGES AND WARNINGS =0: NORMAL PRINT-OUT FOR PRODUCTION RUNS, =1: EXTENDED PRINT-OUT FOR PROGRAM DEBUGGING, =2: AS ITEST=1 WITH ADDITIONAL PRINT-OUT, =3: AS ITEST=2 WITH FURTHER EXTENDED PRINT-OUT, =4, 5, ..9: AS ITEST=3, =10, 11, 12, 13: AS ITEST=0, 1, 2, 3 WITH ADDITIONAL ERROR MESSAGES FOR EACH SIGO VALUE, >13: AS ITEST=13.
IZPUMS	CONTROL OF ITEST FOR DIFFERENT GROUPS <=-1: ITEST IS UNCHANGED, =IGR: BEGINNING WITH THE IGR-TH GROUP UP TO THE NR(3,J)-TH GROUP (CF. CARD 7) ITEST HAS THE NEW VALUE ITUMS (SEE BELOW). IGR MUST BE LESS THAN OR EQUAL TO NR(2,J) (CF. CARD 7). THIS IS VALID FOR ALL J WITH NR(1,J)=3, I. E. WHENEVER MODULE 3 IS CALLED.
ITUMS	NEW VALUE OF ITEST.

IF MODULE 3 IS TO BE UTILIZED BUT NOT WITH THE DEFAULT VALUES NENBER=1, ENBER(1)=-1.0, CONWFU(1)=1.0, OR NOT WITH NWFUN(1)=0 IN CASE OF A CALCULATED COLLISION DENSITY, OR NOT WITH NWFUN(1)=-1 IN CASE OF A POINTWISE GIVEN COLLISION DENSITY (CF. CARD 23) ONE NEEDS THE NEXT TWO CARDS:

CARD 22

@BLOC@	33	INVARIANT

CARD 23

NENBER	NUMBER OF ENERGY INTERVALS WITH DIFFERENT WEIGHTING FUNCTIONS AND/OR DIFFERENT INTEGRATION METHODS,

(ENBER(I),NWFUN(I),CONWFU(I),I=1,NENBER) WITH
ENBER(I): UPPER LIMIT OF I-TH ENERGY INTERVAL, EQUAL TO LOWER LIMIT OF (I+1)-TH ENERGY INTERVAL, SO THAT
ENBER(I) < ENBER(I+1).
THE LOWER LIMIT FOR THE FIRST ENERGY INTERVAL IS TAKEN AS EQUAL TO THE BEGINNING OF THE CURRENT ENERGY GROUP RANGE (SMALLEST ENERGY VALUE) AS SPECIFIED ON CARD 3 (CR IN THE PROGRAM AND IN CARD 7 IN CASE OF SEVERAL DISCONNECTED ENERGY GROUP RANGES).
ENBER(NENBER) MUST BE AT LEAST AS GREAT AS THE LARGEST ENERGY OF THE CURRENT ENERGY GROUP RANGE.
SPECIAL CASE FOR NENBER=1:
ENBER(1)=-1.0. THIS MEANS THE WHOLE SPECIFIED ENERGY GROUP RANGE.
NWFUN(I): TYPE OF WEIGHTING FUNCTION AND METHOD OF INTEGRATION USED IN INTERVAL I.
METHOD OF INTEGRATION:
NWFUN(I)<=0: NUMERICAL INTEGRATION WITH THE ROMBERG METHOD,
NWFUN(I)>0 : ANALYTICAL INTEGRATION.
TYPE OF WEIGHTING FUNCTION:
|NWFUN(I)|=0: ARBITRARY FUNCTION WITH THE NAME DPHI.(DPHI=1./E BY DEFAULT IF NOT GIVEN BY THE USER AS A FUNCTION SUBROUTINE TO THE PROGRAM),
|NWFUN(I)|=1: POINTWISE WEIGHTING FUNCTION,
|NWFUN(I)|=2: DPHI=CONWFU(I)/E (FOR CONWFU SEE NEXT INPUT VARIABLE).
CAUTION: BECAUSE IN SOME CASES ROUNDING ERRORS APPEAR WHEN THE ANALYTICAL INTEGRATION IS CHOSEN, WE RECOMMEND TO USE ONLY NWFUN(I)<=0.
THERE IS NO DIFFERENCE IN THE CPU TIMES BETWEEN ROMBERG AND ANALYTICAL INTEGRATION.
CONWFU(I): FACTOR IN THE WEIGHTING FUNCTION DPHI=CONWFU(I)/E. ONLY USED IF |NWFUN(I)|=2.

*****

THREE DIFFERENT OPTIONS ARE AVAILABLE FOR THE TRANSFER PROBABILITIES NEEDED FOR THE CALCULATION (WITH MODULE 5) OF NORMALIZED TRANSFER MATRICES FOR INELASTIC SCATTERING WITH EXCITATION OF DISCRETE LEVELS AT EXCITATION ENERGIES EJ:
(1) F(EP-->E)=DELTA(EP-E-EJ) IF KINEM=0,
WHERE DELTA DENOTES DIRAC'S DELTA FUNCTION. THIS FORM WAS USED IN THE ORIGINAL VERSION OF MIGROS-2 (KFK 1784).

(2) F(EP-->E)=DELTA(EP-E-EJ*(A+1.)/A) IF KINEM=1
THIS FORM WAS USED IN THE REVISED VERSION OF MIGROS-2 (TRANSFORMATION OF EJ FROM CMS TO LAB COORDINATES).
(3) F(EP-->E)=DELTA(E-EP*(A**2+1.)/(A+1.)**2
+EJ*A/(A+1.)) IF KINEM=2
THIS APPROXIMATION WAS RECOMMENDED BY SEGEV (SEGEV, NSE 45 (1971)269 AND VERTES, NSE 52 (1973)485) AND IS ALSO PROPOSED FOR THE PROCESSING OF ENDF/B DATA (DRAKE, BNL 50274 (T-601) ENDF 102, VOL.1).
FORM (2), I. E. KINEM=1, IS THE DEFAULT OPTION IN MODULE 5. IF EITHER FORM (1) OR (3) IS TO BE USED ONE NEEDS THE FOLLOWING ADDITIONAL INPUT:

CARD 24
@BLOCK 51 INVARIANT
CARD 25
KINEM TAG FOR TREATMENT OF DISCRETE LEVELS (SEE ABOVE).

IF FOR THE MATERIAL OF INTEREST THE NUCLEAR DATA LIBRARY DOES NOT CONTAIN ANY INFORMATION ON THE ENERGY DISTRIBUTION OF SECONDARY NEUTRONS (SED1C, SED2N, SED3N) IN THE ENERGY REGION OF CONTINUOUS LEVEL EXCITATION OF THE RESIDUAL NUCLEUS AN EVAPORATION MODEL IS EMPLOYED IN MODULE 5. THE PARAMETER XNUE FOR THE CALCULATION OF THE NUCLEAR TEMPERATURE, THETA(EP)=SQRT(EP/(XNUE*A)), IS SET EQUAL TO XNUE=0.16/MEV BY DEFAULT. (A= ATOMIC WEIGHT OF THE TARGET NUCLEUS.) IF OTHER XNUE VALUES ARE TO BE USED ONE NEEDS THE FOLLOWING ADDITIONAL INPUT:

CARD 26
@BLOCK 52 INVARIANT
CARD 27
XNUE EVAPORATION MODEL PARAMETER (IN UNITS OF 1/MEV).

IF MODULE 5 IS CALLED THE TRANSFER MATRICES FOR INELASTIC SCATTERING AND FOR (N,2N) ARE CALCULATED BY DEFAULT. IF OTHER REACTION TYPES ARE WANTED ONE NEEDS THE FOLLOWING ADDITIONAL INPUT:

CARD 28
@BLOCK 53 INVARIANT
CARD 29
NIN NUMBER OF REACTION TYPES,
(INTYP(I),I=1,NIN) REACTION TYPE INDICATORS:
INTYP=1 FOR INELASTIC SCATTERING,
INTYP=2 FOR (N,2N) PROCESSES,
INTYP=3 FOR (N,3N) PROCESSES.

*****

IF MODULE 6 IS TO BE USED BUT NOT WITH THE STANDARD VALUES ISEL=2, NLE=5 ONE NEEDS THE FOLLOWING CARDS:

CARD 30
  @BLOC@ 61 INVARIANT
CARD 31
  ISEL TAG FOR POSSIBLE CROSS SECTION MODIFICATION AND ADDITIONAL PRINT-OUT (DEFAULT VALUE: 2)
  |ISEL|=2: NO CROSS SECTION MODIFICATION;
  |ISEL|=1: BELOW 10KEV, IN THE RESOLVED RESONANCE RANGE, THE ELASTIC SCATTERING AND TOTAL CROSS SECTIONS ARE SET EQUAL TO 1 BARN (MAINLY TO SIMPLIFY THE CALCULATION OF APPROXIMATE SCATTERING PROBABILITIES AND AVERAGE ELASTIC SCATTERING COSINES FOR HEAVY ELEMENTS, AND TO SAVE CORE MEMORY SPACE).
  ISEL<0: ADDITIONAL PRINT-OUT OF INTERMEDIATE INFORMATION.
  NLE HIGHEST ORDER IN LEGENDRE EXPANSION (MAX 5) THE ACTUAL VALUE USED IS MAX(1,NLE) BECAUSE OF THE NORMALIZATION OF THE AVERAGE SCATTERING COSINES TO THE KEDAK MUEL VALUES. THE MODULE ALWAYS CALCULATES SCATTERING MATRICES FROM MOMENT ZERO TO MOMENT NLE.

IF MODULE 6 IS CALLED AND FINE-STRUCTURE WEIGHTING WITH 1./SGT**(L+1) IS TO BE EMPLOYED FOR THE L-TH MOMENT ADD THE CARDS 32 UP TO 35:

ARE THE FOLLOWING CARDS:

CARD 32
  @BLOC@ 62 INVARIANT
CARD 33
  NMAT NUMBER OF MATERIALS IN THE MIXTURE WHOSE MACROSCOPIC TOTAL CROSS SECTION IS TO BE USED FOR FINE-STRUCTURE WEIGHTING;
  (NAME(I),TZ(I),I=1,NMAT) WITH
  NAME: MATERIAL NAME (8-BYTE ALPHAMERIC REPRESENTATION),
  TZ : NUCLEAR DENSITY (NUCLEI PER CM**3) TIMES 1.E-24.

IF MODULE 6 IS CALLED AND NOT ALL MOMENTS ARE TO BE WEIGHTED BY THE COLLISION DENSITY F(I,1) (CF. CARD 5) OF THE 0-TH MOMENT, THE FOLLOWING CARDS ARE NEEDED:

CARD 34
  @BLOC@ 63 INVARIANT
CARD 35
  MW TAG FOR WEIGHTING,
  MW=1: WEIGHT F(I,L+1) FOR L-TH MOMENT, NSPEC=NLE+1 MUST OCCUR ON CARD 5 WITH NLE GIVEN ON CARD 31 OR BY DEFAULT;

MW=2: WEIGHT F(I,1)/SGT**(L+1) FOR L-TH MOMENT (CARD 33 MUST PRECEDE).

IF MODULE 6 IS USED BUT NOT WITH THE STANDARD GRID POINT NUMBERS PER GROUP (NK=70, NR=16, SEE BELOW) ONE NEEDS THE FOLLOWING CARDS:

CARD 36
  @BLOC@ 64 INVARIANT
CARD 37
  NK NK*MIN(1,ALOG(ENG(I)/ENG(I-1))/ ALOG(1/ALFA)) IS THE NUMBER OF BASIC GRID POINTS IN THAT ENERGY REGION WITHIN GROUP I FROM WHICH ELASTIC SCATTERING INTO ADJACENT GROUPS IS POSSIBLE, ALFA=((A-1)/(A+1))**2, A= ATOMIC WEIGHT IN NEUTRON MASS UNITS;
  NR NR IS THE NUMBER OF BASIC GRID POINTS IN THAT ENERGY REGION OF EACH GROUP FROM WHICH ELASTIC SCATTERING INTO ADJACENT GROUPS IS IMPOSSIBLE. (THIS REGION POSSIBLY MAY NOT EXIST, THEN NR HAS NO MEANING.)

*****

IF 1/V AVERAGES ARE TO BE CALCULATED (WITH MODULE 8), BUT NOT WITH THE MAXIMUM ADMISSIBLE RELATIVE INTEGRATION ERROR EPS=0.01, ONE NEEDS THE FOLLOWING CARDS:

CARD 38
  @BLOC@ 81 INVARIANT
CARD 39
  EPS MAXIMUM ADMISSIBLE RELATIVE INTEGRATION ERROR.

*****

IF REMC DATA ARE TO BE CALCULATED (WITH MODULE 9) BUT NOT WITH THE STANDARD VALUES (SEE BELOW) ERR=0.01, NJM=10, NUJM=10, ONE NEEDS THE FOLLOWING TWO CARDS:

CARD 40
  @BLOC@ 91 INVARIANT
CARD 41
  ERR MAXIMUM ADMISSIBLE RELATIVE INTEGRATION ERROR;
  NJM 2**NJM+1 IS THE MAXIMUM NUMBER OF GRID POINTS FOR THE ANGULAR INTEGRATION;
  NUJM 2**NUJM+1 IS THE MAXIMUM NUMBER OF GRID POINTS FOR THE ENERGY INTEGRATION.

IF MODULE 9 IS TO BE USED BUT NOT WITH THE DEFAULT VALUES (EXPLAINED BELOW) ISELR=1 FOR ISTRUK=0, ISELR=0 FOR ISTRUK=1, NLRA=0, NLRE=5, NCALL=0, NFG=14, NFI=5, ONE NEEDS THE FOLLOWING CARDS:

CARD 42
  @BLOC@ 92 INVARIANT

CARD 43

ISELR	=1: SCATTERING PROBABILITIES ARE CALCULATED ACCORDING TO EQ. 8.3 OF KFK 1784 WITH THE KEDAK VALUES FOR THE SCATTERING CROSS SECTION SGN(E),
	=0: IN EQ. 8.3 OF KFK 1784 THE SCATTERING CROSS SECTION SGN(E) IS TAKEN AS 1 BARN;
NLRA	LOWEST LEGENDRE ORDER;
NLRE	HIGHEST LEGENDRE ORDER;
NCALL	=0: EACH TIME MODULE 9 IS CALLED ALL ENERGY GROUPS ARE SUBDIVIDED INTO 14 SUBGROUPS WITH 5 ENERGY INTERVALS EACH,
	>0 NUMBER OF CALLS FOR MODULE 9 (MUST BE CONSISTENT WITH CARD 7).

IN CASE NCALL>0 THE FOLLOWING CARD IS NEEDED NCALL TIMES:

CARD 44

NGRE	NUMBER OF ENERGY GROUP RANGES WITH DIFFERENT ENERGY GRIDS;
(N1(I),N2(I),NFG(I),NFI(I),I=1,NGRE)	WITH
	N1 : NUMBER OF FIRST GROUP IN RANGE,
	N2 : NUMBER OF LAST GROUP IN RANGE,
	NFG: NUMBER OF SUBGROUPS PER GROUP,
	NFI: NUMBER OF ENERGY INTERVALS PER SUBGROUP.

*****

THE LAST CARD FOR A GIVEN MATERIAL IS AS FOLLOWS:

CARD 45
  @ENDE@ 111 INVARIANT

*****

CARDS 1 TO 45 HAVE TO BE REPEATED FOR EACH MATERIAL WANTED AND/OR EACH WEIGHTING SPECTRUM TO BE USED. THE LAST CARD FOR THE ENTIRE JOB IS:

CARD 46
  @ENDE@ 112 INVARIANT

*****

PRINTING OF THE PRESENT INPUT DESCRIPTION CAN BE SUPPRESSED BY PLACING THE FOLLOWING CARD (WITH THE M PUNCHED IN COLUMN 1) IN FRONT OF THE FIRST INPUT CARD:

```
CARD C
  MIGR                INVARIANT
```

THIS CARD DOES NOT APPEAR IN THE FREEFO DISPLAY OF INPUT DATA.

*****

THE PROGRAM SYSTEM MIGROS REQUIRES DD-CARDS FOR THE FOLLOWING EXTERNAL STORAGE DEVICES:

```
8     UNIT ON WHICH THE DECODED INPUT IS WRITTEN BY FREEFO,
1     UNIT FROM WHICH THE NUCLEAR DATA LIBRARY IS AVAILABLE,
3     UNIT ON WHICH ALL MODULES WRITE RESULTS,
10    TEMPORARY INTERMEDIATE LIBRARY NEEDED ONLY BY MODULE 6.
```

*****

THE REQUIRED ARRAY LENGTHS DEPEND ON THE INPUT AND ON THE CALLED MODULES. THE NOTATION OF THE INPUT DESCRIPTION IS USED IN WHAT FOLLOWS. ALL ARRAY LENGTHS ARE GIVEN IN TERMS OF 4-BYTE WORDS UNLESS STATED OTHERWISE.

THE CONTROL PHASE NEEDS
2*NTYP+3*NMAT+NFE*(NSPEC+1)+NT+MI+1+3*NE+4*NA*(1+NE) WORDS,
WHERE THE DEFAULT VALUES ARE USED FOR QUANTITIES NOT SPECIFIED IN THE INPUT, VIZ. NTYP=7, NFE=1, NSPEC=1, NT=3, MI=7, NMAT=1, AND NE=26.
TO THIS ONE MUST ADD THE MEMORY SPACE OCCUPIED BY THE UTILIZED MODULE WITH THE LARGEST STORAGE REQUIREMENT. THE STORAGE REQUIREMENTS OF THE VARIOUS MODULES ARE AS FOLLOWS:

MODULE NO.	STORAGE REQUIREMENT (4-BYTE WORDS)
1	7*MI+3*NE+7*MAX(300,NUMBER OF RESONANCES ON KEDAK)+6*MAX(400,MAXIMUM NUMBER OF GRID ENERGIES FOR INTEGRATION OVER ONE ENERGY GROUP) WORDS COMMENT: THE USER CANNOT DETERMINE THE NUMBER OF GRID ENERGIES IN ADVANCE. IF 400 WORDS ARE NOT SUFFICIENT THE SPACE FOR DATA STORAGE IS ENLARGED PROVIDED THE AVAILABLE REGION ADMITS THIS. IF THE REGION IS NOT LARGE ENOUGH THE MODULE IS BY-PASSED. IT IS RECOMMENDED IN THIS CASE TO ENLARGE THE REGION BY AT LEAST 2K BYTES.
2	35*MI WORDS.
3	3*MIBER+6*MI+MXINT+4*(MABWF+MABG1+MABG2+MABG3) +2*KMROM+4*MRF*MI WORDS.

MIBER: MAXIMUM NUMBER OF RANGES WITH DIFFERENT WEIGHTING FUNCTIONS OR DIFFERENT INTEGRATION METHODS. MIBER IS SET EQUAL TO 5 IN THE SUBROUTINE INPUT.

MABWF: MAXIMUM NUMBER OF ENERGY POINTS IN ONE GROUP OF THE POINTWISE GIVEN WEIGHTING FUNCTION. MABWF HAS THE VALUE 0 IF NO POINTWISE GIVEN WEIGHTING FUNCTION IS PROVIDED IN THE INPUT. OTHERWISE IT HAS THE MINIMUM VALUE 50.

MXINT: MAXIMUM NUMBER OF ENERGY POINTS IN ONE GROUP SUMMED OVER ALL PARTICIPATING CROSS SECTIONS (AND EVENTUALLY THE POINTWISE GIVEN WEIGHTING FUNCTION), MINIMUM VALUE= 200.

MABQ1: MAXIMUM NUMBER OF ENERGY POINTS IN ONE GROUP FOR THE CROSS SECTION TYPES SGT, SGA, SGN AND, IF EXISTENT, SGF, MINIMUM VALUE = 200.

MABQ2: MAXIMUM NUMBER OF ENERGY POINTS IN ONE GROUP FOR THE CROSS SECTION TYPE MUEL, MINIMUM VALUE = 200.

MABQ3: MAXIMUM NUMBER OF ENERGY POINTS IN ONE GROUP FOR THE CROSS SECTION TYPE SGT, MINIMUM VALUE = 200.

KMROM: KMROM-1 = MAXIMUM NUMBER OF BISECTIONS IN THE ROMBERG INTEGRATION ROUTINE FSROMB, MINIMUM VALUE = 20.

MRF : 7 FOR NON-FISSIONABLE MATERIAL,
8 FOR FISSIONABLE MATERIAL.

WITH THE MINIMUM VALUES A MINIMUM MEMORY DEMAND OF 3121 4-BYTE WORDS (POINTWISE WEIGHTING SPECTRUM GIVEN, FISSIONABLE MATERIAL) IS NECESSARY TO RUN MODULE 3 (FSTRUK). BUT WE RECOMMEND TO USE ABOUT 10000 4-BYTE WORDS, BECAUSE SOME OR ALL OF THE MINIMUM VALUES MUST BE INCREASED DURING THE CALCULATIONS.

4 6*NE+2*MAX(1500,NUMBER OF SGN VALUES, NUMBER OF SGF VALUES ON KEDAK IN THE ENERGY INTERVAL CONSIDERED) WORDS

5 MAX(7+NE*NE+7*NE+2*NE27+4*NAE+3*ISG+2*NISGD, 4+2*NE*NE+3*NE+NE27+2*NISGC+NISGI+NFP+4*NEP*NF) WORDS

NE27: NUMBER OF ENERGY GROUP BOUNDARIES OF IN-SCATTERING GROUPS. STANDARD ESTIMATE: 27 (THE STANDARD ESTIMATES ARE USED AS STARTING VALUES IN THE PROGRAM BUT MAY BE MODIFIED AUTOMATICALLY DEPENDING ON THE ACTUAL JOB CHARACTERISTICS).

NAE: MAXIMUM NUMBER OF EXCITED LEVELS THAT CONTRIBUTE IN A GIVEN OUT-SCATTERING GROUP. STANDARD ESTIMATE: 30.

ISG : MAXIMUM NUMBER OF ENERGY GRID POINTS IN ONE OF THE CONSIDERED OUT-SCATTERING GROUPS. THIS NUMBER IS DETERMINED BY THE COMBINATION OF THE ENERGY GRID POINTS OF ALL EXCITED LEVELS WHICH MUST BE USED IN THE OUT-SCATTERING GROUP AND OF THOSE GRID POINTS OF THE SPECTRUM THAT LIE IN THE OUT-SCATTERING GROUP. STANDARD ESTIMATE:200

NISGD:ISG+MAXIMUM NUMBER OF ENERGY GRID POINTS OF ANY EXCITED LEVEL (SGIZ) WHICH CONTRIBUTE IN THE OUT-SCATTERING GROUP. STANDARD ESTIMATE: 400.

NISGC:MAXIMUM NUMBER OF ENERGY GRID POINTS OF SGI (SG2N, SG3N) ON KEDAK IN ONE OF THE OUT-SCATTERING GROUPS. STANDARD ESTIMATE: 200.

NISGI:MAXIMUM NUMBER OF ENERGY POINTS AS OBTAINED BY COMBINING THE KEDAK POINTS OF SGI (SG2N, SG3N) AND THE MESH POINTS OF THE SPECTRUM IN ANY OUT-SCATTERING GROUP. STANDARD ESTIMATE: 300.

NEP : NUMBER OF INCIDENT-NEUTRON ENERGIES, FOR WHICH THE DISTRIBUTIONS SEDIC (SED2N, SED3N) ARE GIVEN ON KEDAK. STANDARD ESTIMATE: 30.

NF : NUMBER OF DIFFERENT ANALYTICAL DISTRIBUTIONS GIVEN ON KEDAK FOR SEDIC (SED2N, SED3N) FROM WHICH THE TOTAL DISTRIBUTION MUST BE COMPOSED. STANDARD ESTIMATE: 5

6 APPROXIMATELY 30000 (STANDARD) TO 200000 (MANY GROUPS, LARGE ENERGY DEGRADATION) WORDS. THE EXACT STORAGE REQUIREMENT DEPENDS ON THE MOSTLY UNKNOWN DISTRIBUTION OF THE KEDAK DATA OVER THE ENERGY GROUPS. IT IS RECOMMENDED TO BEGIN WITH THE STANDARD VALUE AND TO INCREASE THE STORAGE SPACE ONLY IF THIS DOES NOT WORK. THE PROGRAM TRIES IN ANY CASE TO ORGANIZE THE CALCULATIONS IN ACCORDANCE WITH THE AVAILABLE MEMORY SPACE.

7 NE WORDS.

8 NE+2*NFE WORDS.

9 45+NM1*IMAX*(3+NUJM)+ICOS*(4+NIV)+IMAX+2*NJM+NF
+15*NMAX+NZM*(2+IZV)+BUF WORDS.

NM1 : NLRE+1.

IMAX: MAXIMUM ENERGY DEGRADATION IN TERMS OF ENERGY GROUPS (=2 FOR SIMPLE SCATTERING INTO THE ADJACENT GROUP).

ICOS: NUMBER OF ANGULAR GRID POINTS OF THE SCNC DATA ON KEDAK.

NIV : NUMBER OF ENERGY GRID POINTS OF THE SCNC DATA ON KEDAK.

NMAX: MAXIMUM NUMBER OF ENERGY GRID POINTS WITHIN ONE ENERGY GROUP FOR THE DATA TYPES SGT, SGN OR NUEL ON KEDAK.

NZM : MAXIMUM NUMBER OF ENERGY INTERVALS IN ONE SUBGROUP TIMES MAXIMUM NUMBER OF SUBGROUPS PER GROUP.
IZV : MAX(4,IMAX*NM1).
BUF : MAX(2+IMAX*NZM,NTOT), WHERE NTOT IS THE MAXIMUM NUMBER OF DATA POINTS WITHIN ONE GROUP FOR THE TYPES SGT, SGN AND MUEL (ALL THREE CONSIDERED AS A JOINT POINT SET) ON KEDAK.

10 NO SPACE FOR DATA ARRAYS REQUIRED.

THE REGION PARAMETER ON THE JOB CARD IS THE SUM OF
- MAXIMUM LENGTH OF DATA ARRAYS,
- 17OK BYTES FOR THE MIGROS PROGRAM,
- BUFFER LENGTH.

2.2 Description of the output

2.2.1 Printed output

Each computational module prints the results. An explanation of the symbols is given in table V.

2.2.2 Unformatted output

Besides the printed output an unformatted output on unit 3 is provided. The arrangement of this output is described in table VI. The unformatted output of MIGRØS serves as input for the program MITRA, /3/. MITRA checks the results of MIGRØS and transforms them into an input of GRUMA, /4/, the management program for the group constant library GRUBA, /4/.

The following tables are given in chapter 2:

Table V : Symbols used in the printed output of MIGRØS-3.

Table VI : Arrangement of the unformatted output.

Table V Symbols used in the printed output of MIGRØS-3

Module 1

Symbol	content	defined by formula	required KEDAK-types
SIGMA G	average group cross section for infinite dilution, radiative capture	(4.6)	
SIGMA N	average group cross section for infinite dilution, elastic scattering	(4.6)	
SIGMA F	average group cross section for infinite dilution, fission	(4.6)	
SIGMAN1	identical with SIGMA N	-	
SIGMAT1	SIGM G + SIGMA N + SIGMA F	-	ISØT1 ISØT2
SIGMA 0	background cross section σ_o	(4.1)	RES
FG FN FF	flux-weighted resonance self shielding factors for { radiative capture; elastic scattering; fission }	(4.1)	
FN1 FT1	current weighted resonance self shielding factors for { elastic scattering; total }	(4.3)	

Temperatures are given in K, the group boundaries in eV, cross sections in barns.

Table V, cont.

Module 2

Symbol	content		defined by formula	required KEDAK-types
SIGMA G	average group cross sections for infinite dilution	radiative capture	(5.32)	
SIGMA N		elastic scattering	(5.33)	
SIGMA F		fission	(5.32)	
SIGMAN1	identical with SIGMA N		-	ISØT1
SIGMAT1	SIGMA G + SIGMA N + SIGMA F		-	ISØT2
SIGMA 0	background cross section σ_o		(5.1)	ST
FG	flux-weighted resonance self shielding factors	radiative capture	(5.1)	STGF
FN		elastic scattering		
FF		fission		
FN1	current-weighted resonance self shielding factors	elastic scattering	(5.8)	
FT1		total		

Tamperatures are given in K, group boundaries in eV, cross sections in barns

Table V, cont.

Module 3

Symbol	content		defined by formula	required KEDAK-types
SIGMA A [+]	average group cross sections for infinite dilution,	absorption	(9.7)	SGA
SIGMA C [+]		capture		
SIGMA N		elastic scattering		
SIGMA F		fission		
SIGMA NO1		$\sigma_e \cdot \bar{\mu}_e$	(9.8)	SGN
SIGMA T1		total	(9.13)	SGF
SIGMA N1	identical to SIGMA NO1			SGT
FA	flux-weighted resonance self-shielding factors,	absorption	(9.3)	MUEL
FC		capture		
FN		elastic scattering		
FF		fission		
FNO1	flux-weighted resonance self-shielding factor for $\sigma_e \cdot \bar{\mu}_e$		(9.5)	
FN1	current-weighted resonance self-shielding factor for $\sigma_e \cdot \mu_e$		(9.10)	
FT1	current-weighted total resonance self-shielding factor		(9.9)	
SIGO	background cross section σ_o			
Group boundaries are given in eV, cross sections in barns				

[+] To calculate SIGMA A the KEDAK type SGA (see /5/) is used. In the case of fissionable materials SIGMA C is produced, which is defined by the formula SIGMA C = SIGMA A - SIGMA F.

Table V, cont.

Module 4

Symbol	content		defined by formula	required KEDAK-types
SGN	average group cross section for	elastic scattering	(3.1)	SGN
SGA[+)]		absorption		SGA
SGF		fission		SGF
SGI		inelastic scattering		SGI
SGC		capture = SGA - SGF		SGA,SGF
SG2N		(n,2n) reaction		SG2N
MUEL	average cosine of elastic scattering		(3.2)	SGN,MUEL
NUE	average number of secondaries per fission		(3.3)	SGF,NUE
ALPHA	average α-value		(3.4)	SGG,SGF
ETA	average η-value		(3.5)	NUE,SGG,SGF

If group averages of other types of cross sections available on KEDAK are calculated, averages in the sense of formula (3.1) are calculated. The names are the same as the names of the underlying KEDAK-types. Cross sections are given in barns.
If SGN for the material HbbØ1 is calculated, also a type STR is calculated, which corresponds to formula (3.6).

[+)] Definition of the absorption cross section (KEDAK-type SGA; compare /5/):

$$\sigma_{ab} = \sigma(n,\gamma) + \sigma(n,f) + \sigma(n,p) + \sigma(n,d) + \sigma(n,\alpha)$$

Table V, cont.

Module 5

Symbol	content	defined by formula	underlying KEDAK-type
PRØBSGI	transfer probabilities for inelastic scattering	(6.21.1) together with (6.21.2), (6.14) and (6.20.1) with (6.20) and (6.20.2)	ISØT1, SGIZ, SGIZC, SGI, SEDIC
PRØBSG2N	transfer probabilities for (n,2n)-reactions	(6.23)	SG2N, SED2N, ISØT1
PRØBSG3N	transfer probabilities for (n,3n)-reactions	(6.23), where (n,2n) has to be replaced by (n,3n)	SG3N, SED3N, ISØT1
In the first column the numbers of the outscattering groups are printed. The numbers above the values of PRØBSGI(PRØBSG2N, PRØBSG3N) are the inscattering groups.			

Table V, cont.

Module 6

Symbol	content	defined by formula	underlying KEDAK-type
SGNC0	zero'th moment	(7.2)	SGNC
SGNC1	1^{st} moment		SGN
SGNC2	2^{nd} moment		MUEL
SGNC3	3^{rd} moment		SGT
SGNC4	4^{th} moment		
SGNC5	5^{th} moment		
	of the elastic scattering matrix normalized to the total elastic cross section		
SGN	total elastic group cross section	(7.1)	SGN
MUEL	group-averaged mean elastic-scattering cosine	(7.3)	SGNC SGN MUEL
SGT	total group cross section with moment-dependent weighting	(7.1')	SGT

Table V, cont.

Module 7

Symbol	content	defined by formula	required KEDAK-types
CHI	fission spectrum	(12.1), (12.2), (12.4), (12.6)	CHICR SEDF

Module 8

Symbol	content	defined by formula	required KEDAK-types
1/V	1/v-group averages in [sec/cm]	(11.1)	-

Module 9

Symbol	content	defined by formula	required KEDAK-types
SGT	average total cross section	(8.1)	SGT
SGN	average elastic-scattering cross section	(8.1)	SGN
MUEL	average cosine of elastic scattering	(8.2)	MUEL
FLUX	average flux (weighting function)	-	-
SGNCn	the n-th legendre moment for elastic scattering	(8.3)	SGN, SGNC
Cross sections are given in barns, the legendre moments are normalized to the total elastic cross section. The interval averages within one group are arranged with increasing energy.			

Table V, cont.

Module 10

In this module the group constants for the thermal group are calculated. The same types as in module 4 are possible. The group constants are defined by the formulas (10.1) to (10.6).

Table VI: Arrangement of the unformatted output

(The symbols of table V are used)

Module 1

1st record:	o ,	'MIGR----'
2nd record:	n ,	material name, temperature in /K/, number of the energy group, lower group boundary in /eV/, upper group boundary in /eV/
3rd record:	n ,	SIGMA G, SIGMA N, SIGMA F, SIGMA N1, SIGMAT1
4th record:	n ,	SIGMA 0, FG, FN, FF, FN1, FT1
.	.	.
.	.	.
.	.	.
.		for all SIGMA 0-values

n is an Integer I x 4 and gives the number of succeeding 4-byte words in the record. The material names are 8-byte alphanumerical words. All other words are REAL*4. The 8-byte alphanumeric words are counted as two words in n. These conventions are the same for all other modules. Exceptions are mentioned. "-" in the label names must be interpreted as blank.

Module 2

1st record:	o ,	'FSTAT---'
2nd record:	n ,	material name, temperature in /K/, number of the energy group, lower group boundary in /eV/, upper group boundary in /eV/.
3rd record:	n ,	SIGMA G, SIGMA N, SIGMA F, SIGMAN1, SIGMAT1
4th record:	n ,	SIGMA 0, FG, FN, FF, FN1, FT1
.		
.		
.		for all SIGMA-0 values

Table VI, cont.

Module 3

1st record: 0, 'STRK----'

The following records are repeated for each energy group.

2nd record: 5, material name (8 Byte), number of the energy group[+)] lower group boundary measured in eV, upper group boundary measured in eV.

3rd record: for non-fissionable materials
5, SIGMA A, SIGMA N, SIGMA NO1, SIGMA N1, SIGMA T1
for fissionable materials
6, SIGMA C, SIGMA N, SIGMA F, SIGMA NO1, SIGMA N1, SIGMA T1

4th record: for non-fissionable materials
6, SIGO, FA, FN, FNO1, FN1, FT1
for fissionable materials
7, SIGO, FC, FN, FF, FNO1, FN1, FT1
record 4 is repeated for all SIGO values.

[+)] An internal numeration is used. The group with the greatest number has the highest energy boundaries.

Module 4

1st record: o , 'SGKE----'
2nd record: n , highest energy group (lowest number), lowest energy group
3rd record: n , material name, name of reaction type (8-byte, alphanumeric)
4th record: n , group constant of the type defined by the 3rd word in the 3rd record, for all energy groups, specified by the 2nd record. The values are ordered with increasing energy and decreasing group numbers.

The records 2 to 4 are repeated for all reaction types, specified by the input.

Table VI, cont.

Module 5

Module 5 produces separately labelled output on unit 3 for inelastic-scattering transfer matrices, for (n,2n)-matrices and for (n,3n)-matrices. In the following the output produced for inelastic-scattering transfer matrices is given first. The output produced for (n,2n)- or (n,3n)-matrices is added in parentheses.

1st record o , 'SMTØT---'('SMTØT2N-';'SMTØT3N-')
2nd record n , material name, total number of outscattering groups
3rd record n , number of the outscattering roup, elements of the matrix PRØBSGI (PRØBSG2N; PRØBSG3N) in the sense, that the first element describes scattering within the group, the second element describes scattering into the neighbouring group etc.
repeated for all outscattering groups.

Module 6

1st record: o , 'FLUM----'
2nd record: n , material name, number of outscattering groups, number of Legendre moments.
3rd record: n , number of the outscattering groups, group averaged total elastic cross section, group averaged cosine for elastic scattering, group averaged ψ_ℓ-weighted total cross sections, ℓ = 0, number of Legendre moments.
repeated for all outscattering groups.
4th record: n , number of the Legendre moment, number of the outscattering group, matrix elements SGNCi (i = number of the moment) arranged in the sense that the first word describes scattering within the group, the next one scattering into the neighbouring group etc.
repeated for all outscattering groups (for a certain Legendre moment)
repeated for all Legendre moments.

Table VI, cont.

Module 7

1st record: o , 'SPALT---'

2nd record: n , material name, energy of the fission-inducing neutron in eV, number of the lowest energy group, number of the highest energy group.

3rd record: n , CHI for all groups specified in the 2nd record, arranged with increasing energy.

Module 8

1st record: o , 'SI/V----'

2nd record: n , 1/V-values for all energy groups defined by the group boundaries in the input, arranged with increasing energy and decreasing group numbers.

Module 9

1st record: o , 'REMØ----'

2nd record: n , material name, total number of outscattering groups, total number of Legnedre moments.

3rd record: n , number of the outscattering group, number of subgroups in the outscattering group, number of intervals in one subgroup (the same for all subgroups in one outscattering group), SGT for all intervals in one group (product of the number of subgroups and the number of intervals in one subgroup) arranged with increasing energy, SGN for all intervals in one group, MUEL for all intervals in one group, FLUX for all intervals in one group.

repeated for all outscattering groups.

4th record: n , number of the Legendre moment, number of the outscattering group, SGNCi (i = Legendre moment) for all intervals in one group arranged in the sense that first the elements describing scattering within the group, then the elements describing scattering into the neighbouring group etc. are stored.

repeated for all outscattering groups (for a fixed Legendre moment)

repeated for all Legendre moments.

Table VI, cont.

Module 10

1st record: o , 'THERM---'

2nd record: n , material name, name of the reaction type, number of the thermal group.

3rd record: n , value of the group constant specified in the 2nd record.

References

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see also chapter II of the KEDAK Program Compendium (KFK 2387, II 2.9)

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Status of the Nuclear Data Library KEDAK-3
October 1975
KFK 2234, NEANDC(E) 171 "U", 1975

3. The calculation of weighted group averages for infinite dilution (from tabulated neutron data). Module 4

3.1 The difference between module 4 in MIGROS-2 and in MIGROS-3 is a more exact method of integration. Again the integration in the averages is done by a trapezoidal rule but the integration points are as well the energy points at which the nuclear data used in the numerator or eventually denominator integral are tabulated on the KEDAK library as the group boundaries as the energy points at which the weighting function is tabulated. The values of the weighting function are linearly interpolated at the energy points of the nuclear data from KEDAK and at the energy group boundaries, and the nuclear data are also linearly interpolated at the energy points of the weighting function and at the energy group boundaries. In the case of a weighting function given as analytical function the integration intervals are given by the energy points of all used nuclear data on KEDAK and the group boundaries. Each interval is divided into three equal parts and the integration is done. Then the integration is repeated once more in the interval now divided into six equal parts. If the results of these two subsequent integrations have a relative deviation greater than 1 %, the interval is now divided into twelf equal parts, the integration is done and the precision is tested once more and so on. If the relative error is less than or equal to 1 % the result of the last integration is taken and the next interval is regarded.

3.2 The average group cross sections are defined by

$$ {}^{k}\sigma_{x,g} = \frac{\int_{(g)} {}^{k}\sigma_{x}(E) \cdot F(E)dE}{\int_{(g)} F(E)dE} \qquad (3.1) $$

k = isotope

x = neutron reaction (n,x)

g = energy group

F(E) is a weighting function given by the input. Normally a slowly varying collision density is used, so that formula (3.1) defines the average group cross section for infinite dilution. The average group cross sections for all types of neutron reactions are calculated by formula (3.1) except:

- the average cosine of the elastic scattering

$$k\bar{\mu}_{e,g} = \frac{\int_{(g)} k\bar{\mu}_e(E) \cdot {}^k\sigma_e(E) \cdot F(E)dE}{\int_{(g)} {}^k\sigma_e(E) \cdot F(E)dE} \tag{3.2}$$

- the average number of secondaries per fission

$$k\nu_g = \frac{\int_{(g)} {}^k\nu(E) \cdot {}^k\sigma_f(E) \cdot F(E)dE}{\int_{(g)} {}^k\sigma_f(E) \cdot F(E)dE} \tag{3.3}$$

- the average α-value

$$k\alpha_g = \frac{\int_{(g)} {}^k\sigma_\gamma(E) \cdot F(E)dE}{\int_{(g)} {}^k\sigma_f(E) \cdot F(E)dE} \tag{3.4}$$

γ = radiative capture

- the average η-value

$$k\eta_g = \frac{k\nu_g}{1+k\alpha_g} \tag{3.5}$$

For which type of neutron reaction an average cross section shall be calculated can be choosen by input. There must be information available on the KEDAK library. If the reaction types σ_a [+)] and σ_f are given in the input, the type $\sigma_c = \sigma_a - \sigma_f$ is automatically calculated.

Besides that, the following group average

$$\sigma_{beH} = \frac{\int_{(g)} \frac{\sigma_e(E)}{E} \cdot F(E)dE}{\int_{(g)} F(E)dE} \qquad (3.6)$$

is calculated for hydrogen. This group average can be used for the production of the elastic scattering matrix.

3.3 The following subroutines are necessary

SUBROUTINE SUND (MM, ENG, NFE, REFE, EFE, ITYP, ITNAM, SGC, DUE,
XINTE, ZINT, XNEN, STREU, LDIM, LDIMP, SE, FSE)

The following parameters are defined by the control program:

MM	Number of energy group boundaries,
ENG(MM)	one-dimensional field containing the energy group boundaries in [eV],
NFE	number of points of the neutron flux density, = 1, if the function PHI(E) is used,
REFE(NFE)	one-dimensional field containing the energy points of the weighting function in |eV|,
EFE(NFE)	one-dimensional field containing the weighting function,
ITYP	number of cross section types,
ITNAM(ITYP)	one-dimensional field containing the names of the reaction types for which the weighted group averages shall be calculated,
LDIM	dimension of the following fields SE and FSE which is max (1500, number of $\sigma_e(E)$ values on KEDAK, number of $\sigma_f(E)$ values on KEDAK in all regarded energy groups).

[+)] The absorption cross section σ_a (KEDAK-type SGA) is defined on KEDAK in the following way:

$$\sigma_a = \sigma(n,\gamma) + \sigma(n,f) + \sigma(n,p) + \sigma(n,d) + \sigma(n,\alpha) \qquad /1/$$

The following parameters are working fields used by the subroutine SUND

SGC, DUE, XINTE, ZINT, XNEN, STREU one-dimensional fields of the length MM,

SE, FSE one-dimensional fields of the length LDIM which are used for the calculation of $^{k}\bar{\mu}_{e,g}$ and $^{k}\nu_{g}$ containing the energies and $^{k}\sigma_{e}(E)$ or the $^{k}\sigma_{f}(E)$ respectively.

The following parameter is calculated in SUND

LDIMP: 0, if the length of the working fields dimensioned with LDIM is sufficient,

n, number by which LDIM should be increased.

The subroutine SUND calls GRUP and FL.

SUBROUTINE GRUP (I, II, M, ENG, SE, FSE, SF, MOD)

The subroutine GRUP is used only for the calculation of $^{k}\nu_{g}$. Because on KEDAK the σ_f-values start to be greater zero at a higher energy than the ν-values, it is not possible to calculate ν_g with formula (3.3) in the lower energy region. A way out of this is to set σ_f internally in this module equal to a positive value (1.E20) for all energies with $\sigma_f = 0$ on KEDAK. The task of subroutine GRUP is to reset σ_f from 1.E20 to 0, if σ_f was not set in the entire actual energy group equal to 1.E20, that means, if σ_f is not zero on KEDAK in the entire energy group.

The following parameters are defined by SUND or by the control program.

I Index of the lower energy group boundary in field ENG,

II beginning index in the field SE for the actual energy group,

M length of the field SE,

ENG one-dimensional field containing the energy group boundaries,

SE(M) one-dimensional field containing the energy points of $^{k}\sigma_{f}$ from KEDAK,

FSE(M) one-dimensional field containing the $^{k}\sigma_{f}$ values from KEDAK,

SF lower integration interval boundary in the actual energy group,

MOD = 0 field SE contains the original σ_f values from KEDAK,

= 1 field SE contains the modified σ_f values (zero modified to 1.E20).

SUBROUTINE FL (EFE1, EFE2, REFE1, REFE2, E, ERG)

The task of FL is to realize the linear interpolation of the weighting function and the cross sections from KEDAK to the boundaries of the integration interval.

The following parameters are defined by SUND.

EFE1 Value of the lower interpolation base,
EFE2 value of the higher interpolation base,
REFE1 energy point of EFE1,
REFE2 energy point of EFE2,
E energy point of the value to be calculated.

The following parameter is filled by FL.

ERG Interpolated value to energy E.

/1/ B. Goel, B. Krieg,
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KFK 2234, 1975

4. The calculation of weighted average group cross sections for infinite dilution and of energy resonance self shielding factors from resolved resonance parameters. Module 1.

4.1 Flux-weighted energy resonance self shielding factors are calculated for capture, fission and elastic scattering. They are defined as

$$ {}^{k}f_{x,g}(\sigma_o, T) = \frac{{}^{k}\sigma_{x,g}(\sigma_o, T)}{{}^{k}\sigma_{x,g}(\sigma_o \to \infty, T)} \qquad (4.1) $$

k = isotope
x = neutron reaction (n,x)
g = energy group
T = temperature in K
σ_o = background cross section in barns

where

$$ {}^{k}\sigma_{x,g}(\sigma_o, T) = \frac{\left\langle \frac{{}^{k}\sigma_x(T,E)\,F(E)}{{}^{k}\sigma_t(T,E) + \sigma_o} \right\rangle}{\left\langle \frac{F(E)}{{}^{k}\sigma_t(T,E) + \sigma_o} \right\rangle} \qquad (4.2) $$

is the microscopic effective cross section.
The weighting function F(E) is the collision density and is assumed to have no resonance structure in the NR-approximation.
F(E) is the weighting function defined by the input.
(See Card 4 of the input description.)

The average is defined as

$$\langle y(E) \rangle = \frac{1}{\Delta E_g} \int_{\Delta E_g} y(E)\, dE$$

where ΔEg is the group width of group g .

The current-weighted resonance self-shielding factors are calculated for elastic scattering and for the total neutron reaction

$$ {}^{k}_{1}f_{x,g}(\sigma_o, T) = \frac{ {}^{k}_{1}\tilde{\sigma}_{x,g}(\sigma_o, T)}{ {}^{k}_{1}\tilde{\sigma}_{x,g}(\sigma_o \to \infty, T)} \qquad (4.3)$$

where

$$ {}^{k}_{1}\tilde{\sigma}_{x,g}(\sigma_o, T) = \frac{\left\langle \frac{ {}^{k}\sigma_x(T,E)\, F(E)}{\{ {}^{k}\sigma_t(T,E) + \sigma_o \}^2} \right\rangle}{\left\langle \frac{F(E)}{\{ {}^{k}\sigma_t(T,E) + \sigma_o \}^2} \right\rangle} \qquad (4.4)$$

is the current weighted microscopic effective cross section. For infinite dilution

$$\lim_{\sigma_o \to \infty} {}^{k}_{1}\tilde{\sigma}_{x,g}(\sigma_o, T) = \lim_{\sigma_o \to \infty} {}^{k}\tilde{\sigma}_{x,g}(\sigma_o, T) = {}^{k}\tilde{\sigma}^{\infty}_{x,g} \qquad (4.5)$$

and

$$ {}^{k}\tilde{\sigma}^{\infty}_{x,g}(T) = \frac{\left\langle {}^{k}\tilde{\sigma}_{x}(E,T)\, F(E) \right\rangle}{\left\langle F(E) \right\rangle} \qquad (4.6) $$

Therefore the denominators of (4.1) and (4.3) may be replaced by (4.6).

Normally ${}^{k}\sigma^{\infty}_{x,g}$ is independent of temperature, but in cases when only few resonances are within an energy group, and the group boundary cuts the wings of an important resonance, ${}^{k}\sigma^{\infty}_{x,g}$ may be temperature dependent.

The averages of (4.2), (4.4) and (4.6) are calculated by numerical integration. The microscopic cross sections $\sigma_x(E)$ are calculated from resonance parameters by a Breit-Wigner single level formula.*

$$ \tilde{\sigma}_{x}(E,T) = \sum_{r=1}^{R} \tilde{\sigma}_{x}(E, E_r, T) \qquad (4.7) $$

r = resonance

R = number of resonances taken into account

E_r = resonance energy

$$ \tilde{\sigma}_{x}(E, E_r, T) = {}_{r}\tilde{\sigma}_{ox} \cdot \psi_{r}(\theta, x) \qquad (4.8a) $$

for radiative capture and fission,

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* (the index for the isotope will be neglected)

$$\sigma_t(E,E_r,T) = \sigma_p + {}_r\sigma_{oc} \cdot \{ \psi_r \cdot \cos 2\delta_l + \chi_r \cdot \sin 2\delta_l \} \qquad (4.8b)$$

and for elastic scattering

$$\sigma_e(E,E_r,T) = \sigma_t(E,E_r,T) - \sum_x \sigma_x(E,E_r,T) \qquad (4.8c)$$

x = radiative capture, fission, where

$${}_r\sigma_{ox} = 4\pi \lambda^2(E)\, g \cdot \frac{\Gamma_n(E)\,\Gamma_x(E_r)}{\Gamma^2(E)} \qquad (4.9)$$

$${}_r\sigma_{oc} = 4\pi \lambda^2(E) \cdot g \cdot \frac{\Gamma_n(E)}{\Gamma(E)} \qquad (4.10)$$

$$\psi(\theta,x) = \frac{\theta}{2\sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{\exp\{-\frac{\theta^2}{4}\cdot(x-y)^2\}}{1+y^2}\, dy \qquad (4.11)$$

$$\chi(\theta,x)=\frac{\theta}{2\sqrt{\pi}}\int_{-\infty}^{+\infty}\frac{y\cdot\exp\left\{-\frac{\theta^2}{4}\cdot(x-y)^2\right\}}{1+y^2}dy \qquad (4.12)$$

$$\theta=\frac{\Gamma}{\Delta}\quad,\quad x=\frac{2(E-E_r)}{\Gamma(E)},\quad y=\frac{2(E'-E_r)}{\Gamma(E)} \qquad (4.13)$$

$\Delta = \left(\frac{4kTE}{A}\right)^{1/2}$: Doppler width

$\Gamma(E) = \Gamma_n(E) + \sum_{x\neq n}\Gamma_x$: total width

$\delta_\ell = \frac{R'}{\lambda\!\!\!^{-}} - \text{arctg}\,\frac{R'}{\lambda\!\!\!^{-}}\cdot\ell$ for $\ell = 0,1$

R' : effective radius of the nucleus

$\lambda\!\!\!^{-}$: reduced neutron length

$\Gamma_n(E) = \Gamma_n(E_r)\left(\frac{E}{E_r}\right)^{1/2}\left[\frac{(R'/\lambda\!\!\!^{-})^2}{1+(R'/\lambda\!\!\!^{-})^2}\right]^\ell$ for $\ell = 0,1$: neutron width

For resonances at negative resonance energies the KEDAK file contains the reduced width Γ_n^ℓ in place of the neutron width $\Gamma_n(E_r)$ and $\Gamma_n(E)$ is calculated as

$$\Gamma_n(E) = \Gamma_n^\ell\sqrt{\frac{E}{1\,eV}}\left[\frac{(R'/\lambda\!\!\!^{-})^2}{1+(R'/\lambda\!\!\!^{-})^2}\right]^\ell$$

Γ_x : fission or radiative capture width

$\sigma_p = 4\pi\lambda\!\!\!^{-2}\sum_{\ell=0}^{l}(2\ell+1)\sin^2\delta_\ell$: potential cross section

For $T \to 0$, that means $\Theta \to \infty$, one obtains the unbroadened resonance profiles

$$\psi(\Theta \to \infty, x) = \frac{1}{1 + x^2}$$

$$\chi(\Theta \to \infty, x) = \frac{x}{1 + x^2}$$

It should be pointed out that eqs. (4.9) - (4.13) and some of the definitions below eq. (4.13) supersede those given in the original description of MIGROS-2 (H. Huschke, B. Krieg, KFK 1784).

Corresponding changes have been made in the subprograms WIRQ and WIRQU in order to improve the accuracy of cross section calculations between resonances and in the thermal region. These changes refer to the energy dependences of Γ_n (hence Γ), Δ and σ_p, which are now fully taken into account.

4.2 The method of integration for the averages in (4.2), (4.4) and (4.6)

The expressions (4.2), (4.4) and (4.6) are calculated by numerical integration. The trapezoidal rule is used. To keep the number of integration points as small as possible the integration points are not taken as equidistant. This is necessary, because the calculation of the function values is very time consuming. To be sure that the resonances are not lost during the integration, the resonance energies are chosen as integration points. Let X_i be the integration points and Y_i the corresponding function values. Then the integration algorithm can be described in the following way:

First step: Initial abscissa and ordinate vectors are defined as

$$X^o = (X_1^o, X_2^o, X_3^o, \ldots X_{n-1}^o, X_n^o) = (E_{g+1}, E_{r,1}, E_{r,2}, \ldots E_{r,n-2}, E_g)$$

$$Y^o = (Y_1^o, Y_2^o, Y_3^o, \ldots Y_{n-1}^o, Y_n^o)$$

with

E_{g+1}: lower group limit,
E_g : upper group limit,
$E_{r,i}$: resonance energy of i-th resonance in energy group g,

and $Y_i^o = F(X_i^o)$, where $Y = F(E)$ is the integrand function.

Second step: The center of the first interval is added to the grid points, and new abscissa and ordinate vectors are defined accordingly,

$$X^1 = (X_1^1, X_2^1, X_3^1, \ldots X_{n+1}^1) = (X_1^o, \tfrac{1}{2}(X_1^o + X_2^o), X_2^o, \ldots X_n^o),$$

$$Y^1 = (Y_1^1, Y_2^1, Y_3^1, \ldots Y_{n+1}^1) = (Y_1^o, F(X_2^1), \quad Y_2^o, \ldots Y_n^o).$$

Furthermore one calculates the contributions from the interval $\left[X_1^1, X_2^1\right]$ to the trapezoidal-rule integral with and without the newly-inserted grid point,

$$a = \tfrac{1}{2}(Y_2^1 + Y_1^1)\ (X_2^1 - X_1^1),$$

$$b = \tfrac{1}{2}(\tilde{Y}_2^1 + Y_1^1)\ (X_2^1 - X_1^1)$$

with $\tilde{Y}_2^1 = \tfrac{1}{2}(Y_3^1 + Y_1^1)$.

This second step is repeated until the criterion

$$\left| \frac{b - a}{a} \right| < \varepsilon \qquad (4.18)$$

is fulfilled twice in succession. To be specific let the condition (4.18) be fulfilled after m-1 and again after m applications of the second step, the last application yielding

$$X^m = (X_1^m,\ X_2^m,\ X_3^m,\ \ldots\ X_{n+m}^m) = (X_1^{m-1},\ \tfrac{1}{2}(X_1^{m-1} + X_2^{m-1}),\ X_2^{m-1},\ \ldots\ X_{n+m-1}^{m-1}),$$

$$Y^m = (Y_1^m,\ Y_2^m,\ Y_3^m,\ \ldots\ Y_{n+m}^m) = (Y_1^{m-1},\ F(X_2^m),\ \qquad Y_2^{m-1},\ \ldots\ Y_{n+m-1}^{m-1}).$$

The calculation proceeds then to the interval $[X_2^m,\ X_3^m]$:

Third step: One calculates the contributions with and without the last inserted grid point from the interval $[X_2^m,\ X_3^m]$,

$$a = \tfrac{1}{2}(Y_3^m + Y_2^m)\ (X_3^m - X_2^m),$$

$$b = \tfrac{1}{2}(Y_3^m + \tilde{Y}_2^m)\ (X_3^m - X_2^m)$$

with $$\tilde{Y}_2^m = \tfrac{1}{2}(Y_3^m + Y_1^m).$$

If the condition

$$\left| \frac{b - a}{a} \right| < \varepsilon \qquad (4.19)$$

is fulfilled the integral over the interval $[X_1^m,\ X_3^m]$ is taken as

$$I_1 = \tfrac{1}{2}(Y_3^m + Y_1^m)\ (X_3^m - X_1^m)$$

and the whole algorithm is now applied to the remaining interval $[X_3^m,\ X_{n+m}^m]$ starting with the ordinate vector

$$X^o = (X_1^o,\ X_2^o,\ \ldots\ X_{n+m-2}^o) = (X_3^m,\ X_4^m,\ \ldots\ X_{n+m}^m).$$

If the criterion (4.10) is not satisfied the integral over the interval $[X_1^m,\ X_2^m]$ is taken as

$$I_1 = \tfrac{1}{2}(Y_2^m + Y_1^m)\ (X_2^m - X_1^m)$$

and the algorithm is repeated in the remaining interval $[X_2^m,\ X_{n+m}^m]$ starting with the ordinate vector

$$X^o = (X_1^o,\ X_2^o,\ \ldots\ X_{n+m-1}^o) = (X_2^m,\ X_3^m,\ \ldots\ X_{n+m}^m)$$

The algorithm is repeated until the integration over the total energy width is performed. The integral over the energy group is given by the sum.

$I = \sum_{i=1}^{N+1} I_i$, where N is the number of repetitions of the algorithm.

4.3 For the calculation of energy resonance self shielding factors and average weighted group constants from resolved resonance parameters the following subroutine are used:

FGEM (NS, SIGO, NE, ENG, NEF, ES, F, NT, TEMP, PR, NMR, NFST, SUM, SUO, IRE, IREP, ER, L, GJ, GAT, GAN, GAG, GAF, ISTE, ISTEP, STE, STE1)

In this subroutine the input of the nuclear data from the Karlsruhe nuclear data library KEDAK and the output of the f-factors and the average cross sections is organized. Also the integration algorithm is performed in this subroutine. The following parameters must be defined:

NS	: number of σ_o-values.
SIGO(NS)	: one-dimensional field containing the σ_o-values [barn].
NE	: number of the group boundaries.
ENG(NE)	: one-dimensional field containing the group boundaries [eV].
NEF	: number of energy points of the weighting spectrum.
ES(NEF)	: one-dimensional field containing the energy points of the weighting spectrum [eV].
F(NEF)	: one-dimensional field containing the weighting. function at the energy points of field ES.

NT : number of temperatures.

TEMP(NT) : one-dimensional field containing the temperatures [K].

PR : error limit ε, as defined in (4.18).

NMR : R/2 as defined in (4.7).

IRE : length of working fields, should be longer than the number of resonances for one isotope.

ISTE : length of a working field for integration, should be longer than the number of integration points necessary for the integration of effective group cross sections within one group.

Working fields:

SUM(NS,7), SUO (NE,3), ER (IRE), GJ (IRE), GAT (IRE), GAN (IRE), GAG (IRE), GAF (IRE), STE (5, ISTE), STE1(ISTE)

The following parameters are calculated in the subroutine:

NFST : number of the first energy group, for which f-factors can be calculated only from statistical resonance parameters. This parameter is important only, if the f-factors are calculated for an energy range, covering both, the range of resolved and the range of unresolved resonances.

IREP : 0, if the length of the working fields dimensioned with IRE is sufficient.

: n number, by which IRE should be increased.

ISTEP : 0, if the length of the working field dimensioned with ISTE is sufficient.

: n number, by which ISTE should be increased.

Information is also transferred by the unlabeled COMMON. It is described in chapter 1.

A description of the output is given in chapter 1.

WIRQ (INR, E, SF, SG, ST, IRE, ER, GJ, GAN, GAT, GAF, L, GAG, T, A, R, RLA)

In this subroutine the contribution of one resonance to the energy dependent cross section at a given energy is calculated by a Breit-Wigner single level formula.
The following parameters must be defined:

INR	: number of the resonance (all resonances of an isotope are numbered with increasing resonance energies).
E	: energy, [eV].
ER(IRE)	: one-dimensional field containing the resonance energies for one isotope, [eV].
IRE	: must be greater or equal to the number of resonances for one isotope.
GJ(IRE)	: one dimensional field containing the statistical parameters g_j for all resonances of one isotope.
GAN(IRE)	: one dimensional field containing the neutron half widths for all resonances of one isotope, [eV].
GAT(IRE)	: one dimensional field containing the total half widths for all resonances of one isotope, [eV].
GAF(IRE)	: one dimensional field containing the fission widths for all resonances of one isotope, [eV].
L(IRE)	: one dimensional field containing the neutron angular momentum for all resonances of one isotope.
GAG(IRE)	: one dimensional field containing the capture widths for all resonances of one isotope, [eV].
T	: temperature in K.
A	: atomic weight.
R	: radius of the nucleus, $[\sqrt{\text{barn}}]$.
RLA	: reduced neutron wave length, $[\sqrt{\text{barn}} \cdot \sqrt{\text{eV}}]$

The following parameters are calculated in the subroutine:

SF : contribution to the fission cross section at the energy E from the resonance with number INR, [barn].

SG : contribution to the capture cross sections at the energy E from the resonance with number INR [barn].

ST : contribution to the total resonance cross section at the energy E from the resonance with number INR, [barn].

WIRQU (NR1, E, SIFG, SIGG, SIGT, NR, IRE, ER, GJ, GAN, GAT, GAF, L, GAG, T, A, R, RLA, NMIN)

In this subroutine the sum of the contribution to the cross section at the energy E from all resonances, that are taken into account, is performed.
The following parameters must be defined:

NR1 : the number of the resonance belonging to the first resonance energy that is greater than the higher energy limit of the actual energy group.
All resonances of an isotope are numbered with increasing resonance energies).

E : energy [eV].

NR : maximum number of resonances for one isotope.

IRE : must be greater or equal to NR.

ER(IRE) : one-dimensional field containing the resonance energies for one isotope.

GJ(IRE) : one-dimensional field containing the statistical parameters g_j for all resonances of one isotope.

GAN(IRE) : one-dimensional field containing the neutron half widths for all resonances of one isotope [eV].

GAT(IRE) : one-dimensional field containing the total half widths for all resonances of one isotope. [eV].

GAF(IRE) : one-dimensional field containing the fission half widths for all resonances of one isotope. [eV].

L(IRE) : one-dimensional field containing the neutron angular momentum for resonances of one isotope.

GAG(IRE) : one dimensional field containing the capture widths for all resonances of one isotope. [eV].

T : temperature in K.

A : atomic weight.

R : radius of the nucleus in [$\sqrt{\text{barn}}$]

RLA : reduced neutron wave length, [$\sqrt{\text{barn}} \cdot \sqrt{\text{eV}}$].

NMIN : the number of resonances at higher and at lower resonance energies than the energy E, that are taken into account for the calculation of the cross sections at the energy E.

The following parameters are calculated in the subroutine:

SIFG : fission cross section at the energy E, [barn].

SIGG : radiative-capture cross section at the energy E, [barn].

SIGT : total cross section at the energy E, [barn].

STOSS (E1, E2, E3, F1, F2, F3, NFE, ES, F)

In this subroutine the macroscopic weighting function (collision density) at the energies E1, E2, E3 is calculated either from an energy point wise given weighting function by interpolation or from a function PHI(E). As standard PHI(E) = 1/E is used.

The following parameters must be defined:

E1, E2, E3 : energies in [eV].

NFE : number of energy points of the weighting spectrum. If NFE = o,1, the standard PHI(E) = 1/E is used.

ES(NFE) : one-dimensional field containing the energy points of the weighting spectrum [eV].

F(NFE) : one-dimensional field containing the weighting spectrum.

The following paramters are calculated in this subroutine:

F1, F2, F3 : weighting spectrum at the energies E1, E2, E3.

PSIXI (X, T, U, V) /1/, /2/.

In this subroutine the functions (4.11) and (4.12) are calculated.

The following parameters must be defined:

X : defined as (4.13)
T : is defined as $\left\{\frac{1}{\theta}\right\}^2$, where θ is given in (4.13).

The following parameters are calculated in the subroutine:

U : defined by (4.11)
V : defined by (4.12)

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On the Evaluation of Integrals Related to the Error Function
Math. of Computation 22, 1968, p. 137 - 143.

5. The calculation of average group cross sections for infinite dilution and of energy resonance self shielding factors from statistical resonance parameters. Module 2

The main change in module 2 compared to the description given in /3/ concerns the calculation of the statistical mean values $\overline{{}^{s}\Gamma_{x} J({}^{s}\beta, {}^{s}\theta)}$ and $\overline{{}^{s}\Gamma J({}^{s}\beta, {}^{s}\theta)}$. In the former version of the programme analytic approximations were used for the integrals under conditions depending on the Doppler width Δ and on the background cross-section σ_o, namely for

$$\frac{\overline{{}^{s}D}}{\sqrt{2\pi}\cdot\Delta} \cdot \frac{\langle {}^{s}\tilde{\sigma}_r \rangle}{{}^{s}\tilde{\sigma}_{p,eff}} \cdot {}^{s}E_r < 0.1$$

(compare formulas (5.28) to (5.32) of /3/). In the new version of the module $\overline{{}^{s}\Gamma_{x} J({}^{s}\theta, {}^{s}\beta)}$ and $\overline{{}^{s}\Gamma J({}^{s}\Gamma, {}^{s}\beta)}$ are in all cases calculated by numerical integration. Although this procedure is more time consuming it was preferred, as the results of the original programme showed deviations from the expected trend of the resonance self shielding factors as function of the temperature, which were removed by use of the modified programme.

5.1 The flux weighted resonance self shielding factors are calculated for radiative capture, fission and elastic scattering. They are defined as

$$ {}^{k}f_{x,g}(\tilde{\sigma}_o, T) = \frac{{}^{k}\tilde{\sigma}_{x,g}(\tilde{\sigma}_o, T)}{{}^{k}\tilde{\sigma}_{x,g}(\tilde{\sigma}_o \to \infty, T)} \qquad (5.1)$$

${}^{k}\sigma_{x,g}$ = microscopic effective group cross section (group cross section for a certain background cross section σ_o and a certain temperature T)

k = isotope

x = neutron reaction (n,x)

g = energy group

T = temperature in K

σ_o = background cross section in barns.

The following approximation is used:

$$ {}^{k}\tilde{\sigma}_{x,g}(\tilde{\sigma}_o \to \infty, T) \cong {}^{k}\tilde{\sigma}_{x,g}(\tilde{\sigma}_{o,max}, T) \qquad (5.2)$$

with

$$\tilde{\sigma}_{o,max} = max(10^6, \text{highest } \sigma_o \text{ value given by the input}) \qquad (5.3)$$

The microscopic effective group cross section may be represented by

$$\tilde{\sigma}_{x,g}(\sigma_o,T)=\frac{\sum_j \phi_j \cdot \tilde{\sigma}_{x,g}(\sigma_o,T,E_j)\cdot\Delta E_j}{\sum_j \phi_j \cdot \Delta E_j} \qquad (5.4)$$

ϕ_j is a slowly varying, resonance free flux density at the energy E_j, normally approximated by a collision density (The weighting function defined by the input is used. See card 4 of the input description.)

ΔE_j = energy interval around E_j

$\sigma_{x,g}(E_j)$ $(=\sigma_{x,g}(\sigma_o,T,E_j))$ **is the effective cross section in the energy interval ΔE_j around E_j belonging to energy group g) for the temperature T and the background cross section σ_o.**

The $\sigma_{x,g}(E_j)$ are slowly varying with energy when calculated from statistical resonance parameters. The group average of (5.4) is therefore performed in the following approximate way

$$\tilde{\sigma}_{x,g}(\sigma_o,T)\simeq\frac{\sum_j \phi_j \cdot \tilde{\sigma}_{x,g}(E_j)}{\sum_j \phi_j} \qquad (5.5)$$

where for the E_j are chosen: the upper and the lower group boundary of group g, E_g and E_{g+1}, and $(E_g + E_{g+1})/2$.

$\sigma_{x,g}(E_j)$ is composed of the contributions of all resonance series s.

$$\tilde{\sigma}_{x,g}(E_j) = \sum_s {}^s\tilde{\sigma}_{x,g}(E_j) \tag{5.6}$$

for radiative capture and fission, and

$$\tilde{\sigma}_{e,g}(E_j) = \sum_s \left\{ {}^s\tilde{\sigma}_{t,g}(E_j) - {}^s\tilde{\sigma}_{c,g}(E_j) - {}^s\tilde{\sigma}_{f,g}(E_j) \right\} + \tilde{\sigma}_p \tag{5.7}$$

${}^s\sigma_{r,g}(E_j)$ is the total resonance cross section, (c = radiative capture, f = fission).

The current weighted resonance self shielding factors are calculated for the total neutron reaction and for elastic scattering. They are defined as :

$${}^k_1 f_x(\sigma_0, T) = \frac{{}^k_1\tilde{\sigma}_{x,g}(\sigma_0, T)}{{}^k_1\tilde{\sigma}_{x,g}(\sigma_0 \to \infty, T)} \tag{5.8}$$

where

$${}^k_1\tilde{\sigma}_{x,g}(\sigma_0 \to \infty, T) \cong {}^k_1\tilde{\sigma}_{x,g}(\sigma_{0,max}, T) \tag{5.9}$$

$\sigma_{o,max}$ is given by (5.3).
The microscopic effective cross section for the neutron reaction (n,x) in the energy group g may be written as :

$$ {}_1\sigma_{x,g} = \frac{\sum_j {}_1\phi_j \cdot {}_1\sigma_{x,g}(E_j) \cdot \Delta E_j}{\sum_j {}_1\phi_j \cdot \Delta E_j} \qquad (5.10) $$

${}_1\phi_j$ is a slowly varying, resonance free current density, normaly approximated by a collision density. (In the programme the weighting function defined by the input is used; card 4 of the input description.)

For (5.10) the same approximation for averaging as for (5.5) is used.

${}_1\sigma_{x,g}(E_j)$ is composed of the contributions of the single resonance series s.

$$ {}_1\sigma_{e,g}(E) = \sum_s \left\{ {}^s{}_1\sigma_{r,g}(E_j) - {}^s{}_1\sigma_{c,g}(E_j) - {}^s{}_1\sigma_{f,g}(E_j) \right\} + \sigma_p \qquad (5.11) $$

$$ {}_1\sigma_{t,g}(E) = \sum_s {}^s{}_1\sigma_{r,g} + \sigma_p \qquad (5.12) $$

The effective resonance cross section at the energy E_j and the series s is calculated by a theory, first developed by R. Froelich /1/, /2/ and modified by H. Huschke. This modified theory is given in appendix I of /3/.

$$ {}^s\sigma_{x,g}(E) = {}^s\sigma_{p,\mathrm{eff}} \frac{\left[1 + \frac{\langle {}^s\sigma_r \rangle}{\langle \sigma_t \rangle}\right] \cdot \frac{\overline{{}^s\Gamma_x \cdot J({}^s\beta, {}^s\theta)}}{{}^s\overline{D} \cdot \cos 2\delta_l} - \frac{{}^s\overline{D}\,\langle {}^s\sigma_x \rangle \langle {}^s\sigma_r \rangle}{\Delta \sqrt{2\pi} \cdot \langle \sigma_t \rangle^2} \cdot \varepsilon}{1 - \left[1 + \frac{\langle {}^s\sigma_r \rangle}{\langle \sigma_t \rangle}\right] \cdot \frac{\overline{{}^s\Gamma \cdot J({}^s\beta, {}^s\theta)}}{{}^s\overline{D}} + \frac{{}^s\overline{D}\,\langle {}^s\sigma_r \rangle^2}{\Delta \sqrt{2\pi} \langle \sigma_t \rangle^2} \cdot \varepsilon} \qquad (5.13) $$

for fission and capture

and

$$ {}^{s}\tilde{\sigma}_{r,g}(E) = {}^{s}\tilde{\sigma}_{p,eff} \frac{\left[1+\frac{\langle {}^{s}\tilde{\sigma}_r\rangle}{\langle \tilde{\sigma}_t\rangle}\right]\frac{\overline{{}^{s}\Gamma . J({}^{s}\beta,{}^{s}\theta)}}{\overline{{}^{s}D}} - \frac{\overline{{}^{s}D}\,\langle {}^{s}\tilde{\sigma}_r\rangle^2}{\Delta\sqrt{2\pi}\,\langle \tilde{\sigma}_t\rangle^2}\cdot\varepsilon}{1-\left[1+\frac{\langle {}^{s}\tilde{\sigma}_r\rangle}{\langle \tilde{\sigma}_t\rangle}\right]\frac{\overline{{}^{s}\Gamma . J({}^{s}\beta,{}^{s}\theta)}}{\overline{{}^{s}D}} + \frac{\overline{{}^{s}D}\,\langle {}^{s}\tilde{\sigma}_r\rangle^2}{\Delta\sqrt{2\pi}\,\langle \tilde{\sigma}_t\rangle^2}\cdot\varepsilon} \qquad (5.14) $$

for the total resonance cross section.

${}^{s}\Gamma_x$ width for the neutron reaction (n,x) and the resonance series s

${}^{s}\Gamma$ total width for the resonance series s.

$$ J(\beta,\theta) = \int_0^\infty \frac{\psi(\theta,x)}{\psi(\theta,x)+\beta}\,dx \qquad (5.15) $$

$$ \psi(\theta,x) = \frac{\theta}{2\sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{\exp\left\{-\frac{\theta^2}{4}\cdot(x-y)^2\right\}}{1+y^2}\,dy \qquad (5.16) $$

$$ \theta = \frac{\Gamma}{\Delta} \quad , \quad \Delta = \sqrt{\frac{4kTE}{A}} \qquad (5.17) $$

k = Boltzmann constant

E = energy

A = mass number

T = temperature

$\delta_l = \frac{R}{\lambda\!\!\!^{-}} - \operatorname{arctg} \frac{R}{\lambda\!\!\!^{-}} \cdot l$ for $l = o,1$; $\delta_2 = \frac{R}{\lambda\!\!\!^{-}} - \operatorname{arctg} \left(\frac{3\frac{R}{\lambda\!\!\!^{-}}}{3-\left(\frac{R}{\lambda\!\!\!^{-}}\right)^2}\right)$

R = effective radius of the nucleus

$\lambda\!\!\!^{-}$ = reduced neutron wave length

$\overline{{}^{s}D}$ = average level distance for the resonance series s.

$$\overline{\Gamma_n \Gamma_f} \equiv \int_0^\infty \Gamma_n \Gamma_f \, {}^{s}F_n({}^{s}\Gamma_n) \cdot {}^{s}F_f({}^{s}\Gamma_f) \, d{}^{s}\Gamma_n \, d{}^{s}\Gamma_f \qquad (5.18)$$

where ${}^{s}F_n({}^{s}\Gamma_n)$ is the distribution of the neutron width of the resonance series s and ${}^{s}F_f({}^{s}\Gamma_f)$ is the distribution of the fission width of the resonance series s.

$\langle {}^{s}\sigma_x \rangle$ *) average cross section of the neutron reaction (n,x) for the series s (See formula (5.28))

$\langle {}^{s}\sigma_r \rangle$ average resonance cross section of the series s. (See formula (5.33))

$$\langle \sigma_t \rangle \equiv \sigma_o + \sigma_p + \sum_s \langle {}^{s}\sigma_r \rangle \quad , \qquad (5.19)$$

with

$$\sigma_o = \frac{1}{N} \left\{ \langle \Sigma_t \rangle - N \cdot \left(\sigma_p + \sum_s \langle {}^{s}\sigma_r \rangle \right) \right\} \qquad (5.20)$$

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*) $\langle y(E) \rangle = \frac{1}{\Delta E} \int_{\Delta E} y(E) dE$

the average background cross section.
Σ_t is the total cross section of the mixture.

$$ {}^s\tilde{\sigma}_{p,eff} = \langle \tilde{\sigma}_t \rangle - \langle {}^s\tilde{\sigma}_r \rangle \tag{5.21} $$

$$ {}^s\beta = \frac{\langle \tilde{\sigma}_t \rangle}{{}^s\tilde{\sigma}_{oc}} \tag{5.22} $$

$$ {}^s\tilde{\sigma}_{oc} = 4\pi \lambda^2 \cdot g \cdot \frac{{}^s\Gamma_n}{{}^s\Gamma} \cdot \cos 2\delta_l \tag{5.23} $$

$$ \varepsilon = 2 \cdot \int_0^\infty \exp\left\{ -\frac{D^2}{2\Delta^2} \right\} \cdot \Omega(D)\, dD \tag{5.24} $$

There must be noted that the expression (5.24) for the correction is only correct for Doppler broadened resonances, so that $\Gamma/\Delta << 1$. The formalism cannot be used for the natural line shape of the resonances.

$$ \Omega(D) = \frac{1}{D} \sum_{\mathcal{H}=1}^{\nu/2} \cos\left\{ \frac{4\pi}{\nu}\mathcal{H} + \frac{\nu \cdot D}{2\overline{D}} \sin \frac{4\pi}{\nu}\mathcal{H} \right\} \exp\left\{ \frac{\nu D}{2\overline{D}} \left(\cos \frac{4\pi}{\nu}\mathcal{H} - 1 \right) \right\} \tag{5.25} $$

with ν = 1o.

To calculate the current weighted effective cross sections for the resonance series s, an approximation of H. Huschke* is used. That means, that the current weighted effective cross section can be calculated by the formulas (5.13) to (5.25), when $\langle\sigma_t\rangle$ is replaced by $\langle\sigma_t\rangle/2$. This also means, that ${}^s\sigma_{p,eff}$ is replaced by $\{{}^s\sigma_{p,eff} - \langle {}^s\sigma_r\rangle\}/2$.

The average level distance $\overline{{}^sD}$ for the resonance series s at the energy E is given by

$$\overline{{}^sD} = \overline{{}^{os}D} \cdot \frac{\{{}^sE_B + E\}^2}{\{{}^sE_B\}^2} \cdot \exp\left\{-\sqrt{89{,}72\,({}^sE_B + E)} + \sqrt{89{,}72\,{}^sE_B}\right\} \qquad (5.26)$$

$\overline{{}^{os}D}$ average level distance of resonance series s for low energies, $E \ll E_B$.

E_B binding energy of the last neutron in the compound nucleus in MeV.

E energy in MeV.

The statistical mean values of $\overline{{}^s\Gamma_x \cdot J({}^s\beta, {}^s\theta)}$ are calculated by numerical integration. For the distribution of the neutron half widths $F_n(\Gamma_n)$ and the fission half widths $F_f(\Gamma_f)$ χ^2-distribution are used.

$$F(\Gamma)\,d\Gamma = \frac{\nu}{2\overline{\Gamma}\cdot G\left(\frac{\nu}{2}\right)} \left(\frac{\nu\cdot\Gamma}{2\overline{\Gamma}}\right)^{\frac{\nu}{2}-1} \cdot \exp\left\{-\frac{\nu}{2}\frac{\Gamma}{\overline{\Gamma}}\right\} d\Gamma \qquad (5.27)$$

ν degree of freedom

G here is the Γ-function

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* see appendix II of /3/.

The average cross sections of the neutron reaction (n,x) for the resonance series s are given by

$$\langle {}^{s}\tilde{\sigma}_x \rangle = \frac{2\pi^2}{{}^{s}D} \cdot \lambda^2 \cdot g \cdot \overline{{}^{s}\Gamma_n} \cdot {}^{s}S_x \qquad (5.28)$$

with

$${}^{s}S_x = \frac{\overline{\left[\frac{{}^{s}\Gamma_n \cdot {}^{s}\Gamma_x}{{}^{s}\Gamma}\right]}}{\overline{{}^{s}\Gamma_n}} \qquad (5.29)$$

and

$$\langle {}^{s}\tilde{\sigma}_r \rangle = \frac{2\pi^2}{{}^{s}D} \cdot \lambda^2 \cdot g \cdot \overline{{}^{s}\Gamma_n} \cdot \cos 2\delta_\ell \qquad (5.30)$$

with

$$\delta_\ell = \frac{R}{\lambda} - \text{arc tg}\left(\frac{R}{\lambda} \cdot \ell\right) \qquad \text{for } \ell = 0,1 \text{ and}$$

$$\delta_2 = \frac{R}{\lambda} - \text{arc tg}\left(\frac{3\frac{R}{\lambda}}{3-\left(\frac{R}{\lambda}\right)^2}\right)$$

The ${}^{s}S_{x}$ are calculated by numerical integration with the χ^2-distributions defined in (5.27)

The average neutron half widths are calculated from the reduced average neutron half widths

$$\overline{{}^{s}\Gamma_n} = \overline{{}^{os}\Gamma_n} \cdot \sqrt{E} \cdot \nu_\ell \qquad (5.31)$$

with

$$\nu_\ell = \frac{R^2+(1+\ell)\lambda^2}{R^2+\lambda^2} \quad \text{for } \ell = 0,1 \text{ and}$$

$$\nu_2 = \frac{(R/\lambda)^4}{(R/\lambda)^4+3(R/\lambda)^2+9}$$

The average group cross sections for infinite dilution are calculated in the following way:

$$\sigma^{\infty}_{x,g} = \frac{\sum_j \phi_j \left\{ \sum_s \langle {}^{s}\sigma_x \rangle \right\}}{\sum_j \phi_j} \qquad (5.32)$$

for capture and fission,

$$\sigma^{\infty}_{e,g} = \frac{\sum_j \phi_j \left\{ \sum_s \left(\langle {}^{s}\sigma_r \rangle - \langle {}^{s}\sigma_c \rangle - \langle {}^{s}\sigma_f \rangle \right) + \sigma_p \right\}}{\sum_j \phi_j} \qquad (5.33)$$

for elastic scattering, where ϕ_j is the weighting function(provided by the input) at the group boundaries and in the middle of the group.

5.2 The numerical procedure in calculating the statistical averages.

Statistical averages of the following type have to be calculated:

$$\overline{f(\Gamma)} = \int_0^\infty f(\Gamma)\, F(\Gamma)\, d\Gamma \tag{5.34}$$

where $f(\Gamma)$ is a function, which depends on Γ, $F(\Gamma)$ is a probability distribution. $F(\Gamma)$ is a χ^2-distribution of the degree of freedom ν.

The procedure of integration is the following. The whole range of integration is divided into n intervals so that

$$\int_{\Gamma_i}^{\Gamma_{i+1}} F(\Gamma)\, d\Gamma = \frac{1}{n} \qquad \text{for all intervals } i=1,n \tag{5.35}$$

In the interval i the average $\overline{\Gamma}_i$ is calculated

$$\overline{\Gamma}_i = \frac{\int_{\Gamma_i}^{\Gamma_{i+1}} \Gamma\, F(\Gamma)\, d\Gamma}{\int_{\Gamma_i}^{\Gamma_{i+1}} F(\Gamma)\, d\Gamma} = n \cdot \int_{\Gamma_i}^{\Gamma_{i+1}} \Gamma\, F(\Gamma)\, d\Gamma \tag{5.36}$$

For χ^2-distributions for several degrees of freedom

$$\chi_i = \frac{\overline{\Gamma}_i}{\overline{\Gamma}} \quad ; \quad i = 1, n \tag{5.37}$$

are tabulated.

$$\overline{\Gamma} \equiv \int_0^\infty \Gamma \cdot F(\Gamma)\, d\Gamma \tag{5.38}$$

The integral (5.34) then is approximated by

$$\overline{f(\Gamma)} = \sum_{i=1}^{n} f(\overline{\Gamma} \cdot \chi_i) \cdot \int_{\Gamma_i}^{\Gamma_{i+1}} F(\Gamma)\, d\Gamma = \frac{1}{n} \sum_{i=1}^{n} f(\overline{\Gamma} \cdot \chi_i) \tag{5.39}$$

This approximation reproduces $\overline{\Gamma}$ exactly

$$\overline{\Gamma} = \frac{1}{n} \sum_{i=1}^{n} \overline{\Gamma} \cdot \chi_i = \frac{1}{n} \sum_{i=1}^{n} \overline{\Gamma_i}$$

Using equation (5.36) one gets

$$\overline{\Gamma} = \sum_{i=1}^{n} \int_{\Gamma_i}^{\Gamma_{i+1}} \Gamma \cdot F(\Gamma)\, d\Gamma = \int_0^\infty \Gamma \cdot F(\Gamma)\, d\Gamma .$$

In the same way the statistical averages of the type

$$\overline{f(\Gamma_1, \Gamma_2)} = \int_0^\infty d\Gamma_1 \int_0^\infty d\Gamma_2\, f(\Gamma_1, \Gamma_2) \cdot F_1(\Gamma_1) \cdot F_2(\Gamma_2) \tag{5.40}$$

are approximated by

$$\overline{f(\Gamma_1, \Gamma_2)} = \frac{1}{n_1 \cdot n_2} \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} f(\overline{\Gamma_1} \cdot \chi_{1,i}\, ,\, \overline{\Gamma_2} \cdot \chi_{2,j}) \tag{5.41}$$

with

$$\chi_{1,i} = \frac{\overline{\Gamma_{1,i}}}{\overline{\Gamma_1}} \quad , \quad \chi_{2,j} = \frac{\overline{\Gamma_{2,j}}}{\overline{\Gamma_2}} \quad . \tag{5.42}$$

5.3 For the calculation of energy resonance self shielding factors and average group constants from statistical resonance parameters the following subroutines are used:

FSTAT (MI, SIGO, J, ENG, NFE, REFE, EFE, MT, TEMP, SE, SM, XEUGZ)

In this subroutine the average group cross sections and the energy resonance self shielding factors are calculated from statistical parameters residing on the KEDAK-file. After the subroutine QUER has calculated the microscopic average cross sections and the effective microscopic cross sections at three energy points E numerical integration is performed and the average group cross sections and the self shielding factors are printed on paper and are stored on an external unit.

MI	: number of values of the background cross section σ_o
SIGO(MI)	: one-dimensional field containing the background cross sections [barns].
J	: number of energy group limits.
ENG(J)	: one-dimensional field containing the energy group limits in [eV].
NFE	: number of points of the collision density, 0 or 1, if the function PHI(E) = 1/E is used.
REFE(NFE)	: one-dimensional field containing the energy points of the collision density in [eV].
EFE(NFE)	: one-dimensional field containing the flux density for all energy points in REFE.
MT	: number of temperatures.

TEMP(MT) : one-dimensional field containing the temperatures in [K].

SE(3,5,MI) : three-dimensional field which is calculated in the subroutine QUER .

SM(3,5,MI) : three-dimensional field which is calculated in the subroutine QUER .

XEUG(5,MI) : two-dimensional field containing the resonance self shielding factors for all σ_o-values. The first index indicates the reaction type

1: radiative capture, flux-weighted
2: elastic scattering, flux-weighted
3: fission, flux-weighted
4: elastic scattering, current-weighted
5: total, current-weighted

A description of the CØMMØN and of the output is given in chapters 1 and 2.

QUER (E, TT, N, SE, SM, XNYN, FXNY, DEL, RQU, CHI, DN, EBI, XA, XL, GN, GG, NEY, EY, GFA, GI, IT, MI, SIGO, NEXTGR, ENEXT, INEXT, SSSSNE)

In this subroutine the effective microscopic cross sections for the resonance series s at the energy E as defined by equation (5.13) and (5.14) are calculated. Also the effective microscopic cross sections at the energy E including the contributions of all resonance series s as defined by the equations (5.6), (5.7), (5.11) and (5.12) are calculated in this subroutine. The following parameters must be defined:

E : energy in [eV], at which the effective cross section should be calculated

TT : temperature in [K].

N : n-th energy point within an energy group at which the microscopic effective cross sections are calculated for the evaluation of the effective group cross sections.

XNYN(1o) : one-dimensional field containing the ν_n, the degree of freedom of the χ^2-distributions for the neutron width, for all resonance series s ($s \leq 1o$).

FXNY(1o) : one-dimensional field containing the ν_f, the degree of freedom of the χ^2-distribution for the fission width, for all resonance series.

DEL : $(4k/A) \cdot 1o^6$, k = Boltzmann constant in [eV/ K], A = mass number.

RQU : R^2 [barn], R = effective radius of the nucleus.

CHI(25,4) : 2-dimensional field, containing the χ_i as defined in equation (5.37) for several degrees of freedom for the χ^2-distribution (n = 25, ν = 1, 2, 3, 4).

DN(1o) : one-dimensional field containing the average level distance at low energies $\overline{os}_D$ for all resonance series s ($s \leq 1o$) [meV].

EBI : binding energy of the last neutron in the compound nucleus [eV].

XA : $\lambda_o^2 = E \cdot \lambda^2$ [eV barn].

XL(1o) : one-dimensional field containing the quantum numbers l for the angular momentum in all resonance series.

GN(1o) : one-dimensional field containing the average reduced neutron widths $\overline{\Gamma}_n^o \cdot 1o^3$ for all resonance series. $\overline{\Gamma}_n^o$ in [$eV^{1/2}$].

GG(1o) : one-dimensional field containing the average capture widths for all resonance series in [meV].

NEY : number of energy points, for which the fission widths are tabulated on the KEDAK-library.

EY(199) : one-dimensional field containing the energy points, for which the fission widths are read from the nuclear data library [eV]; maximum number of points is 199.

GFA(1o, 199) : two dimensional field containing the average fission widths at the energies EY for all resonance series in [meV],
first parameter for the series,
second parameter for the energy points.

GI(1o) : one-dimensional field containing the statistical parameter $\frac{2J+1}{2(2I+1)}$ for all resonance series. (J=spin of the compound nucleus. I=spin of the target nucleus.)

IT : number of resonance series

MI : number of values of the background cross section σ_o.

SIGO(MI) : one-dimensional field containing the values of the background cross sections.

The following parameters are calculated in the subroutine

SE(3,5,MI) : three-dimensional field containing the microscopic effective group cross section in / barn /,
first index for energy,
second index for the reaction type.

1: capture, see formula (5.6)
2: elastic scattering, see formula (5.7)
3: fission, see formula (5.6)
4: elastic scattering, see formula (5.11)
5: total, see formula (5.12)

third index for the background cross section σ_o.

SM(3,5,MI) : three-dimensional field containing the microscopic average group cross sections in [barn], as given by formulas (5.19), (5.28) and (5.30)
First index for energy,
second index for the reaction type as for SE,
third index for the background cross section σ_o,
(not significant, because the average cross section does not depend on σ_o).

Only local variables are: NEXTGR, ENEXT, INEXT, SSSSNE

EZZ (E, NS, EZG, EZC, EZF, DRSG, DRFS, CHI, XNYN, FXNYN, GN, RQU, XL, XA, GG, NEY, EY, GF)

In this subroutine the statistical mean values, defined by equation (5.29) are calculated.

The following parameters must be defined:

E : energy [eV].

NS : number of the resonance series to be calculated.

CHI(25,4) : two-dimensional field containing the χ_i as defined in equation (5.37) for several degrees of freedom for the χ^2-distribution (n = 25, ν = 1, 2, 3, 4).

XNYN(1o) : one-dimensional field containing the ν_n, the degree of freedom of the χ^2-distribution for the neutron half width, for all resonance series s ($s \leq 1o$).

FXNYN(1o) : one-dimensional field containing the ν_f, the degree of freedom of the χ^2-distribution for the fission width, for all resonances.

GN(1o) : one-dimensional field containing the average reduced neutron widths $\overline{\Gamma}^o_n \cdot 1o^3$ for all resonance series. $\overline{\Gamma}^o_n$ in [$\sqrt{eV}$].

RQU : R^2 [barn], R = **effective radius of the nucleus.**

XL(1o) : one-dimensional field containing the quantum numbers l for the angular momentum for all resonance series.

XA : $\lambda^2_o = E \cdot \lambda^2$ [eV barn].

GG(1o) : one-dimensional field containing the average capture widths for all resonance series [meV].

EY(99) : one-dimensional field containing the energy points, for which the fission widths are read from the nuclear data library [eV]; maximum number of points is 199.

GF(1o,199) : two-dimensional field containing the average fission widths at the energies EY for all resonance series in [meV],
first index for the series,
second index for the energy points.

The following parameters are calculated in the subroutine:

EZG : defined by equation (5.32) of /3/, for capture, not used in the present version of the programme.

EZC : defined by equation (5.31) of /3/; not used in the present version of the programme.

EZF : defined by equation (5.32) of /3/, for fission; not used in the present version of the programme.

DRSG : defined by equation (5.29), for capture.

DRFS : defined by equation (5.29), for fission

TAB(XT, XK, LG, DSJ, XABCJ, DJK)

In this subroutine the $J(\beta,\theta)$-function and the derivatives $\frac{\partial J}{\partial \beta}$ and $\frac{\partial J}{\partial \theta}$ are calculated.

The following parameters must be defined:

XT : $\theta = \frac{\Gamma}{\Delta}$, Γ and Δ in [eV], (5.17).

XK : k, where k is defined by $\beta = 2^k \cdot 10^{-5}$, β is defined by (5.22).

LG : 1, if XABCJ is calculated
2, if DJK is calculated
0, if DSJ is calculated
negative, if XABCJ, DJK and DSJ are calculated

The following parameters are calculated by the subroutine:

XABCJ : $J(\beta,\theta)$-function as defined by (5.15).

DSJ : $\frac{\partial J(\beta,\theta)}{\partial \theta}$

DJK : $\frac{\partial J(\beta,\theta)}{\partial k}$, with $\beta = 2^k \cdot 10^{-5}$.

SUCH (E, NSU, NEY, EY)

This is an auxiliary subroutine

Besides the subroutines the following functions are necessary:

DMIT (E, NS, DN, EBI)

In this function the average level distance at the energy E is calculated by formula (5.26).

E : energy in [eV].
NS : number of the resonance series.
DN(1o) : one-dimensional-field containing the $\overline{^{os}D}$ for all resonance series s [meV].
EBI : binding energy E_B of the last neutron in the compound nucleus [eV].
DMIT : $\overline{^{s}D}$ at the energy E for the resonance series NS in [meV].

GAMN (E, NS, GN, RQU, XL, XA)

In this function the average neutron width at the energy E is calculated by the formula (5.31).

E : energy in [eV].
NS : number of the resonance series.
GN(1o) : one-dimensional field containing the reduced average neutron half widths $\overline{^{o}\Gamma_n}$ for all resonance series in [meV].
RQU : R^2 in [barn], R = effective radius of the nucleus
XL(1o) : one-dimensional field containing the quantum numbers for the angular momentum for all resonance series.
XA : $\lambda\!\!\!^{-2}\cdot E$ in [eV•barn], $\lambda\!\!\!^{-}$ is the neutron wave length.
GAMN : $\overline{\Gamma_n}$, the average neutron half width at the energy E for the resonance series NS [meV].

GAMG (E, NS, GG)

In this subroutine the average capture half width at the energy E is provided.

E	: energy in [eV].
NS	: number of the resonance series.
GG(1o)	: one-dimensional field containing the average capture half widths for all resonance series in [meV].
GAMG	: average capture half widths at the energy E for the resonance series NS in [meV].

GAFM (E, NS, NEY, EY, GF)

In this subroutine the average fission half width at the energy E is interpolated from the tabulated values.

E	: energy [eV].
NS	: number of the resonance series.
EY(199)	: one-dimensional field, containing the energies, at which the average fission widths are tabulated [eV].
GF(1o,199)	: one-dimensional field, containing the tabulated average fission widths in [meV].
GAFM	: average fission width at the energy E for the resonance series NS in [meV]

POL (X, X1, FX1)

Auxiliary function for a linear interpolation

X	: argument, for which an arbitrary function should be interpolated.
X1(2)	: one-dimensional field, containing two arguments of the function.
FX1(2)	: one-dimensional field, containing the values of the function at the arguments X1.
POL	: value of the function at X.

EPSI (E, T, NS, DN, EBI, DEL)

In this function the overlapping correction ε, defined by formula (5.24) is calculated.

E	: energy in [eV].
T	: temperature in [K].
NS	: number of resonance series.
DN(1o)	: one-dimensional field containing the $\overline{{}^{os}D}$ for all resonance series s [meV].
EBI	: binding energy E_B of the last neutron in the compound nucleus [eV].
DEL	: $(4k/A)\cdot 1o^6$, k = Boltzmann constant in [eV/ K], A = mass number.

DELTA (E, T, NS, DEL)

In this function the Doppler width, formula (5.17), is calculated.

E	: energy in [eV].
T	: temperature in [K],
NS	: number of resonance series.
DEL	: $\frac{4k}{A} \cdot 1o^6$; k = Boltzmann constant in [eV/ K], A = mass number.

PHASE (E, NS, XA, RQU, XL)

In this function cos $2\delta_1$ is calculated, where $\delta_1 = R/\lambda\!\!\!^{-} - \text{arctg}\,\frac{R}{\lambda\!\!\!^{-}} \cdot 1$. R is the effective radius of the nucleus, $\lambda\!\!\!^{-}$ is the reduced neutron wave length.

E	: energy in [eV].
NS	: number of resonance series.

XA : $\lambda\!\!\!^{-2}_{o} = E \cdot \lambda\!\!\!^{-2}$ [eV·barn].

XL(1o) : one-dimensional field containing the quantum numbers l for the angular momentum in all resonance series.

SIGC(E, NS, XA, GI, DN, EBI, GN, RQU, XL)

In this function the average radiative capture cross section at the energy E for a single resonance series is calculated

E : energy in [eV].

NS : number of resonance series.

XA : $\lambda\!\!\!^{-2}_{o} = E \cdot \lambda\!\!\!^{-2}$ [eV·barn].

GI(1o) : one-dimensional field containing the statistical parameter $\frac{2J+1}{2(2I+1)}$ for all resonance series.

DN(1o) : one-dimensional field containing the average level distance at low energies $\overline{{}^{os}D}$ for all resonance series in [meV].

EBI : binding energy of the last neutron in the compound nucleus in [eV]

GN(1o) : one-dimensional field containing the average reduced neutron widths $\overline{\Gamma}^{o}_{n} \cdot 1o^{3}$ for all resonance series, $\overline{\Gamma}^{o}_{n}$ in [$eV^{1/2}$].

RQU : R^2 in [barn], R = effective radius of the nucleus.

XL(1o) : one-dimensional field containing the quantum number l of the angular momentum for all resonance series.

5.4 Description of the (not selfexplaining) warnings, produced by module 2

xxx WARNING 2.04

Comment: To get a correct overlapping correction, Γ/Δ should be much smaller than one. Normally it is assumed, that $\Gamma/\Delta < 0.5$ is small enough. See the discussion following formula (5.24).

xxx WARNING 2.05

Comment: For the calculation of the current weighted resonance self shielding factors an approximation is used, which in some cases is not valid for small σ_o-values. (See also Appendix II, formula (25) of /3/). In these cases a warning is produced and the smallest σ_o-value, for which the applied approximation is valid, is printed out.

xxx WARNING 2.06

Comment: The reason for this warning might be the same as in xxx WARNING 2.04. If not, the formalisme for approximating the overlapping correction is insufficient.
The warning is given, when the denominator in formula (5.14) becomes negative. If the resulting ${}^s\sigma_{r,g}$ in (5.14) is small against the contribution of all other resonance series, this warning may be ignored.

References

/1/ R. Froelich
Theorie der Dopplerkoeffizienten schneller Reaktoren unter Berücksichtigung der gegenseitigen Abschirmung der Resonanzen.
KFK 367 (1965)

/2/ H. Huschke
Gruppenkonstanten für dampf- und natriumgekühlte Reaktoren in einer 26-Gruppendarstellung.
KFK 77o, p 2-7, (1968)

/3/ H. Huschke, B. Krieg
MIGRØS-2: A Program Written in FORTRAN for the Calculation of Microscopic Group Constants from Nuclear Data.
KFK 1784 (1973)

6. The calculation of normalized transfer matrices for inelastic scattering, (n,2n)- and (n,3n)-reactions. Module 5.

6.1 Changes with respect to module 5 in MIGRØS-2

Module 5 has been nearly completely rewritten for MIGRØS-3. The reasons for this were partly connected with the introduction of KEDAK 3,/1/. In addition to the KEDAK-3-materials evaluated at Karlsruhe those materials have to be processed by the new module, that have been transferred from ENDF/B,/2/,by the code BRIGITTE,/3/.

Information about new cross-section types (SGIZC, SEDIC, SED2N, SED3N) is available on KEDAK 3 and is used in the new module 5. At the time, when the first version of module 5, /4/, was written, these types did not contain information and therefore were not taken account of in that first version of the module.

Moreover the physical, numerical and code-procedures have been refined in the MIGRØS-3-version.

The following points give the main differences in detail:

1.) The convention of KEDAK-2, /5/, that for one material the energy points, at which the cross-sections are stored, are the same for all cross-section types has been given up on KEDAK-3 in order to save storage on the nuclear data library. Especially for the calculation of transfer matrices for inelastic scattering this means, that the excitation cross-sections for the different discrete levels (SGIZ(E_j,E)) are no longer stored at the same energy points E.

2.) On KEDAK-2 there were two clearly separated energy regions in connection with inelastic scattering: one region of low neutron incident energies, by which discrete levels of the residual nucleus are excited and an adjacent region of higher neutron incident energies, by which continuous levels of the residual nucleus are excited. On KEDAK-3 the energy regions (regions of primary neutron energy), which are connected with excitation of discrete or continuous levels of the residual nucleus may overlap.

3.) In contrary to KEDAK-2 the nuclear library KEDAK-3 provides energy distributions for the secondary neutrons produced in inelastic scattering processes, by (n,2n)-reactions and by (n,3n)-reactions (types SEDIC, SED2N, SED3N). Therefore the corresponding transfer matrices can now be calculated with the information taken from the nuclear data library.

4.) Three different options are given to choose the physical approximation by which the partial transfer matrix connected with the excitation of discrete levels of the residual nucleus is calculated.

5.) The method of numerical integration over the outscattering energy group has been refined for the calculation of transfer probabilities, that are in connection with discrete excitation levels of the residual nucleus and for those, that are connected with the excitation of continuous levels of the residual nucleus.

6.) The nuclear data are no longer kept in core storage for the entire energy region given on KEDAK but are kept in core storage only for the outscattering group just treated.

6.2 Formulas used

In correspondence with /4/ the general formula for the calculation of the inelastic scattering transfer probability from energy group g to energy group h is given by

$$ {}^{k}\sigma_{i,g\to h} = \frac{\int_{E_{h+1}}^{E_h} dE \int_{E_{g+1}}^{E_g} dE' \; {}^{k}\sigma_i(E')\phi(E')P(E'\to E)}{\int_{E_{g+1}}^{E_g} \phi(E')dE'} \qquad (6.1) $$

Again E' is the energy of the incident neutron and E the energy of the scattered neutron. ${}^{k}\sigma_i(E')$ is the inelastic cross section of material k [+)] at energy E', $\phi(E')$ is the energy dependent neutron flux and P(E'→E) the probability

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[+)] The index k will be omitted in the following.

that an incident neutron of energy E' produces a secondary neutron of energy E by inelastic scattering. (6.1) is valid for (n,2n)- and (n,3n)-processes as well.

In the programme to be described for $\phi(E')$ the weighting function given by the input (see BLØC2 in the input description, chapter 2) is inserted. This weighting function (given by input) may be chosen by the user. In general it will be a collision density ($F(E') = \Sigma_t(E') \cdot \phi(E')$), where $\Sigma_t(E')$ is the total cross-section of the material composition under consideration and $\phi(E')$ the neutron flux. Weighting by $F(E')$ instead of weighting by $\phi(E')$ means that most of the energy dependent structure in the weighting function is neglected. It has to be considered however, that for all materials the threshold for inelastic scattering lies above the resonance region of the heavy materials. (In the (200 - 300) energy group representation, /6/, the full energy dependence of the total cross-section of the material composition is taken into account in the weighting flux $\phi(E') = \frac{F(E')}{\Sigma_t(E')}$.)

To make quite clear, that the weighting function supplied by the input, $w(E')$, is used for the calculation of the transfer probabilities formula (6.1) is rewritten as

$$k_{\sigma_{i,g\to h}} = \frac{\int_{E_{h+1}}^{E_h} dE \int_{E_{g+1}}^{E_g} dE'\, \sigma_i(E')\, w(E')\, P(E'\to E)}{\int_{E_{g+1}}^{E_g} dE'\, w(E')} \qquad (6.1.1)$$

6.2.1 Calculation of the partial inelastic transfer matrices connected with the excitation of discrete levels of the residual nucleus

For our calculations we have to start from formula (6.1.1). The inelastic cross-section for the excitation of discrete levels of the residual nucleus is given separately for each excitation level E_j as $\sigma^{E_j}(E')$. The total inelastic cross-section for excitation of discrete levels of the residual nucleus is $\sum_j \sigma_i^{E_j}(E')$ ($\sum_j$ means summation over j). The

probability, that an incident neutron of energy E' by excitation of the level E_j produces a scattered neutron of energy E is $\sigma_i^{E_j}(E')\ P_j(E'\to E)$. For an exact calculation of the neutron energy loss in inelastic processes, the scattering angle-energy correlation has to be taken fully into account, /7/, /8/, /9/. In module 5 three different approximations to this exact treatment are applied:

1.) $$P_j(E'\to E) = \delta(E'-E-E_j) \qquad (6.2)$$

δ is the Dirac δ-function.
This approximation corresponds to the one applied in MIGRØS-2 ,/4/. Here the excitation energy E_j of the residual nucleus is used as it is given on the nculear library, that means in the center of mass system. If the transformation of E_j into the laboratory system is carried out the second possibility to calculate the transfer probability in the new version of module 5 is given.

2.) $$P_j(E'\to E) = \delta\left(E'-E-\frac{AT+AN}{AT}E_j\right), \qquad (6.3)$$

where AT is the atomic mass of the target nucleus and AN that of the neutron. The atomic weights given on KEDAK (type ISØT1) are referred to the atomic mass of C12 = 12 AMU. In this system the mass of the neutron is 1.008665 AMU, so that

$$P_j(E'\to E) = \delta\left(E'-E-\frac{AT+1.008665}{AT}E_j\right) \qquad (6.3.1)$$

The third approximation used in module 5 has been recommended by Segev ,/7/, /9/. This is the approximation used on ENDF/B, /2/.

3.) $$P_j(E'\to E) = \delta\left(E-\frac{(AT)^2+1.008665^2}{(AT+1.008665)^2}E' + \frac{AT}{AT+1.008665}E_j\right) \qquad (6.4)$$

To obtain the inelastic transfer probabilities from outscattering group g to inscattering group h the relations 1.) to 3.) have to be inserted into formula (6.1.1). The integration using the transfer probability given in relation 1.) (formula (6.2)) has been carried out in /4/. Here we shall insert relations 2.) and 3.) into the general formula (6.1.1). First the relation 2.).

$$\sigma_{i,g\to h} = \frac{\int_{E_{h+1}}^{E_h} dE \int_{E_{g+1}}^{E_g} dE' \sum_j \sigma_i^{E_j}(E')w(E')\delta(E'-E-\frac{AT+AN}{AT}E_j)}{\int_{E_{g+1}}^{E_g} dE' w(E')} \quad (6.5)$$

First the double integration in the numerator is carried out starting with the integration over E' using the relationship /10/:

$$\left.\begin{aligned} &\text{if } f_2(x_o) = 0, \\ &\int_{x_1}^{x_2} f_1(x)\delta[f_2(x)]dx = \frac{f_1(x_o)}{\left|\frac{df_2}{dx}\right|_{x=x_o}}, \\ &\text{if } x_1 \le x_o \le x_2 \end{aligned}\right\} \quad (6.6)$$

This results in

$$\int_{E_{h+1}}^{E_h} dE \int_{E_{g+1}}^{E_g} dE' \sum_j \sigma_i^{E_j}(E')w(E')\delta(E'-E-\frac{AT+AN}{AT}E_j) \quad (6.7)$$

$$= \int_{E_{h+1}}^{E_h} dE \sum_j \sigma_i^{E_j}(E+\frac{AT+AN}{AT}E_j)w(E+\frac{AT+AN}{AT}E_j)\cdot\chi(E_{g+1}\le E+\frac{AT+AN}{AT}E_j\le E_g)$$

with

$$\chi(E_{g+1}\le E+\frac{AT+AN}{AT}E_j\le E_g) = \begin{cases} 1, \text{ if the inequality in the argument is valid} \\ 0, \text{ if the inequality in the argument is not valid} \end{cases}$$

Transformation of the integration over E in (6.7) to an integration over $E_o' = E + \frac{AT+AN}{AT}E_j$ results in

$$\left.\begin{aligned} &\int_{E_{h+1}}^{E_h} dE \int_{E_{g+1}}^{E_g} dE' \sum_j \sigma_i^{E_j}(E')w(E')\delta(E'-E-\frac{AT+AN}{AT}E_j) \\ &= \int_{E_{h+1}+\frac{AT+AN}{AT}E_j}^{E_h+\frac{AT+AN}{AT}E_j} dE'_o \sum_j \sigma_i^{E_j}(E'_o)w(E'_o)\chi(E_{g+1}\leq E'_o \leq E_g) \end{aligned}\right\} \quad (6.8)$$

The function $\chi(E_{g+1} \leq E'_o \leq E_g)$ may be replaced by a modification of the integration region, so that the numerator of (6.5) is finally given by

$$\left.\begin{aligned} &\int_{E_{h+1}}^{E_h} dE \int_{E_{g+1}}^{E_g} dE' \sum_j \sigma_i^{E_j}(E')w(E')\delta(E'-E-\frac{AT+AN}{AT}E_j) \\ &= \int_{E_u}^{E_o} dE'_o \sum_j \sigma_i^{E_j}(E'_o)w(E'_o) \end{aligned}\right\} \quad (6.9)$$

with

$$\left.\begin{aligned} E_u &= \mathrm{Max}(E_{g+1},\ E_{h+1}+\frac{AT+AN}{AT}E_j) \\ E_o &= \mathrm{Min}(E_g,\ E_h+\frac{AT+AN}{At}E_j) \end{aligned}\right\} \quad (6.9.1)$$

In (6.9.1) the function Max means the maximum value of the two numbers in the argument. Correspondingly the function Min means the minimum value of the two numbers in the argument.

If instead of relation 2.) relation 1.) (formula (6.2)) for $P_j(E' \to E)$ is inserted into the numerator of (6.11) the result of the integration corresponds to the one given in formulas (6.9), (6.9.1), if the constant $\frac{AT+AN}{AT}$ is replaced by 1 in these formulas. (See /4/, (6.4) and (6.5).)

If the option 3.) for $P_j(E' \to E)$ (formula (6.4)) is chosen the formula (6.1.1) for the inelastic transition probability becomes:

$$\sigma_{i,g\to h} = \frac{\int_{E_{h+1}}^{E_h} dE \int_{E_{g+1}}^{E_g} dE' \sum_j \sigma_i^{E_j}(E')w(E')\delta\left(E - \frac{AT^2+AN^2}{(AT+AN)^2}E' + \frac{AT}{AT+AN}E_j\right)}{\int_{E_{g+1}}^{E_g} dE' w(E')} \tag{6.10}$$

The double integral in the numerator is reduced to a single integral by the δ-function. Using (6.6) the result of the integration over E' is

$$\left.\begin{aligned} &\int_{E_{g+1}}^{E_h} dE \int_{E_{g+1}}^{E_g} dE' \sum_j \sigma_i^{E_j}(E')w(E')\delta\left(E - \frac{AT^2+AN^2}{(AT+AN)^2}E' + \frac{AT}{AT+AN}E_j\right) \\ &= \frac{(AT+AN)^2}{AT^2+AN^2}\int_{E_{h+1}}^{E_h} dE \sum_j \sigma_i^{E_j}(E_o')w(E_o') \cdot \chi(E_{g+1}\leq E_o' \leq E_g) \end{aligned}\right\} \tag{6.11}$$

with

$$E_o' = \frac{(AT+AN)^2}{AT^2+AN^2}\left(E + \frac{AT}{AT+AN}E_j\right) \tag{6.11.1}$$

To carry out the integration over the inscattering group $h = (E_{h+1}, E_h)$, the integration over E is transformed into an integration over E_o', so that the right hand side of (6.11) becomes:

$$\int_{\frac{(AT+AN)^2}{AT^2+AN^2}\left(E_{h+1} + \frac{AT}{AT+AN}E_j\right)}^{\frac{(AT+AN)^2}{AT^2+AN^2}\left(E_h + \frac{AT}{AT+AN}E_j\right)} dE_o' \sum_j \sigma_i^{E_j}(E_o')w(E_o') \cdot \chi(E_{g+1}\leq E_o' \leq E_g) \tag{6.11.2}$$

The restriction given by the function χ may be taken into account by modification of the integration limits, so that for the application of option 3.) (6.4) in the numerator of formula (6.1.1) the following result is obtained:

$$\left.\begin{aligned} &\int_{E_{h+1}}^{E_h} dE \int_{E_{g+1}}^{E_g} dE' \sum_j \sigma_i^{E_j}(E')w(E')\delta\left(E - \frac{AT^2+AN^2}{(AT+AN)^2}E' + \frac{AT}{AT+AN}E_j\right) \\ &= \int_{E_u}^{E_o} dE'_o \sum_j \sigma_i^{E_j}(E'_o)w(E'_o) \end{aligned}\right\} \quad (6.12)$$

with

$$\left.\begin{aligned} E_u &= \mathrm{Max}\left(E_{g+1}, \frac{(AT+AN)^2}{AT^2+AN^2}\left(E_{h+1} + \frac{AT}{AT+AN}E_j\right)\right) \\ E_o &= \mathrm{Min}\left(E_g, \frac{(AT+AN)^2}{AT^2+AN^2}\left(E_h + \frac{AT}{AT+AN}E_j\right)\right) \end{aligned}\right\} \quad (6.12.1)$$

In formulas (6.9) and (6.12) the integration over E'_o is carried out by a trapezoidal rule. Integration points are the combination of all energy points of the KEDAK-type SGIZ(E_j, E'_o) for all E_j contributing between E_u and E_o and the energy points of the weighting function. If w(E') is not given energy-pointwise, an energy grid is constructed for the weighting function PHI(E'), so that all points between the grid points can be obtained by linear interpolation with a relative error of less than 1 $^o/_{oo}$. For the trapezoidal integration this energy grid is combined with the energies of KEDAK.

6.2.2 Short summary of formulas derived for the calculation of partial inelastic transfer matrices connected with the excitation of discrete levels of the residual nucleus

Given are the results for the normalized partial inelastic transfer probabilities $P^d_{i,g\to h}$, when options 1.), 2.) or 3.) are inserted into (6.1.1). The superscript d refers to discrete levels. The general

formula for $P^d_{i,g\to h}$ is:

$$P^d_{i,g\to h} = \frac{\sigma^d_{i,g\to h}}{\sigma^d_{i,g}} \tag{6.13}$$

with

$$\sigma^d_{i,g} = \frac{\int_{E_{g+1}}^{E_g} \sum_j \sigma_i^{E_j}(E')w(E')dE'}{\int_{E_{g+1}}^{E_g} w(E')dE'} \tag{6.13.1}$$

For the three options 1.) (6.2), 2.) (6.3) and 3.) (6.4) the transfer probability $P^d_{i,g\to h}$ is given by

$$P^d_{i,g\to h} = \frac{\int_{E_u}^{E_o} dE'_o \sum_j \sigma_i^{E_j}(E'_o)w(E'_o)}{\int_{E_{g+1}}^{E_g} \sum_j \sigma_i^{E_j}(E')w(E')dE'} \tag{6.14}$$

The different approximations used for the inelastic energy transfer (options 1.), 2.), 3.)) are expressed in the result (6.14) by different integration limits E_u and E_o.

If approximation 1.) (6.2) is applied the integration limits are given by:

$$\left.\begin{aligned} E_u^{(1)} &= \mathrm{Max}(E_{g+1},\ E_{h+1} + E_j) \\ E_o^{(1)} &= \mathrm{Min}(E_g,\ E_h + E_j) \end{aligned}\right\} \tag{6.15}$$

The superscript on E_u, E_o refers to options 1.), 2.) or 3.)

$$\left.\begin{aligned} E_u^{(2)} &= \mathrm{Max}(E_{g+1},\ E_{h+1} + \frac{AT+AN}{AT} E_j) \\ E_o^{(2)} &= \mathrm{Min}(E_g,\ E_h + \frac{AT+AN}{AT} E_j) \end{aligned}\right\} \qquad (6.16)$$

and finally

$$\left.\begin{aligned} E_u^{(3)} &= \mathrm{Max}(E_{g+1},\ \frac{(AT+AN)^2}{AT^2+AN^2} (E_{h+1} + \frac{AT}{AT+AN} E_j)) \\ E_o^{(3)} &= \mathrm{Min}(E_g,\ \frac{(AT+AN)^2}{AT^2+AN^2} (E_h + \frac{AT}{AT+AN} E_j)) \end{aligned}\right\} \qquad (6.17)$$

6.2.3 Calculation of partial inelastic transfer matrices connected with the excitation of continuous levels of the residual nucleus

Again formula (6.1.1) has to be evaluated inserting now the nuclear data that describe the excitation of continuous levels. In the following formulas the superscript c refers to "continuous" level excitation.

$$\sigma^c_{i,g\to h} = \frac{\int_{E_{h+1}}^{E_h} dE \int_{E_{g+1}}^{E_g} dE' \sigma_i^c(E') P_i^c(E'\to E) w(E')}{\int_{E_{g+1}}^{E_g} dE' w(E')} \qquad (6.18)$$

The continuous level inelastic scattering cross-section, $\sigma_i^c(E')$, is given by the type SGIZC on KEDAK. For some materials this type is not filled. In these cases $\sigma_i^c(E')$ is equal to the total inelastic cross-section (KEDAK-type SGI) above the last energy point of the type SGIZ and is set equal to zero in the energy region where excitation cross-sections for discrete levels, SGIZ, are given. $P_i^c(E'\to E)$ may be analytic or tabulated functions of E and E'. In the present version of MIGRØS-3 (summer 1976) only evaporation distributions can be processed. Additional subroutines are being worked on, to enable module 5, to process secondary neutron energy distributions, that are given by tabulated functions.

The evaporation distribution is given by

$$P_i^c(E'\to E)\begin{cases} = \frac{E}{I}\, e^{-E/\Theta(E')}, \text{ if } 0\le E\le E'-U \\ = 0, \text{ else} \end{cases} \qquad (6.19)$$

U is the threshold energy of the inelastic scattering process and Θ the nuclear temperature, which on KEDAK is given as a tabulated function of E'. The normalization constant I depends on the nuclear temperature and the threshold energy U of the inelastic scattering process.

$$I = \Theta^2(E')\left[1-e^{-(E'-U)/\Theta(E')}\left(1+\frac{E'-U}{\Theta(E')}\right)\right] \qquad (6.19.1)$$

Θ and U are given in the KEDAK-type SEDIC. If SEDIC is not filled an evaporation model with a nuclear temperature $\Theta(E') = \sqrt{\frac{E}{\nu \cdot A}}$ [MeV], /11/, is used by module 5. A is the atomic weight of the target nucleus, read from KEDAK, and ν an adjustable parameter, that is set equal to 0.16 MeV^{-1} in the standard case but may be modified by input. If SEDIC is not filled U is read from KEDAK as the threshold of SGI.

P_i^c in (6.19) is a continuous function of E and E'. In (6.18), (6.19) the integration over E may be carried out first with the result

$$\sigma^c_{i,g\to h} = \frac{\int_{E_{g+1}}^{E_g} dE'\sigma_i^c(E')w(E')\, P_i^c(E'\to h)}{\int_{E_{g+1}}^{E_g} w(E')dE'} = \qquad (6.20)$$

$$\frac{\int_{E_{g+1}}^{E_g} dE' \frac{1}{I}\,\sigma_i^c(E')w(E')\Theta^2(E')\left[\exp\left(-\frac{E_{h+1}}{\Theta(E')}\right)\left(\frac{E_{h+1}}{\Theta(E')}+1\right) - \exp\left(-\frac{E_h}{\Theta(E')}\right)\left(\frac{E_h}{\Theta(E')}+1\right)\right]}{\int_{E_{g+1}}^{E_g} w(E')dE'}$$

The normalized transfer probability is

$$P^c_{i,g\to h} = \frac{\sigma^c_{i,g\to h}}{\sigma^c_{i,g}} \tag{6.20.1}$$

$$\sigma^c_{i,g} = \frac{\int_{E_{g+1}}^{E_g} \sigma^c_i(E')w(E')dE'}{\int_{E_{g+1}}^{E_g} dE'w(E')} \tag{6.20.2}$$

The integrations over E' in (6.20) and (6.20.2) is done by Simpson's rule. The energy grid, with which the integration is started is the combination of the energy points of $\sigma^c_i(E')$ on KEDAK and the energy points of the weighting function, if w(E') is given energy-pointwise. If w(E') is given as a function the integration starts with the energy points of $\sigma^c_i(E')$.

6.2.4 Total inelastic scattering transfer matrix

The group constant sets need the total inelastic transfer-matrix, which is the combination of the inelastic transfer matrix for discrete level excitation, $P^d_{i,g\to h}$ and the inelastic transfer matrix for continuous level excitation $P^c_{i,g\to h}$. Combination of formulas (6.13) and (6.20.1) gives the total inelastic scattering transfer matrix:

$$P_{i,g\to h} = \frac{\sigma^d_{i,g}\, P^d_{i,g\to h} + \sigma^c_{i,g}\, P^c_{i,g\to h}}{\sigma^d_{i,g} + \sigma^c_{i,g}} \tag{6.21}$$

or, written in a slightly modified manner:

$$P_{i,g\to h} = \frac{R^d_{i,g}\, P^d_{i,g\to h} + R^c_{i,g}\, P^c_{i,g\to h}}{R^d_{i,g} + R^c_{i,g}} \tag{6.21.1}$$

$$R^{d}_{i,g} = \int_{E_{g+1}}^{E_g} \sigma^{d}_{i}(E')w(E')dE' \qquad R^{c}_{i,g} = \int_{E_{g+1}}^{E_g} \sigma^{c}_{i}(E')w(E')dE' \qquad (6.21.2)$$

6.2.5 Calculation of transfer probabilities for (n,2n)- and (n,3n)-reactions

The transfer probabilities for (n,2n)- and (n,3n)-reactions are calculated with formulas corresponding to those used in chapter 6.2.3 for the calculation of inelastic transfer matrices in connection with excitation of continuous levels of the residual nucleus. In correspondence with (6.18) we have:

$$\sigma_{(n,2n)g\to h} = \frac{\int_{E_{h+1}}^{E_h} dE \int_{E_{g+1}}^{E_g} dE' \sigma_{(n,2n)}(E')w(E')P_{(n,2n)}(E'\to E)}{\int dE'w(E')} \qquad (6.22)$$

The same formula is valid for (n,3n)-reactions, if (n,2n) is replaced by (n,3n).

For $P_{(n,2n)}(E'\to E)$ and $P_{(n,3n)}(E'\to E)$ the information of the KEDAK type SED2N and SED3N is used. In the present version of KEDAK evaporation distributions are given, which from (6.19), (6.19.1) differ by the values of Θ and U. Again, if no information is contained in SED2N, SED3N the nuclear temperature is taken as an analytic function of E' with an adjustable parameter ν, which may be chosen by input.

After integration over the inscattering group the normalized element of the transfermatrix is

$$P_{(n,2n)g\to h} = \qquad (6.23)$$

$$\frac{\int_{E_{g+1}}^{E_g} dE' \frac{1}{I}\sigma_{(n,2n)}(E')w(E')\Theta^2(E')\left[\exp(-\frac{E_{h+1}}{\Theta(E')})(\frac{E_{h+1}}{\Theta(E')}+1)-\exp(-\frac{E_h}{\Theta(E')})(\frac{E_h}{\Theta(E')}+1)\right]}{\int_{E_{g+1}}^{E_g} dE'\sigma_{(n,2n)}(E')w(E')}$$

again the integration over E' is carried out by Simpson's rule.

6.3 Description of the code

The main subroutine of module 5, SCAT, is a subroutine of the organizing subroutine of MIGRØS-3, INPUT. SCAT itself calls two subroutines, SCATD, that provides the transition probabilities for inelastic scattering reactions, that occur by excitation of discrete levels of the residual nucleus and SCATC, which provides transfer probabilities for inelastic scattering processes, that excite continuous energy levels of the residual nucleus. SCATC also calculates the transfer matrices of (n,2n)- and (n,3n)-processes.

6.3.1 Description of the subroutine SCATD and its subprogrammes

SCATD has been developed from the former subroutine SCAT[+] (see /4/). The main differences are, that now the KEDAK-data are read for each outscattering group separately and that instead of formula (6.2) only formulas (6.2), (6.3) or (6.4) may be used for the calculation of the energy transfer by inelastic scattering. The subroutine SCATD calculates the integration limits E_u and E_o given in equations (6.15), (6.16) or (6.17) and carries out the numerical integration over the outscattering group in formulas (6.9) and (6.12). The integration is done in a threefold nested doloop, in which the inner index treats the excitation levels, the second index treats the inscattering groups and the outer index treats the outscattering groups.

```
Subroutine SCATD(NX,EG,NFE,EF,FI,NE27,WEIN,QUØT,WAHR,VW,E,AE,SU,LBA,
                 SGIT,IANF,SGIP,WERT,EZ,NISG,NISGP,NAE,NAEP,ISG,ISGP,
                 KINEM,NEA,NAB)
```

Arguments, that have to be defined, when SCATD is called:

EG(NX)	provided by the input, energy group boundaries of the outscattering groups. Internally in the programme the energy group limits are numbered starting with 1 for the lowest energy (internal energy group count). EG(NX) may or may not contain the thermal group.
NX	number of energy group boundaries of outscattering groups.
EF(NFE)	provided by the input: energy grid of the weighting spectrum

[+] SCAT (/4/) was originally developed by B. Schatz

FI(NFE) — points of the weighting spectrum

NFE — number of energy points of the weighting spectrum (NFE is set equal to 1 internally, if the weighting spectrum is given by an analytical function)

NE27 — number of energy group boundaries of the inscattering groups. The inscattering groups contain the thermal group.

NISG, NAE, ISG — estimations of needed lengths of fields, that are used in SCATD and related subroutines

KINEM — provided by the input: decides, whether approximation (6.2), (6.3) or (6.4) is chosen, to describe the energy transfer connected with the excitation of discrete levels of the residual nucleus

Arguments, that are transferred by SCATD to the calling subroutine SCAT.

NEA — number of energy group of lowest energy (internal group count), for which transfer matrices are calculated in SCATD (provided by DAØRG).

NAB — number of energy group of highest energy (internal group count), for which transfer matrices are calculated in SCATD (provided by DAØRG).

WEIN(NX,NX) — transfer probabilities for inelastic scattering with excitation of discrete levels of the residual nucleus (corresponding to formula (6.14)). The first index gives the group number of the outscattering group (1 being the number of the energy group with lowest energy), the second index refers to the inscattering group. Second index 1 means inscattering group is equal to outscattering group, second index 2 means the inscattering group is the energetically next lower group, second index I means inscattering group is the energy group, that energetically lies (I-1) groups below the outscattering group.

QUØT(NX) — $\int_{E_{g+1}}^{E_g} dE' \sum_j \sigma_i^{E_j}(E')w(E')$ (internal group count)

(calculated in AKED)

$= R^d_{i,g}$ given by formula (6.21.2)

NISGP, NAEP, ISGP — numbers, that have to be added to NISG,NAE,ISG to get sufficient field lengths for the tasks to be carried out by SCATD and its subprogrammes. NISGP,NAEP and ISGP are provided by the subroutine DAØRG.

The following arguments are working fields in SCATD:

local working fields: WAHR(NX), VW(NX), E(NE27) (E(NE27) = energy group boundaries , containing thermal group , LBA(NX).
Working fields, supplied by subroutine AKED:
AE(NAE),SU(NX),SGIT(ISG),IANF(NAE),SGIP(ISG,NAE),WERT(ISG),EZ(NISG)

The subroutine AKED, called by SCATD is a modified version of the subroutine AKED[+)] described in /4/. AKED calculates

$$\int_{E_{g+1}}^{E_g} \sum_j \sigma_i^{E_j}(E')w(E')dE' \quad \text{and}$$

$$\int_{E_{g+1}}^{E_g} w(E')dE'$$

Subroutine AKED(I,E,EZ,SGIP,JMAT,LMAX,SU,QUØT,WERT,AE,IA,NAB,IE,INF,NFE,
EF,FI,NE,NX,SGIT,NAE,NAEP,ISG,ISGP,IANF,NISG,NISGP,EJMAX)

Arguments, that have to be defined, when AKED is called:

I	group number of outscattering group (internal energy group count).
E(NE)	energy group boundaries (containing thermal group)
IE	number of energy group of lowest energy required by input
INF	number of energy group of highest energy required by input
NFE,EF(NFE),FI(NFE)	see arguments of SCATD
NE	number of energy boundaries, including thermal group
NX	number of energy boundaries given by input
NAE, ISG, NISG	needed field lengths, provided by DAØRG

Arguments, that are supplied by AKED to calling subroutine SCATD.

EZ(ISG)	energy field, containing combination of energy points of the excitation cross-sections $\sigma_i^{E_j}(E')$, contributing in energy group I together with the energy points of the

[+)] AKED(/4/) was originally developed by B. Schatz.

weighting function, energy points of the weighting function given energy-pointwise by input or energy points constructed by the subroutine SPECTI for the representation of an analytic weighting spectrum given by a function subprogramme. (provided by DAØRG)

SGIP(ISG,NAE) level excitation cross-sections from KEDAK $\sigma_i^{E_j}$ (KEDAK-type SGIZ(E_j,E')).First index refers to the energy point E' in the^{j}field EZ, the second index gives the number of the excitation level (provided by SIØRG)

JMAT number of excitation levels, contributing in energy group I (provided by DAØRG)

LMAX actual length of energy field EZ, needed to store cross-section and spectrum points for energy group I (provided by DAØRG)

SU(NX) energy group integral of the weighting function:

$$\int_{E_{g+1}}^{E_g} w(E')dE'$$

QUØT(NX) energy group integral of discrete level inelastic cross-section* weighting function

$$\int_{E_{g+1}}^{E_g} \sum_j \sigma_i^{E_j}(E')w(E')dE'$$

WERT(ISG) contains values of the weighting function w ateneergy points EZ(1)... EZ(LMAX)

AE(NAE) excitation energies of discrete levels contributing in energy group I (provided by SIØRG)

SGIT(ISG) $\sum_j \sigma_i^{E_j}(E')$. SGIT(II) is the total discrete level inelastic cross-section at the energy point EZ(II).(provided by SIØRG)

IANF(NAE) IANF(J) : number of first energy point of field EZ, for which an excitation cross-section of level J, $\sigma_i^{E_j}(E')$, is given on KEDAK. This first cross-section value is stored in SGIP(1,J), the corresponding energy is stored in EZ(IANF(J)):

EZ(IANF(J)) ...	SGIP(1,J)
EZ(IANF(J)+1) ...	SGIP(2,J)
.	.
.	.
.	.
EZ(LMAX)	SGIP(LMAX-IANF(J)+1)

(provided by SIØRG)

EJMAX energy of excitation level of the highest energy, contributing in energy group I (provided by DAØRG)

local variables: NAEP,ISGP,NISGP,IA,NAB.

The subroutine DAØRG has two tasks. The first time DAØRG is called (by the subroutine SCATD for all energy groups required by input) its task is to find out

1. The common range of outscattering energies, that is required by the input and for which inelastic scattering reactions to excited levels occur, that means the range of energy groups, for which the calculation of inelastic scattering matrices to discrete levels is actually performed (IA,NAB).

2. The maximum values of the fieldlengths NISG,ISG and NAE, that are needed in any of the energy groups to be treated. If the values, of NISG, ISG NAE, estimated by the organizing subroutine SCAT are not sufficient, numbers NISGP,ISGP and NAEP are provided, that have to be added to NISG,ISG,NAE, to get sufficient field lengths.

The second call (subroutine DAØRG called by subroutine AKED) provides the energy field EZ.

Subroutine DAØRG(I,KEN,EZ,E,AE,EF,FI,J,KMAX,NISG,NISGF,NISGP,NE27,NAE,
NAEF,NAEP,ISG,ISGF,ISGP,IA,NAB)

Arguments, that have to be defined, before DAØRG is called:

I	number of energy group
KEN=NFE	number of energy points of the weighting spectrum
EF(KEN)	energy points of the weighting spectrum
FI(KEN)	weighting spectrum
NE27	number of energy boundaries including thermal group
E(NE27)	energy group boundaries including thermal group
NISG,NAE, ISG	field lenghts estimated by subroutine SCAT

Quantities, that are supplied by DAØRG to the calling programme:

EZ(KMAX)	energy field, that contains all energy points of the partial inelastic excitation cross-section within energy group I and the energy points of the weighting spectrum.
KMAX	actual dimension of energy field described above.

AE(J)	excitation energies, that may be excited by primary neutron energies belonging to energy group I
J	actual length of field AE
NISGP NAEP ISGP	if ≠ 0, they give the numbers, that have to be added to NISG, NAE,ISG, to get sufficient field lengths.
IA	number of energy group of lowest energy, from which discrete levels can be excited and which is lying within the energy-group-range required by input. IA = 0, if nuclear data are available for lowest energy group required by input
NAB	number of energy group of highest energy, from which discrete levels can be excited, and which is lying within the energy-group range, required by input. NAB = NE27-1, if nuclear data are available for highest energy group required by input.

If no excitation levels for discrete levels are available on the nuclear data library for the material in question, a return is made to the calling programme.

NISGF,NAEF,ISGF	not used in the calling programme in the present version of the module.

The subroutine NDREAD reads from KEDAK the energy points, for which excitation cross-sections of the excitation level next higher to a given excitation level XLEVEL are stored within given energy limits.
NDREAD is called by DAØRG.

```
Subroutine NDREAD(I,EZ,E,AE,XLEVEL,J,KMAX,NENRE,NISG,NISGF,NISGP,NE27,NAE,
                  NAEF,NAEP,NETMAX,IL,IB,IH,*)
```

Variables, that have to be defined, when NDREAD is called:

I	number of energy-group, for which data are to be read.
NE27	see DAØRG
E(NE27)	see DAØRG
XLEVEL	Real*8-number, that is set equal to 0.0 by the calling programme, when the first excited level is to be found on KEDAK and that has to be slightly higher than the excitation energy of the level just below the one, that has to be read next /13/.
NISG	maximum possible length of field EZ
NAE	maximum possible length of field AE

KMAX — EZ(1)...EZ(KMAX) is already filled with energy points of excitation cross-sections belonging to preceding levels.

Arguments, that are results of NDREAD:

KMAX — After the return to the calling subroutine KMAX gives the number of energy points EZ, stored before calling NDREAD plus the number of energy points of the excitation cross-section of the energy level treated by the latest call of NDREAD.

EZ(KMAX) — after returning to the calling programm EZ(KMAX) contains the energy points of the excitation cross-sections of the first J excitation levels. The energy points of the first (J-1) excitation levels are ordered according to ascending energies, following in the field EZ are the energypoints of the excitation cross-section of level number J.

AE(J) — energy levels, whose excitation cross-sections have already been treated.

XLEVEL — after return to the calling programme, XLEVEL contains the excitation energy of the excitation level, that has been read during the latest run of NDREAD.

J — number of excitation levels, already treated by NDREAD.

NENRE — NENRE = 2: The excitation level read during the latest run of NDREAD cannot be excited by neutrons with primary energies belonging to energy group I.

NISGF, NAEF, NISGP, NAEP — quantities needed for the calculation of the field lengths NISG,NAE

NETMAX — maximum number of energy points within group I, at which the excitation cross-sections of any excitation level are stored (maximum needed length of NISG = maximum needed length of ISG+NETMAX).

IL,IB,IH — local variables of the calling subroutine, that are commented on in the FØRTRAN-programmes (NDREAD,DAØRG)

The subroutine ØRDNEN arranges the numbers, contained in the double precision array FELD(NTT), according to increasing quantities. ØRDNEN is called by DAØRG and SPECT1.

Subroutine ØRDNEN(KMAX,EMIN,EMAX,FELD,NTT,EPS)

Arguments, that have to be known, before the subroutine ØRDNEN is called:

KMAX — used length of array FELD

FELD(1)...FELD(KMAX) — array, that has to be ordered according to increasing numbers

NTT — available length of array FELD

EPS — if the relative deviation between any two members of FELD(KMAX) is less or equal EPS:

$$\left|\frac{FELD(I+1) - FELD(I)}{FELD(I+1)}\right| \leq EPS,$$

FELD(I) is set equal to FELD(I+1). In the present version of the module EPS = 0

Arguments, that are supplied by the subroutine ØRDNEN:

EMIN — value of lowest number of FELD

EMAX — value of highest number of FELD

KMAX — number of members of FELD after eliminating equal numbers.

The subroutine CUTS cuts array FELD (that is ordered according to increasing quantities) at lower energy limit UGG and at upper energy limit ØGG. CUTS is called by DAØRG and by ENØRG.

Subroutine CUTS(UGG,ØGG,FELD,NFE,KA,KE,KMAX1)

Arguments, that have to be defined, before CUTS is called:

UGG — lowest energy value, that shall be contained in FELD after cutting

ØGG — highest energy value, that shall be contained in FELD after cutting

NFE — length of array FELD

FELD(NFE) — array (ordered according to increasing quantities), that has to be cut

Arguments, that are supplied by CUTS:

KA — FELD(KA) = lowest value to be kept in array FELD after cutting

KE — FELD(KE) = highest value to be kept in array FELD after cutting

KMAX1 — KMAX1 = KE-KA+1 = number of values left in FELD after cutting low and high values

The subroutine SPECT1 checks, whether the energy field EZ(KMAX) contains enough points, to represent the analytical weighting function in such a way, that all points of the spectrum may be obtained by linear interpolation with a deviation of less than EPSI from the exact value. Actually it is checked, whether the midpoints between two given energy points may be obtained

by linear interpolation with sufficient accuracy. If not, the corresponding midpoints are added to the field EZ and the procedure is repeated until the condition

$$\left| \frac{PHI_{interpolated} - PHI_{exact}}{PHI_{exact}} \right| < EPSI$$

is fulfilled. SPECT1 is called by DAØRG.

Subroutine SPECT1(KMAX,EZ,NISG,NISGF,NISGP,EPSI,EPS)

Arguments, that have to be defined, before SPECT1 is called:

KMAX	actual length of energy field EZ
NISG	available length of energy field EZ
EZ(KMAX)	field containing energy points (constructed from the energy points of the excitation cross-sections of all levels, that may be excited by neutrons of energy group I).
EPSI	required accuracy of linear interpolation. In the present version EPSI is set equal to 0.001
EPS	argument for the subroutine ØRDNEN (called by SPECT1)

Arguments, that are results of SPECT1:

KMAX	actual length of array EZ after adding energy points of the analytic weighting function.
EZ(KMAX)	energy points of EZ after adding analytic weighting spectrum
NISGF, NISGP	if $\neq 0$, the field length NISG of EZ is not sufficient. NISGF,NISGP give information about necessary field length

The subroutine TRA corresponds to the subroutine of the same name in /4/. TRA supplies the values FIS of the (tabulated or analytic) weighting function at energy points EFI. TRA is called by AKED and SCATD.

Subroutine TRA(EFI,FIS,NF,EF,FI)

Arguments, that have to be defined, before TRA is called:

EFI	energy point, at which the weighting function has to be calculated
NF	field length of tabulated weighting function
EF(NF) FI(NF)	tabulated weighting function

supplied by TRA is FIS

FIS	value of the weighting function at energy EFI

The subroutine SIØRG organizes the interpolation of the excitation cross-sections read from KEDAK into the energy grid EZ(KMAX) provided by DAØRG. Moreover it calculates at each point of the energy grid the sum of the excitation cross-sections over all excitation levels: $\sum_j \sigma_i^{E_j}(E')$.

The reading of the cross-sections from the KEDAK-library is done by SGINT, the interpolation is performed by XINPØL. The subroutine SIØRG is called by AKED.

Subroutine SIØRG(I,EZ,AE,SGIP,SGIT,IANF,JMAX,KMAX,NISG,ISG,NAE)

Arguments, that have to be known, before calling SIØRG:

I	number of energy group
KMAX	length of energy grid EZ, established by DAØRG and its subroutines
EZ(KMAX)	energy grid, established by DAØRG and its subroutines
NISG ISG NAE	available lengths of arrays, given in the dimension statement

Arguments, that are supplied by SIØRG:

JMAX	number of excitation levels, that may be excited by neutrons with primary energies of energy-group I
AE(JMAX)	excitation levels
SGIP(KMAX,JMAX)	excitation cross-sections at KMAX energy points and for JMAX levels

SGIT(KMAX) $\sum_j \sigma_i^{E_j}(E')$: total discrete level excitation inelastic cross section

IANF(JMAX) IANF(J): pointer, that gives the number of the energy point of the field EZ, at which the excitation cross-section for level AE(J) starts (pointer for the threshold of the excitation cross-section of AE(J))

The subroutine SGINT reads for level XLEVEL excitation cross-sections from KEDAK, that lie within the energy limits EZ(1)...EZ(KMAX). SGINT is very similar to the subroutine NDREAD, however SGINT reads energy-points and cross-section-points. SGINT is called by SIØRG.

Subroutine SGINT(EZ,AE,SGIT,KMAX,KMAX1,XLEVEL,J,NISG,NAE,ISG,NENRE,IH)

Arguments, that have to be defined, before SGINT is called:

KMAX — the energy field EZ is already in use until EZ(KMAX): EZ(KMAX+1) may be used, to store the first energy point read from KEDAK

XLEVEL — the following excitation energy to be read from KEDAK has to be higher than XLEVEL /13/.

NISG, NAE, ISG — available lengths of arrays

quantities, that are supplied by SGINT:

KMAX1 — KMAX1-KMAX: number of energy points of excitation cross-section of level AE(J), that are stored on the nuclear library within the energy region EZ(1)...EZ(KMAX)

EZ(KMAX+1)... EZ(KMAX1): energy points of excitation cross-section of AE(J) on KEDAK (within the energy limits EZ(1)...EZ(KMAX)).

AE(J) — excitation energy, that was treated in the latest call of SGINT

J — number of energy level, that was the latest one, that was read from the library

SGIT(ISG) — SGIT(1)...SGIT(KMAX1-KMAX): excitation cross-section of level AE(J) read from KEDAK

XLEVEL — AE(J), when SGINT returns to SIØRG.

quantities, that are of local significance in SIØRG: NENRE,IH.

The subroutine XINPØL performs the following task: The cross-sections SGIT(1) ... SGIT(NETACT) with the corresponding energy-points EZ(KMAX+1)...EZ(KMAX+NETACT) are to be interpolated (linear interpolation) into the energy field EZ(1)... EZ(KMAX). The subroutine XINPØL is called by SIØRG.

Subroutine XINPØL(EZ,SGIT,SGP,NISG,NETACT,KMAX,KANF,KEND)

Arguments, that have to be defined, when XINPØL is called:

EZ(1)...EZ(KMAX)	energy field, into which the cross-sections are to be interpolated
EZ(KMAX+1)...EZ(KMAX+NETACT)	energy points of the cross-section
SGIT(NETACT)	cross-sections
NISG	available length of field EZ
NETACT	number of energy points of the cross-section
KMAX	length of the energy field, into which the cross-section are to be interpolated

Arguments, that are results of the subroutineXINPØL:

SGP(KMAX)	values of cross-sections, interpolated into energy-field EZ(1)...EZ(KMAX)
KANF	pointer, that gives the number of the first energy point of EZ, for which a value of SGP is given: EZ(KANF)...SGP(1) EZ(KANF+1)...SGP(2)
KEND	pointer, that gives the number of the last energy point of EZ, for which a value of SGP is given. EZ(KEND)...SGP(NETACT)

The function FIPØLA performs linear interpolation to one point lying between two given points

FIPØLA is called by TRA,SPECT1,RENUDA,SINPØL.

Function FIPØLA(XA,XB,XC,YA,YC)

XA	abscissa of first given point
YA	ordinate of first given point
XC	abscissa of second given point
YC	ordinate of second given point
XB	abscissa of point, to which the interpolation has to be carried out.

All arguments are REAL*4-variables.

When returning to the calling programme, FIPØLA contains the ordinate corresponding to XB.

The function FIPØLD corresponds to the function FIPØLA, however the arguments, containing the given and required abscissa are REAL*8-variables.

The function FIPØLD is called by SCATD,AKED,XINPØL.

Function FIPØLD(XAD,XBD,XCD,YA,YC)

XAD	abscissa of first given point (REAL*8)
YA	ordinate of first given point (REAL*4)
XCD	abscissa of second given point (REAL*8)
YC	ordinate of second given point (REAL*4)
XBD	abscissa of point, to which the interpolation has to be carried out (REAL*8)

6.3.2 Description of the subroutine SCATC and its subprogrammes

The subroutine SCATC together with its subprogrammes calculates transfer probabilities for inelastic scattering with excitation of continuous levels of the residual nucleus according to formulas (6.20), (6.20.1) and (6.20.2). Moreover transfer matrices for (n,2n)- and (n,3n)-reactions are calculated according to formula (6.23). For the calculation of the total inelastic scattering transfer matrices in the programme SCAT $R^{c}_{i,g}$ (formula 6.21.2) is provided by SCATC. SCATC organizes for the outscattering groups required by input (and for which continuous level inelastic scattering occurs) and for all inscattering groups the calculation of the transfer matrices and of the reaction rates.

```
Subroutine SCATC(NX,EG,XNUE,NFE,EF,FI,NE27,INTYP,WEINC,QUØTC,ENG,EZ,SGIZC,
                 EI,EP,F1,F2,F3,F4,NISG,NISGP,NISGI,NISGIP,NEP,NEPP,NF,NFP,
                 IA,NAB)
```

Arguments, that have to be defined, when the subroutine SCATC is called

NX	number of energy group boundaries of outscattering groups (may or may not contain thermal group)
EG(NX)	energy boundaries of outscattering groups (internal energy group count: EG(1) refers to the lowest energy value)
XNUE	parameter of the evaporation model; used only, if type SEDIC(SED2N,SED3N) is not given on KEDAK for the material in question
NFE	number of points of the weighting function given by the input
EF(NFE)	energy points of the weighting function
FI(NFE)	values of the weighting function
NE27	number of energy boundaries of inscattering groups (contains thermal group)
INTYP	gives type of reaction, for which the transfer probabilities have to be calculated:

INTYP = { 1: inelastic scattering with excitation of continuous levels of the residual nucleus
2: (n,2n)-reactions
3: (n,3n)-reactions

NISG,NISGI,NEP,NF : estimated lengths of arrays, used as working fields by SCAT and its subroutines.

Arguments, that are results of SCATC and its subroutines:

WEINC(NX,NX) normalized transfer probabilities for the reaction type given by INTYP. The first index refers to the outscattering group (internal energy-group count). The second index refers to the inscattering group in the following manner: second index = 1: inscattering group = outscattering group; second index = 2: inscattering group lies energetically one group lower than the outscattering group; second index = 3: inscattering group lies energetically two groups lower than the outscattering group and so on.

QUØTC(NX) $R^{c}_{i,g}$, given in formula (6.21.2). The reaction rate is calculated for the reaction, defined by INTYP

IA number of outscattering group of lowest energy, for which transfer probabilities are provided by SCATC

NAB number of outscattering group of highest energy, for which transfer probabilities are provided by SCATC

The following arguments are working fields:

ENG(NE27) energy group boundaries containing thermal group; given in internal energy-group count

EZ(NISG) energy points of SGIZC (SG2N,SG3N), read from KEDAK

SGIZC(NISG) array, that contains continuous level inelastic cross-sections (or (n,2n)-cross-sections or (n,3n)-cross-sections), read from KEDAK

NISGP if ≠ 0, NISGP has to be added to NISG, to obtain sufficient field lengths

EI(NISGI) array, in which the combination of EZ and EF is stored

NISGIP if ≠ 0,NISGIP has to be added to NISGI, to obtain sufficient field length

EP(NEP), F1(NF,NEP), F2(NF,NEP), F3(NF,NEP), F4(NF,NEP) filled by subroutine RENUDA (see below)with information of KEDAK-type SEDIC (or SED2N or SED3N)

NEPP if ≠ 0, NEPP(NFP) has to be added to

NFP NEP(NF), to obtain sufficient array lengths

Subroutine RENUDA reads from the nuclear data library continuous level inelastic cross-sections (SGIZC) (or (n,2n)-cross-sections (SG2N), or (n,3n)-cross-sections (SG3N))within given energy limits. If the type SGIZC is not available on KEDAK (for the material in question) the points of type SGI, lying above the energy region of discrete level inelastic scattering, (above the highest energy point of SGIZ) are interpreted as points of SGIZC.

RENUDA is called by SCATC.

Subroutine RENUDA(TYP,KØNT,SGIZC,EZ,EU,EØ,NACT,NISG,NISGP)

Arguments, that have to be defined, before RENUDA is called:

TYP	type of cross-section, that has to be read from the nuclear data library
EU	lower limit of energy region, within which the cross-section has to be read from KEDAK
EØ	upper limit of energy region, within which the cross-section has to be read from KEDAK
NISG	length of array EZ, available to store energy points read from KEDAK

Arguments, that are results of RENUDA

KØNT	= 0: the required cross-section type is not available on the nuclear data library = 1: the required cross-section type is available on the nuclear data library
NISGP	see description of SCATC
NACT	contains actual length of fields EZ and SGIZC, if NACT ≤ NISG
EZ(NACT)	energy points — read from KEDAK
SGIZC(NACT)	cross-sections of type TYP — read from KEDAK

The subroutine ENØRG constructs the energy field EI(KMAX), that consists of the energy points EZ(NACT) (energy points of the cross-sections read from KEDAK) and the energy points of the weighting functions EF(NFE) in case the weighting function is given energy pointwise by the input). If the weighting function is given by an analytical function, ENØRG is not called. The

resulting energy field EI(KMAX) has the lower energy limit EU and the upper energy limit EØ and is ordered according to growing energy values.

The subroutine ENØRG is called by SCATC.

Subroutine ENØRG(EU,EØ,EI,EF,NACT,KMAX,KEN,NISGI,NISGIP)

Arguments, that have to be defined, when ENØRG is called:

EU	lower energy limit for the resulting energy field EI
EØ	upper energy limit for the resulting energy field EI
EI(NACT)	when ENØRG is called EI contains the energy field EZ(NACT)
EF(KEN)	energy points of the weighting function given by the input
NACT	length of the field EI, that is to be combined with the energy points EF, that lie within the energy limits EU, EØ
KEN	total number of energy points of the weighting function, given by the input (=NFE)
NISGI	available length of field EI

Arguments, that are results of the subroutine ENØRG.

KMAX	gives length of energy field, that is the combination of EI(NACT) and EF(NFE)
EI(KMAX)	resulting combined energy field
NISGIP	if ≠ 0, NISGIP gives number, that has to be added to NISGI, to get sufficient field length for EI

The subroutine CUTS, called by ENØRG is described in the preceding chapter 6.3.1.
The subroutine ØRD1, called by ENØRG has the same task as the subroutine ØRDNEN described in chapter 6.3.1. However, the field FELD(NTT), to be ordered according to increasing values is a REAL*4 variable in ØRD1 and a REAL*8 variable in ØRDNEN.

The subroutine REPRØB reads from KEDAK the energy distribution of secondary neutrons for continuous level inelastic scattering or (n,2n)-processes or (n,3n)-processes respectively. The corresponding KEDAK-types are SEDIC, SED2N and SED3N. In the present status the programme can handle an evaporation model only. The nuclear temperature may be given as tabulated function of the incident neutron energy or as analytic function of the incident neutron energy. An extension to secondary energy distributions given by tables (types CHII, CHI2N, CHI3N on KEDAK) is being worked on.

If the KEDAK-types SEDIC (or SED2N or SED3N respectively) do not contain information, an evaporation model is used with the nuclear temperature given by $\Theta = \sqrt{\frac{E'}{\nu \cdot A}}$ (compare chapter 6.2.3). The atomic weight A is obtained by reading the KEDAK-type ISØT1 /13/. The threshold U for the wanted reaction type is obtained by reading from KEDAK the respective cross-section (SGI,SG2N,SG3N) and finding the energy point, where the cross-section starts to be greater than zero.

The subroutine REPRØB is called by SCATC.

Subroutine REPRØB(INTYP,KØNT,EP,F1,F2,F3,F4,NEP,NEPP,NF,NFP)

Arguments, that have to be known, before REPRØB is called

INTYP — gives reaction type, for which the energy distribution of secondary neutrons has to be read from KEDAK.

$$\text{INTYP} = \begin{cases} 1: \text{type SEDIC has to be read (or A from ISØT1 and U from SGI)} \\ 2: \text{type SED2N (or A from ISØT1 and U from SG2N)} \\ 3: \text{type SED3N (or A from ISØT1 and U from SG3N)} \end{cases}$$

NEP — available length of array EP and of second index of F1, F2, F3, F4

NF — available length of first index of F1, F2, F3, F4

Arguments, that are results of REPRØB:

KØNT
- 1: required type (SEDIC,SED2N,SED3N) available on KEDAK
- 0: required type not available on KEDAK, an evaporation model with $\Theta = \sqrt{\frac{E'}{\nu \cdot A}}$ has to be used

EP(NEP) primary neutron energies, obtained from KEDAK as further name from types SEDIC,SED2N,SED3N (see /13/)

F1(NF,NEP): K
F2(NF,NEP): P
F3(NF,NEP): Θ
F4(NF,NEP): U

from types SEDIC,SED2N, SED3N (see /13/)

If there is no information stored in types SEDIC or SED2N or SED3N respectively two quantities from KEDAK are stored in the field F4:

F4(1,1) is filled with A, the atomic weight of the material considered

F4(1,2) is filled with U, the threshold energy of the reaction

NEPP if ≠ 0, NEPP gives number, which has to be added to NEP, to obtain sufficient lengths of arrays

NFP if ≠ 0, NFP gives number, which has to be added to NF, to obtain sufficient lengths of arrays

The labelled CØMMØN APØINT contains the information about the actual lengths of fields EP,F1,F2,F3,F4, in case NEP and NF were sufficient.

CØMMØN/APØINT/INEP,INF

INEP actual value of NEP

INF actual value of NF

The subroutine SIMPSI performs the integration in numerator and denominator of formulas (6.20) and (6.20.2) and (6.23) using the Simpson-rule /12/.

SIMPSI is called by SCATC

Subroutine SIMPSI(NUGRE,U,AW,XNUE,A,B,EPS,NMAXX,RESINT,N,EZ,SGIZC,
EF,FI,ENG,NACT,NFE,NE,NN,EP,F1,F2,F3,F4,NEP,NF,
KØNT,ERR)

Arguments, that have to be defined, when SIMPSI is called:

NUGRE — group number of inscattering group in internal energy group count (NUGRE is used only, if NN=1)

U — threshold energy for reaction under consideration

AW — atomic weight as given by the KEDAK-type ISØT1

XNUE — parameter of the evaporation model (ν), used if no information is given in the KEDAK-type SEDIC(SED2N,SED3N)

A — lower energy limit of integration

B — upper energy limit of integration

the values of A and B are the energy points of the field EI, constructed by ENØRG. If the weighting spectrum is given as an analytic function, A and B are given by the array EI, that contains the energy points of the corresponding cross-section on KEDAK and the energy group boundaries.

EPS — required accuracy of the integration (1 % in the present version). EPS means the relative deviation of two subsequent integrations

NMAXX — maximum number of integration intervals during Simpson integration. (NMAXX = 100 000 in the present version; see the discussion of the warning printed out by SIMPSI)

EZ(NACT), SGIZC(NACT), EF(NFE), FI(NFE), ENG(NE), EP(NEP), F1(NF,NEP), F2(NF,NEP), F3(NF,NEP), F4(NF,NEP), NACT, NFE, NE, NEP, NF — quantities, described before in connection with subroutines RENUDA, REPRØB and SCATC

KØNT
- if = 0, the nuclear temperature has to be calculated from $\Theta = \sqrt{\frac{E'}{\nu \cdot A}}$ (no information in types SEDIC(SED2N,SED3N) on KEDAK)
- if = 1, the nuclear temperature is given on KEDAK (SEDIC,SED2N,SED3N)

NN — characterizes function, that has to be integrated by SIMPSI

NN = 0: $\int_A^B \sigma_i^c(E')w(E')dE'$ has to be calculated (formula (6.21.2))

NN = 2: $\int_A^B w(E')dE'$ has to be calculated (denominator of (6.20))

NN = 1: $\int_A^B \sigma_i^c(E')w(E')P_i^c(E'\to h)dE'$

(see numerator of formula (6.20))

Arguments, that are results of SIMPSI:

RESINT	result of integration
N	number of integration intervals, actually used
ERR	accuracy of integration, actually obtained (relative deviation between the two last subsequent integrations)

Warning printed out by SIMPSI

In case the required integration accuracy, EPS, is not obtained after using NMAXX integration points in the energy region (A,B), a message is printed out by SIMPSI. It contains information about

N	number of integration intervals, actually used
NMAX	maximum number of integration intervals (which is 100 000 in the present version, but may be reduced, if A and B are very close to each other; see below)
RESINT	result of integration
ERR	integration accuracy, actually obtained
NN	type of function, that has to be integrated
A	lower integration limit
B	upper integration limit
INUGRE	number of inscattering group in external energy group count (group number one refers to energy group of highest energy)

This message is often produced for the case NN=1, when the integration limits lie within an outscattering group, that contains the threshold of the considered reaction. To get an impression of the error, that may be

introduced into the final result, the integral (NN=1) over the entire outscattering group into group INUGRE is printed out by SCATC. This write-statement gives number of outscattering group, number of in-scattering group (both in external group count)and the integral (NN=1) over the entire outscattering group

$$\int_{Eg+1}^{Eg} \sigma_i^c(E')w(E')P_i^c(E'\to h)dE'$$

In some cases the maximum number of intervals, that may be generated during the Simpson-integration is restricted, in order to save computer time: If the integration interval (A,B) is very small, ($\frac{B-A}{B}$ less or equal 1.1E-5) the integration is carried out by the trapezoidal rule. For $\frac{B-A}{B}$ less or equal 5.E-5 the maximum number of integration intervals, NMAX, is restricted to 20. (The integration interval (A,B) becomes small, if energy points on KEDAK are very close to each other, or if one of the KEDAK energy points lies very close to one of the energy points of the weighting function.)

If the threshold of the reaction lies within the outscattering group and the upper energy boundary of the inscattering group is less or equal 101 eV, the number of integration intervals is restricted to 100.

If during the integration the interval H becomes small compared to the lower integration limit A, $\frac{H}{A}$ less or equal 0.5E-6, and the number of integration intervals is already greater than 100, the Simpson-integration is stopped and the message explained above is printed out.

The function, that has to be integrated by SIMPSI is provided by the function FINT. This may be $\sigma_i^c(E')w(E')$ (6.21.2)

$w(E')$

$\sigma_i^c(E')w(E')P_i^c(E'\to h)$ (numerator of (6.20))

FINT is called by SIMPSI.

Function FINT(E,NUGRE,U,AW,XNUE,EZ,SGIZC,EF,FI,ENG,NACT,NFE,NE,NN,EP,F1, F2,F3,F4,NEP,NF,KØNT)

Arguments of function FINT:

E	energy point of outscattering group, at which the function is to be calculated. This corresponds to E' in formulas (6.20), (6.21.2)
NUGRE U AW XNUE	same meaning as in SIMPSI
EZ(NACT) SGIZC(NACT) EF(NFE) FI(NFE) ENG(NE) EP(NEP) F1(NF,NEP) F2(NF,NEP) F3(NF,NEP) F4(NF,NEP)	quantities, described before in connection with subroutines RENUDA,REPRØB and SCATC
NACT NFE NE NEP NF	described in connection with RENUDA, REPRØB, SCATC
NN	characterization of function, that has to be calculated (see discussion of argument list of SIMPSI)
KØNT	see description of argument list of SIMPSI

The function SINPØL performs linear interpolation to a given abscissa, starting from a tabulated function. SINPØL calls the function FIPØLA. SINPØL is called by FINT, to interpolate the cross-section and the weighting function.

Function SINPØL(EINT,EFELD,FELD,NFELD)

discussion of the arguments of the function SINPØL:

EINT	energy point, at which the value of the tabulated function has to be obtained by linear interpolation
NFELD	number of tabulated values
EFELD(NFELD)	abscissa of tabulated function (energy points)
FELD(NFELD)	function value FELD(I) corresponds to energy EFELD(I)

The function PRØB calculates the transfer probabilities $P_i^c(E' \to h)$ (see formula (6.20)) for inelastic scattering, (n,2n) or (n,3n)-reactions.
PRØB is called by FINT

Function PRØB(E,NUGR,U,A,XNUE,ENG,NE,EP,F1,F2,F3,F4,NEP,NF,KØNT)

E	energy point of outscattering group, for which the transfer probability has to be calculated (corresponds to E'in formulas)
NUGR	group number of inscattering group (internal group count)
U	threshold of reaction
A	atomic weight as given by KEDAK-type ISØT1
XNUE	parameter for the calculation of the nuclear temperature
KØNT	= 0, if nuclear temperature is not given on KEDAK
	= 1, if nuclear temperature is given on KEDAK

NE,NEP,NF
ENG(NE)
EP(NEP)
F1(NF,NEP),F2(NF,NEP)
F3(NF,NEP),F4(NF,NEP)

} described in connection with SCATC and REPRØB

The double precision function EXD(X) calculates (with double precision) the series (exp(x)-1), which is needed for a good numerical evaluation of $P_i^c(E' \to h)$ in the numerator of formula (6.20) for inscattering groups of small energy, (see /4/, chapter 6, page 6.8)

The function EXD is called by PRØB.

The double precision function DNFAK(NN) calculates (with double precision) NN!
DNFAK is called by EXD.

The function TEMP calculates the nuclear temperature used for the evaporation model by linear interpolation of the data given by the KEDAK types SEDIC, SED2N, SED3N.
TEMP is called by PRØB.

Function TEMP(EFS,EP,F3,NEP,NF)

description of the arguments:

EFS	energy point of outscattering group, at which the nuclear temperature has to be calculated
EP(NEP)	energy points (energies of incident neutron) given on KEDAK (KEDAK types SEDIC, SED2N, SED3N) /13/
F3(NF,NEP)	nuclear temperatures given on KEDAK. If the energy distribution of secondary neutrons is given by a linear combination of different analytic functions on KEDAK, the first index of F3 refers to the number of the analytic function. In most cases the distribution is described by one analytic function only. The second index refers to the primary energy given in EP.
NEP,NF	available field lengths

The actual field lengths of EP and F3 given by the KEDAK data are transferred by the common |APØINT|

INEP	actual value of NEP
INF	actual value of NF

The function THETA calculates the nuclear temperature for the evaporation model, in case no information is contained in SEDIC (or SED2N or SED3N respectively).
THETA is called by PRØB.

Function THETA(E,XN)

E	energy point, for which the nuclear temperature is to be calculated (E' in formulas)
XN	XNUE*A, prepared in PRØB

6.3.3 The organizing subroutine of module 5, SCAT

One task of the subroutine SCAT is to organize the working field X(MMAXX) for the use in SCATD and SCATC. In the programme MIGRØS-2, /4/, the organizing of the working fields used in module 5 was done by the subroutine INPUT. In the new version of module 5 the inelastic scattering to discrete levels of the residual nucleus and the inelastic scattering to continuous levels of the residual nucleus are treated in completely separated sets of subroutines, SCATD and SCATC, with completely different working fields and consequently completely different storage requirements. In order to avoid too many changes in the subroutine INPUT (call and organization of two different modules (instead of one) for the calculation of inelastic transfer matrices) the organization of the working fields of SCATD and SCATC is now done in SCAT.

If the length of the working field, MMAXX, is not sufficient to carry out the calculations in SCATD or SCATC, control is returned to the calling subroutine INPUT. The subroutine INPUT checks, whether transfer matrices for further reactions ((n,2n) or (n,3n)) are required by the programme input. In that case SCAT is called again and it is tried, to calculate the (n,2n)- or (n,3n)-matrices; otherwise the module with the next module number required by the programme-input is called. The second task of SCAT is, to calculate the total inelastic scattering transfermatrix from the results of SCATD and SCATC according to formula (6.21.1) in chapter 6.2.4. $R_{i,g}^{d}, R_{i,g}^{c}$ and $P_{i,g\to h}^{d}, P_{i,g\to h}^{c}$ are given as results of SCATD and SCATC.

Finally SCAT organizes the output of module 5 on listing and produces the unformatted output.
SCAT is called by the subroutine INPUT.

```
Subroutine SCAT(NX,EG,XNUE,NFE,EF,FI,NE27,KINEM,NIN,NINA,INTYP,X,IX,MMAXX,
                MFELD)
```

The first eleven variables of the argument list are input quantities, that are transferred by the calling programme INPUT.

NX	number of group boundaries of outscattering groups
EG(NX)	energy group boundaries of outscattering groups
XNUE	parameter of the evaporation model
NFE	number of points of the weighting function
EF(NFE)	abscissa of the weighting function
FI(NFE)	ordinates of the weighting function
NE27	number of energy group boundaries of the inscattering groups (includes thermal group)
KINEM	parameter, that selects, how the energy loss of the incident neutron is calculated in inelastic scattering processes with excitation of discrete levels of the residual nucleus: KINEM=0: formula (6.2) is applied KINEM=1: formula (6.3) is applied (this is the standard input in the present version) KINEM=2: formula (6.4) is applied
NIN	number of reaction types, for which transfer matrices are to be calculated. Possible are inelastic scattering, (n,2n)-processes and (n,3n)-processes (standard input is NIN=2)
INTYP(NIN)	characterization of the reaction types INTYP(I)=1: inelastic scattering INTYP(I)=2: (n,2n)-reactions INTYP(I)=3: (n,3n)-reactions (standard input is INTYP(1)=1, INTYP(2)=2)

Moreover the subroutine INPUT defines the available length of the working field:

MMAXX	available length of the working field
X(MMAXX),IX(MMAXX)	working field, available in SCAT

Results from SCAT, that are returned to the calling programme INPUT.

MFELD	actually needed length of working field
NINA	number of reactions, for which calculations in SCAT have already been carried out or had to be interrupted because of unsufficient length of the working field

In the following the most important variables used in SCAT are described

1. Correspondence between the working fields in SCAT and the results of the subroutine SCATD:

X(L1)...X(L1+NX*NX-1): corresponds to WEIN(1,1)...WEIN(NX,NX) in SCATD and contains normalized transfer probabilities of inelastic scattering processes connected with excitations of discrete levels of the residual nucleus as given in formula (6.14)

X(L2)...X(L2+NX-1): corresponds to QUØT(1)...QUØT(NX) in SCATD and contains the resonance integrals $R^{d}_{i,g}$ as given in formula (6.21.2).

Explanation of some variables used in SCAT, to handle the results of SCATD (in the statements following "CALL SCATD").

IG	external count of group numbers (1 corresponds to energy group with highest energy)
MG	internal count of group numbers (1 corresponds to energy groups with lowest energy)
NXMH	number of downscattering (inscattering) groups (containing outscattering group)
MH	group count for downscattering (inscattering) groups

MH=1: inscattering group corresponds to outscattering group

MH=2: inscattering group is the energy group, energetically next lower to the outscattering group

MH=3: inscattering group is the energy group, that energetically is two groups lower than the outscattering group

MH=NXMH: inscattering group is that energy group, that energetically is (NXMH-1) groups below the outscattering group

Detailed correspondence between X(L1)...X(L1+NX*NX-1) and WEIN(1,1)... WEIN(NX,NX) and X(L2)...X(L2+NX-1) and QUØT(1)...QUØT(NX)

X(L1) corresponds to WEIN(1,1):

transfer probability (for inelastic scattering with excitation of discrete levels) from outscattering group of lowest energy into the same group: (EG(1),EG(2))

X(L1+MG-1) corresponds to WEIN(MG,1):

transfer probability from energy group MG (internal group count) into energy group MG.

X(L1+MG+NX-1) corresponds to WEIN(MG,2):

transfer from energy group MG (internal count) to that inscattering group, that energetically lies one group below MG.

X(L1+MG+2*NX-1) corresponds to WEIN(MG,3):

transfer from group MG to that group, that energetically lies two groups below MG.

finally:
X(L1+MG+(NXMH-1)*NX-1) corresponds to WEIN(MG,NXMH):

transfer from group MG to that group, that energetically lies (NXMH-1) groups below MG.

X(L2) corresponds to QUØT(1):

resonance integral (according to formula (6.21.2) for outscattering group of lowest energy (EG(1), EG(2))

X(L2+1) corresponds to QUØT(2):

resonance integral for outscattering group of second lowest energy

X(L2+NX-1) corresponds to QUØT(NX):

resonance integral for outscattering group of highest energy (EG(NX-1), EG(NX))

2. Correspondence between the working fields in SCAT and the results of the subroutine SCATC:

X(L3)...X(L3+NX*NX-1) correspond to WEINC(1,1)...WEINC(NX,NX), the normalized transfer probabilities for inelastic scattering with excitation of continuous levels (or for (n,2n) - or (n,3n) - transfer probabilities). See formulas (6.20)-(6.20.2) (or (6.23)).

X(L4)...X(L4+NX-1) correspond to QUØTC(1)...QUØTC(NX) and contain the resonance integrals $R^{c}_{i,g}$ according to formula (6.21.2)

The relations between X(L3)...X(L3+NX*NX-1) and WEINC(1,1)...WEINC(NX,NX) and between X(L4)...X(L4+NX-1) and QUØTC(1)...QUØTC(NX) correspond to the relations between the working fields in SCAT and the results of SCATD:

X(L3) corresponds to WEINC(1,1)
X(L3+MG-1) corresponds to WEINC(MG,1)
X(L3+MG+NX-1) corresponds to WEINC(MG,2)
X(L3+MG+(NXMH-1)*NX-1) corresponds to WEINC(MG,NXMH)

X(L4) corresponds to QUØTC(1)
X(L4+NX-1) corresponds to QUØTC(NX)

The results of SCAT, which are total inelastic scattering matrices (INTYP=1) or transfer matrices for (n,2n) - reactions (INTYP=2) or for (n,3n)-reactions (INTYP=3) are finally stored in X(L1)...X(L1+NX*NX-1)

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KFK 2387 II 2.9, 1977

7. Calculation of Normalized Elastic Scattering Matrices and of Elastic and Total Group Cross Sections. Module 6.

In neutronic assemblies in which neutrons with energies above 100 keV essentially determine reaction rates, neutron leakage etc. anisotropic elastic scattering has to be taken account of. In widely used S_N-transport calculations this is achieved with a Legendre-expansion of the elastic scattering kernel in the multigroup transport equation. Especially extended transport approximations, consistent /1/ or inconsistent /2/ with the Boltzmann equation, turned out to be well suited for anisotropic calculations. The MIGROS-module to be described here provides the needed microscopic multigroup cross sections up to a Legendre-order L = 5. The Legendre-moments of the neutron flux density in suitably chosen subzones of the reactor under consideration, being needed as weighting-functions, are approximated by $\psi_\ell(E) = F(E)/[\Sigma_t(E)]^{\ell+1}$, $\ell = 0,1,\ldots,5$, where F(E) is the total collision density and $\Sigma_t(E)$ is the macroscopic total cross section of the subzone. Additionally, simpler weighting options may be applied. For a detailed discussion on weighting the reader is referred to /1/.

Since the first report on MIGROS-2 /3/ in 1973 this module has undergone some modifications. These are

- the additional determination of ψ_ℓ-weighted total group cross sections for S_N-calculations in extended transport approximations

- a reduction in weighting options (options for test purposes are cancelled)

- an improved calculation of hydrogen scattering matrices (transfer elements for scattering into the last group had been erroneous)

- improvements in fine-structure weighting in connection with the calculation of total group cross sections

- substitution of the non-linear interpolation procedure to smoothe interpolated values

- initial determination of the need of computer storage to save computing time in case of a restart

- cancellation of the restriction to four fine-groups per macro-group to save time in many-group calculations (more than 200 groups)

- changes in output format to compact the written output

- changes in messages (errors and warnings)

In Tab. 1 the modified and unmodified subroutines are listed separately. For the performance of each subroutine see below (chapter 7.3).

Tab. 1: Subroutines of the modified module 6

Modified	Unmodified
FLUMMI, SUM, IPØLA, PUSUM^{+}, MAKRØ, MIXSGT^{+}, INFØRM^{+}, PUNK, LØØKO^{+}, LØØK1^{+}, LØØK2^{+}, GRUPIN, SPRAL, TRAPEZ^{++}, MUKØN^{+}, PRINT	ADD, TRAFØ, LØØK3, LECAL, LEGPØL, LEGINT, G, LEGIST, LEGANS, IPØLIN, PHI

$^{+}$ only slightly modified, $^{++}$ eliminated

Along with these modifications a change in the overlay structure was necessary (see chapter 1, Table II).

7.1 Definition of the quantities calculated in this module

Given are the KEDAK data

$\sigma(E)$ = microscopic cross section for elastic neutron scattering at energy E (KEDAK type SGN),

$\bar{w}(E,\bar{\mu}_o)$ = angular distribution in the c.m.-system for elastic neutron scattering with

$$2\pi \int_{-1}^{+1} d\bar{\mu}_o \; \bar{w}(E,\bar{\mu}_o) = 1$$

E = energy of the incoming neutrons

$\bar{\mu}_o$ = scattering cosine in the c.m.-system (KEDAK type SGNC),

$\sigma_t(E)$ = total microscopic neutron reactions cross section at energy E (KEDAK type SGT).

Then for energy groups (E_g, E_{g-1}), $E_1 > E_2 > \ldots > E_G$, G = number of groups, the module calculates the elastic group cross sections[+]

$$\sigma^g = \int_g dE\ \sigma(E)\psi_o(E) / \int_g dE\ \psi_o(E), \qquad g = 1,2,\ldots,G, \tag{7.1}$$

the total ψ_ℓ-weighted group cross sections

$$\sigma^g_{t,\ell} = \int_g dE\ \sigma_t(E)\psi_\ell(E) / \int_g dE\ \psi_\ell(E), \qquad \ell = 0,1,\ldots,5; \quad g = 1,2,\ldots,G, \tag{7.1'}$$

the normalized ℓ-th order matrixelements for elastic scattering from group g' to group g

$$s_\ell^{g'\to g} = \frac{1}{\sigma^{g'}} \int_{g'} dE\ \sigma(E) w_\ell(E\to g)\psi_\ell(E) / \int_{g'} dE\ \psi_\ell(E) \qquad \ell = 0,1,\ldots,5; \quad g',g = 1,2,\ldots,G, \tag{7.2}$$

and the mean scattering cosine in group g

$$\bar{\mu}^g = \sum_{g'\geq g} s_1^{g\to g'}, \qquad g = 1,2,\ldots,G. \tag{7.3}$$

In (7.2) the quantity $w_\ell(E\to g)$ is defined as

[+] in the following $\int_{E_g}^{E_{g-1}} dE\ldots$ is shortened by $\int_g dE\ldots$

$$w_\ell(E\to g) = \int_g dE'\; w_\ell(E,E'), \tag{7.4}$$

where

$$w_\ell(E,E') = \begin{cases} \dfrac{d}{dE'} \displaystyle\int_{-1}^{\mu_o(E,E')} d\mu_o\; 2\pi\; w(E,\mu_o) P_\ell(\mu_o) & \\ \qquad\qquad \text{if } E' \le E \le E'/\alpha & \\ 0 \text{ otherwise} & \end{cases} \tag{7.5}$$

with $\alpha = \left(\frac{A-1}{A+1}\right)^2$, A = atomic weight of the scattering nucleus in neutron mass units.

$P_\ell(\mu_o)$ is the Legendre-polynomial of degree ℓ, $P_o(\mu_o) = 1$, $P_1(\mu_o) = \mu_o$ etc., and $\mu_o(E,E')$ is the scattering cosine in the laboratory system for elastic scattering from energy E to energy E':

$$\mu_o(E,E') = \frac{A+1}{2}\sqrt{E'/E} - \frac{A-1}{2}\sqrt{E/E'}\;. \tag{7.6}$$

Further $w(E,\mu_o)$ is the angular distribution for elastic neutron scattering in the <u>laboratory system</u>, related to $\bar{w}(E,\bar{\mu}_o)$ through

$$w(E,\mu_o) = \bar{w}(E,\bar{\mu}_o)\;\frac{d\bar{\mu}_o(\mu_o)}{d\mu_o}, \tag{7.7}$$

where

$$\bar{\mu}_o(\mu_o) = \frac{1}{A}\left(\mu_o^2 - 1 + \mu_o\sqrt{\mu_o^2 - 1 + A^2}\right)$$

The quantity $w_o(E\to g)$ gives the probility for elastic scattering from energy E into the interval (E_g, E_{g-1}), the energy group g.

For computation the righthand side of the defining equation (7.4) which involves a double-integration as it stands can easily be simplified.

In the case of isotropy in the s.m.-system we have $\bar{w}(E,\bar{\mu}_o) = 1/4\pi = \text{const.}$ and therefore according to (7.5) and (7.7)

$$w_\ell(E\to g) = \frac{1}{2}\int_{\hat{\mu}_o(E,E_g)}^{\hat{\mu}_o(E,E_{g-1})} d\mu_o \frac{d\bar{\mu}_o(\mu_o)}{d\mu_o} P_\ell(\mu_o), \tag{7.8}$$

where

$$\hat{\mu}_o(E,E_g) = \begin{cases} -1 & \text{if } E \geq E_g/\alpha \text{ and } E_g > \hat{E} \\ +1 & \text{if } E \leq E_g \text{ and } E_g > \hat{E} \\ \mu_o(E,E_g) & \text{if } E_g < E < E_g/\alpha \text{ and } E_g > \hat{E} \\ -1 & \text{if } E_g = \hat{E} \end{cases} \tag{7.9}$$

Here $\hat{E}$ is the lower limit of the considered energy region, usually $\hat{E}$=0.001 eV. (In the subroutine LECAL $\hat{E}$ = ABN(IM+1)). With (7.9) scattering to energies below $\hat{E}$ is avoided, in particular: there is no scattering out of the lowest group.

In the case of anisotropy in the c.m.-system, normally for energies above 10 keV, we have

$$w_\ell(E\to g) = 2\pi \int_{\hat{\mu}_o(E,E_g)}^{\hat{\mu}_o(E,E_{g-1})} d\mu_o \; w(E,\mu_o)\; P_\ell(\mu_o) \tag{7.10}$$

7.2 Integration, interpolation, energy and cosine grid, weighting

The multigroup constants to be determined according to (7.1), (7.1') and (7.2) contain integrals over products of cross sections and weighting functions, these two factors generally behaving differently and being given at different grids of energy points. Additionally, in (7.2) the elastic cross section is multiplied by the transfer "probilities", $w_\ell(E\to g)$, which are angular integrals over the product of angular distributions and the Legendre-

polynomials according to (7.8) and (7.10). Expecially these $w_\ell(E\to g)$ are strongly fluctuating functions, a fact that requires great care during integration.

The techniques of integration, interpolation, and the choice of meshpoints applied in this module result from a comparison of the results of the totally numerical procedure with the analytical ones in special cases as well as from a comparison of different numerical methods. So

- angular integration is performed with Simpson's rule,

- energy integration is done with a modified trapezoidal rule because of the varying density of discrete cross section energies and the need for a fine mesh in the outgroup scattering region (defined below),

- interpolation of the elastic (SGN) and total cross sections (SGT) and the mean scattering cosines (MUEL) is linear, energy and angle interpolation of the elastic scattering distributions (SGNC) is performed with polynomials up the third order - a detailed description of this non-linear interpolation procedure is given in ref. 1, p. 140.

In particular, in the angular integrals (7.8) and (7.10) there is partial cancellation since the Legendre-polynomial $P_\ell(\mu_o)$ has ℓ zeros in $[-1, +1]$ and therefore the integrand changes sign. This effect of cancellation increases with ℓ, but can be overcome by a cosine grid with a number of meshpoints increasing with ℓ.

For the computation of the integral (7.10) - anisotropy in the c.m.-system - table 7.2 gives the number NST(L) of cosine meshpoints for the L-th moment in $[-1, +1]$.

Table 7.2: Number of cosine meshpoints in $[-1, +1]$ (scattering anisotropic)

L	0	1	2	3	4	5
NST(L)	81	81	161	161	321	321

The integration according to (7.10) is performed by LEGANS.

The integral (7.8) - isotropy in the c.m.-system - does not depend on energy. The values

$$B_\ell(\omega) = \frac{1}{2}\int_{-1}^{\omega} d\mu_o \frac{d\bar{\mu}_o(\mu_o)}{d\mu_o} P_\ell(\mu_o) \qquad (7.11)$$

$$\ell = 0,1,\ldots,5$$

with $\bar{\mu}_o(\mu_o)$ from (7.7) need be calculated only once for all groups in the region of isotropic scattering. So we can afford to determine the $B_\ell(\omega)$ at 321 ω-points in $[-1, +1]$. The integration is done analytically with suitable different approximations for A = 1, 1 < A $\leq$ 30, and A > 30.

The $w_\ell(E\to g)$ according to (7.8) are calculated by LEGIST by interpolating in the table of the $B_\ell(\omega)$ which a determined with LEGINT.

In concern with energy integrations the choice of the energy grid is strongly influenced by the oscillatory behaviour of the transfer probilities $w_\ell(E\to g)$ which is qualitatively shown in fig. 7.1 for ℓ = 5.

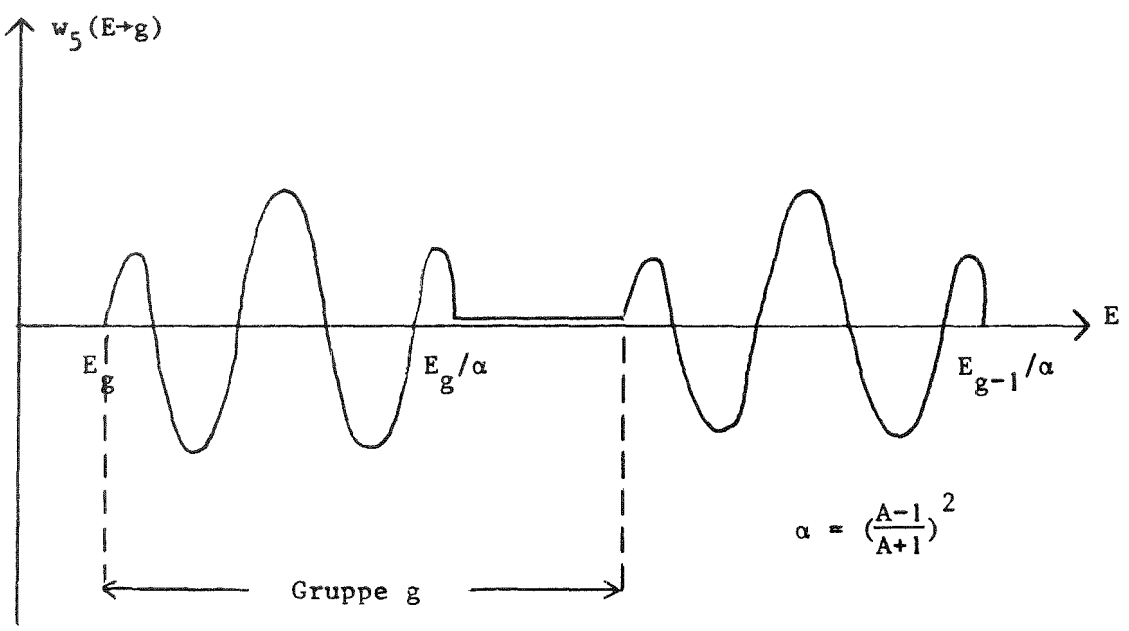

Fig. 7.1: Behaviour of the $w_\ell(E\to g)$ for ℓ = 5

Thus the energy integrals that require the finest energy mesh are the numerator in (7.2), namely

$$\int_{g'} dE\ \sigma(E) w_\ell(E \to g) \psi_\ell(E) \qquad (7.12)$$

The intervall $\left[\overline{E}_g,\ E_g/\underline{\alpha}\right]$ from which scattering to energies $E < E_g$ is possible is called outgroup scattering region; if $E_g/\alpha < E_{g-1}$, the intervall $\left[\overline{E}_g/\alpha,\ E_{g-1}\right]$ from which scattering occurs only to energies $E \geq E_g$ within group g is called ingroup scattering region.

In the outgroup scattering region $w_\ell(E \to g)$ may change its sign several times due to the zeros of the Legendre-polynomials in (7.5). To describe this behaviour properly we need a sufficiently fine energy grid (independent of α). In the ingroup scattering region there is only a weak dependence on energy so that a coarse mesh will do.

Comparisons with analytical cases show that for $\ell \leq 5$ and for a group lethargy $\ln(E_{g-1}/E_g) = \Delta u_g \leq 0.7$ an appropriate choice is NK = 70 and NR = 16 where NK(NR) is the number of discrete energies in the outgroup (ingroup) scattering region used for the representation of the $w_\ell(E \to g)$; other values can be specified by input.

NR should be large enough to guarantee a sufficiently accurate representation of an analytically given macroweighting spectrum (see below) if there are only a few discrete SGN-energies.

The whole group g is an outgroup scattering region if $E_g/\alpha \geq E_{g-1}$; in this case $NK \cdot \ln(E_{g-1}/E_g)/\ln(1/\alpha)$ - instead of NK in the first version of this module - discrete energy points are assigned to the group. In case of hydrogen 100 energy points per energy decade are taken.

These discrete energies are called basic points; they are determined in PUNK. Together with the discrete SGNC-energies found on KEDAK they form the <u>coarse energy grid</u> corresponding to which the $w_\ell(E \to g)$ we calculated in LECAL.

In GRUPIN the coarse grid, the SGN-energies and, if given, the energy points of the macroweighting spectrum are joined by means of PUSUM to form the <u>fine energy grid</u>. Linear interpolation of the $w_\ell(E \to g)$ and the elastic cross

sections $\sigma(E)$ to the fine grid yields a pointwise representation of the transfer cross sections $\sigma_\ell(E\to g) = \sigma(E) \cdot w_\ell(E\to g)$ which contains on one hand the information available from KEDAK and on the other hand the oscillatory behaviour of the $\sigma_\ell(E\to g)$ in the outgroup scattering region. For the representation of $\sigma_t(E)$ in (7.10) the energy points of SGT found on KEDAK are used.

For the final integration, which is performed groupwise in SPRAL, in case of a fine-structure weighting with $1/\Sigma_t^{\ell+1}$ the energy points of the macroscopic total cross section $\Sigma_t(E)$ - the sum of the energy points of the constituent σ_t's - are added to the fine grid, and the $\sigma_\ell(E\to g)$ are interpolated linearly to the resulting grid. In case of a mere macroweighting the fine grid is used.

The modified trapezoid integration procedure in SPRAL was developed from the usual trapezoid rule which treats the integrand as a whole linearly between to neighbouring points. The procedure applied here merely requires a linear behaviour of the components of the integrand. That this is a less severe restriction is clear from the fact that the product of two linear functions does not show a linear but a quadratic behaviour. For a detailed description see ref. /1/, p. 136.

The weighting function $\psi_\ell(E)$ is approximated by the product of a macro- and a micro-spectrum, representing the slowly varying collision density and the possibly strongly fluctuating fine-structure of the neutron flux density, respectively.

The possible weighting options are listed in the table 7.3.

Table 7.3: The fine-weighting options of module 6

Opt.	Macro-spectrum	Micro-spectrum	MW	NSPEC
1	$1/E$	1	-	-
2	$1/E$	$\left[1/\Sigma_t(E)\right]^{\ell+1}$	2	-
3	$F_o(E)$	1	-	1
4	$F_o(E)$	$\left[1/\Sigma_t(E)\right]^{\ell+1}$	2	1
5	$F_\ell(E)$	1	1	$\ell+1$

MW and NSPEC are the corresponding input parameters.

7.3 The routines of this module: purpose and a description of the argument lists and the commons

Subroutine:	Purpose:
FLUMMI	main control program
SUM	summation
IPØLA	interpolation with polynomials up to degree 3
PUSUM	joining of point sets
MAKRØ	construction of a macro-group structure dependent on given density of data points
MIXSGT, ADD	calculation of the total macroscopic cross section for fine-structure weighting
TRAFØ	transformation of angular distributions
INFØRM	printing of additional information
PUNK	generation of the basic energy grid
(NDF)	reading of KEDAK
LØØKO	reading of ISØT1 (atomic weight) using NDF
LØØK1	reading of SGN, MUEL, SGT using NDF
LØØK2	reading of SGNC using NDF
LØØK3	reading of SGNC-energies using NDF
LECAL	control of the calculation of the $w_\ell(E \to g)$ according to (7.8) and (7.10)
LEGPØL	calculation of pointwise Legendre polynomials
LEGINT	calculation of Legendre integrals according to (7.11)
G(FUNCTIØN)	$G(N,X,Y) = (X^N - Y^N)/(X-Y)$
LEGIST	calculation of partial Legendre coefficients according to (7.8)
LEGANS	calculation of partial Legendre coefficients according to (7.10)
GRUPIN	preparing of weighted energy integration
IPØLIN	linear interpolation
SPRAL	weighted energy integration
PHI(FUNCTIØN)	PHI(E) = 1/E
MUKØN	final determination of group constants according to (7.1), (7.1'), (7.2), (7.3)
PRINT	printing and reserving of final results

In the following a description of the argument lists and the commons of the subroutines is given. Under the heading "Arguments" those quantities are found which must be defined before computation will start. Under the heading "Results" those quantities are listed which are calculated by the routine.

```
SUBRØUTINE FLUMMI (A,B,EA,EB,E,EN,SGN,ECØ,SCØ,V,W,F,AR,FU,ABN,INT,
                   GR,FEKØE,EG,R,RSP,ESP,SPEK,SGNC,FEKØ,ELSIG,ELTØT,
                   ET,ST,MAT,DAT,NLA,NLE,ISEL,NMAX,NX,NE27,NSPEK,
                   LSPEK,MAZ,NTK,KT,NTTT,NTTP,ICØS,ICØSP,NECU,NECUP,
                   ISM,ISMP,ISØ,ISØP,ISCØ,ISCØP,ISEC,ISECP,KIM,NS,
                   NK,NR,GE,SG,SGTØT)

CØMMØN STØFF,ISTRUK,ISPA,NØUT,KPR,IM,IL,KL
```

Purpose:

- Construction of macro-groups by means of MAKRØ;
- calculation of unnormalized scattering matrices for each macro-group by means of LECAL and GRUPIN,
- calculation of normalized scattering matrices etc. by means of MUKØN,
- printing and reserving of results with PRINT

Arguments:

NX — number of energy group boundaries (input or standard)

EG(NX) — energy group boundaries (increasing) (input or standard)

NE27 — NX + 1

Comment: the group boundaries will be modified and rearranged in the following manner:

ABN(I) = EG(NX - I+1), I = 1,2,...,NX,

if ABN(NX) $\begin{cases} > 10^{-3} : \text{NEGR} = \text{NE27}, \text{ABN(NEGR)} = 10^{-3}\ \text{eV} \\ = 10^{-3} : \text{NEGR} = \text{NX} \\ < 10^{-3} : \text{ERRØR 6.8} \end{cases}$

NGR = NEGR-1

NGR — number of energy groups

NEGR — number of group boundaries

ABN(NEGR)	group boundaries (decreasing)
IL,IM	indices of the first and last energy group for which scattering matrices etc. shall be calculated (input)
NMAX	highest Legendre order which can be treated (NMAX = 5 in this version)
NLA	first Legendre moment to be calculated (input or standard, but finally NLA = 0 always)
NLE	last Legendre moment to be calculated (input or standard)
NSPEK	macro-weighting spectrum control parameter (= 1: spectrum from FUNCTIØN PHI > 1: NSPEK = number of discrete energies of the macro-weighting spectrum)
LSPEK	number of values of the macro-weighting spectrum if NSPEK > 1, = 1 otherwise
ESP(NSPEK)	discrete energies of the macro-weighting spectrum if NSPEK > 1, no meaning otherwise (input)
SPEK(LSPEK)	values of the macro-weighting spectrum (the first NSPEK values for the 0. moment, the second NSPEK values for the 1. moment etc. if MAZ(1) = 1, the first NSPEK values - there will be no more in this case - for all moments if MAZ(1) = 0)
NTK	micro-weighting spectrum pointer (= 1: the fine-structure mixture from which the micro-weighting spectrum is to be calculated is given in the arrays MAT and DAT; = 0: no fine-structure weighting)
KT	number of different nuclei in the fine-structure mixture (input), if NTK = 1; = 1 otherwise
MAT(KT)	nuclei in KEDAK notation in the fine-structure mixture (input)
DAT(KT)	densities in particles per ccm times 10^{-24} of the nuclei in the fine-structure mixture (input)
NTTT	estimated number of discrete energies of the micro-spectrum
MAZ(2)	pointers for the weighting of the higher moments (see SPRAL: MZ)
ISM	estimated number of energy meshpoints of the coarse mesh per macro-group
ISD	estimated number of energy meshpoints of the fine mesh per macro-group

ICØS	number of angular meshpoints of the angular distributions (SGNC) on KEDAK
NECU	scattering width
ISCØ	Max (NECU•ISD, ISM•ICØS)
ISEC	Max (ISD, ISM•NECU)
NS	maximum number of energy groups per macro-group (input or standard)
NK	number of basic points in the outgroup scattering region per group (input or standard)
NR	number of basic points in the ingroup scattering region per group (input or standard)
STØFF	nucleus in KEDAK notation for which scattering matrices etc. shall be calculated
NØUT	printed-output unit (usually NØUT=6)
KPR	unit on which the final results are stored
ISEL	pointer for additional output (input or standard)
KL	MIGRØS counting index

Auxiliary arrays:

A(ISM),B(ISM),EA(ISM),EB(ISM),E(ISM),EN(ISD),SGN(ISD),ECØ(ISD),SCØ(ISD),
V(ISD),W(ISD),F(ISD),AR(ICØS),FU(ICØS),ABN(NE27),INT(NE27),GR(NE27),
FEKØE(NE27),R(NX),RSP(6,NX),SGNC(ICØS,ISM),FEKØ(ISM,NECU),ELSIG(6,NECU,NX),
ELTØT(2,NX),ET(NTTT),ST(NTTT),GE(ISD),SG(ISD),SGTØT(6,NX)

Results:

NTTP	increment of NTTT if NTTT is found to be for small during execution
ICØSP	increment of ICØS if ICØS is found to be too small during execution
NECUP ISMP ISDP ISCØP ISECP	analogous

KIM	downward extension in groups of the energy region to be calculated in order to treat outscattering in the low energy groups correctly

SUBRØUTINE SUM(M,A,S)

Purpose: Summation of real numbers different in sign and magnitude with minimization of rounding errors

Arguments:

M	number of summands
A(M)	summands

Results:

S	$\sum_{I=1}^{M} A(I)$

SUBRØUTINE IPØLA(M,A,B,N,X,Y,T)

Purpose: Interpolation with polynomials up to degree three (for details see ref. 1, p. 140)

Arguments:

M	number of given points
A(M)	given abszissae
B(M)	given ordinates
N	number of the given new abszissae
X(N)	given new abszissae with X(1) = A(1), X(N) = A(M), X(I-1) < X(I), I = 2, N

Auxiliary array:

T(M)

Results:

Y(N)	new ordinates corresponding with the given new abszissae

SUBRØUTINE PUSUM (ISD,KA,A,KE,E,B)

Purpose: Joining of point sets

Arguments:

KA	number of elements in the array A
A(KA)	first point set (increasing)
KE	number of elements in the array E
E(KE)	second point set (increasing)

Auxiliary array:

B(KE)

Results:

KE	number of different points in A and E
E(KE)	different points in A and the given E (increasing)

SUBRØUTINE MAKRØ (ALFA,ALLN,ISØ,IL,IM,NGR,ABN,R,ISD,ISM,ISDP,NS,NK,NR,
NEN,NECU,NUEB,V,W,F,LST,INTT,INT,NEGR,KSPE,NSPEK,ESP,
NTK,KT,MAT,NTTT,NTTP,NF,ISEL,ISGT)

CØMMØN STØFF,ISTRUK,ISPA,NØUT

Purpose: A macro-group is defined as an energy region consisting of one group or several connected groups. MAKRØ subdivides the given energy region (ABN(IM +1), ABN(IL)) into macro-groups meeting the following conditions:

each macro-group contains

a) as many groups as possible
b) NS groups at most
c) ISD - ISM SGN-meshpoints at most
d) either groups with only isotropic outscattering in the c.m.-system or groups with only anisotropic outscattering in the c.m.-system

Arguments:

ALFA	$((A-1)/(A+1))^2$ where A is the atomic weight of the scattering nucleus in neutron mass units
ALLN	ln ALFA

IL,IM	indices of the first and last group for which scattering matrices shall be calculated
ISØ	index of the first group with only isotropic outscattering in the c.m.-system
NUEB	scattering width
NS	maximum number of groups per macro-group
NK	number of basic points in the outgroup scattering region per group, reduced if NUEB > 2
NR	number of basic points in the ingroup scattering region
NEN	total number of SGNC-energies
NGR	number of energy groups
NEGR	number of energy group boundaries
ABN(NEGR)	energy group boundaries
R(NGR)	group lethargy widths
NECU	maximum scattering width
ISM	maximum number of basic points plus discrete SGNC-energies per macro-group
ISD	ISM plus maximum number of discrete SGN-energies per macro-group
KSPE	pointer for macro-weighting (=0: 1/E-weighting, = 1: weighting with a spectrum given pointwise)
NSPEK	number of energy points of the macro-spectrum if KSPE = 1, = 1 otherwise
ESP(NSPEK)	energy points of the macro-spectrum
NTK	pointer for micro-weighting (= 0: No micro-weighting with $1/\Sigma_t^{\ell+1}$)
KT	number of materials for micro-weighting if NTK = 1; = 1 if NTK = 0
MAT(KT)	materials for micro-weighting if NTK = 1; no meaning if NTK = 0
NTTT	maximum number (estimated) of energy points per group for micro-weighting
NF	unit for temporary storage purposes
ISEL	pointer for additional output

STØFF	nucleus in KEDAK notation for which scattering matrices etc. shall be calculated
NØUT	printed-output unit

Auxiliary arrays:

V(ISD), W(ISD), LST(2, NGR), F(ISD)

Results:

INTT	number of macro-group boundaries
INT(INTT)	macro-group boundaries given by group indices
ISDP	increment of ISD if ISD is found to be too small during execution
NTTP	increment of NTTT if NTTT is found to be too small during execution
ISGT	interrupt indicator (= 0: no interrupt; = 1: an interrupt with printing of an error message has occurred)

comment: the determined macro-groups are as follows:

1. macro-group: [ABN(INT(2)+1), ABN(IN(1))]

I-th macro-group: [ABN(INT(I+1)+1), ABN(INT(I)+1]

I = 2,3,...,INTT-1

SUBRØUTINE MIXSGT(KT,MAT,DAT,NTT,NTP,NT,ET,ST,EA,EE,ISGT)

CØMMØN STØFF, ISTRUK, ISPA, NØUT

Purpose: Calculation of the total macroscopic cross section of a given mixture according to

$$\Sigma_t(E) = \sum_{I=1}^{KT} d_I \cdot \sigma_{t,I}(E)$$

where d_I = density in nuclei per ccm times 10^{-24} of the I-th nucleus in the mixture and $\sigma_{t,I}$ = total microscopic cross section of the I-th nucleus in the mixture; KT see below. E stands for the joint set of discrete energies for which for at least one nucleus in the mixture a σ_t is found on KEDAK.

Arguments:

KT	number of different nuclei in the mixture
MAT(KT)	nuclei in the mixture
DAT(KT)	densities (DAT(I) = d_I)
EA,EE	lower and upper boundary of the energy intervall in which Σ_t shall be calculated
NTT	estimated number of discrete energies of the mixture in the intervall $\boxed{EA,EE}$.
NØUT	printed-output unit

Results:

NT	number of discrete energies of the mixture in the intervall $\boxed{EA,EE}$
ET(NT)	discrete energies in $\boxed{EA,EE}$
ST(NT)	total macroscopic cross sections of the mixture corresponding to the ET(I)
NTP	increment of NTT if NTTT is found to be too small during execution
ISGT	interrupt indicator (see MAKRØ)

SUBRØUTINE ADD(K,NTT,NTP,NT,ET,ST,NU,D,E,S,EV,SV,EW,SW,EA,EE)

Purpose: Determination of $P_{K,NU+1}(F|ET,ST)$ from $P_{K,NU}(F|ET,ST)$

(definition of $P_{I,J}(F|ET,ST)$ see below.)

Arguments:

K	index of the nucleus which shall be added to the hitherto calculated mixture of the first K-1 nuclei
EA,EA,NTT	see MIXSGT
NT	number of the hitherto determined discrete energies of the mixture = number of ET(J) in $P_{K,NU}(E/ET,ST)$
ET(NT)	hitherto determined discrete energies
ST(NT)	hitherto determined total cross sections
NU	index of the highest energy up to which the K-th nucleus has been taken into account

D	density of the K-th nucleus
E,EV	energy points of the polygonial to be added
S,SV	microscopic total cross sections at E and EV
EW	ET(NU) before the last modification
SW	ST(NU) before the last modification

Results:

NT	number of discrete energies of the mixture up to E
ET(NT)	discrete energies up to E
ST(NT)	total macroscopic cross sections up to E
NU	index of the highest energy up to which the K-th nucleus has been taken into account
NTP	see MIXSGT

Definition of $P(E|ET,ST)$ and $P_{I,J}(E|ET,ST)$:

Be

$$P(E|ET,ST) = P(E|ET(1),ET(2),\ldots,ET(NT);\ ST(1),ST(2),\ldots,ST(NT))$$

$$= \begin{cases} 0 & \text{if } E < ET(1) \text{ or } E > ET(NT) \\ ST(J) & \text{if } E = ET(J) \\ ST(j-1) + \dfrac{ST(J) - ST(J-1)}{ET(J) - ET(J-1)}\,(E-ET(J-1)) & \\ \qquad \text{if } ET(J-1) < E < ET(J) & \end{cases}$$

provided $ET(1) < ET(2) < \ldots < ET(NT)$.

Be now

$$P_{I,J}(E|ET,ST) = \sum_{K=1}^{I-1} P_{K,NT_K}(E|ET,ST)$$

$$+ P(E|ET_I(1),\ ET_I(2),\ \ldots\ ,\ ET_I(J);$$

$$ST_I(1),\ ST_I(2),\ \ldots\ ,\ ST_I(J))$$

where the $ET_I(K)$ are the discrete σ_t-energies of the I-th nucleus and the $ST_I(K)$ are the corresponding macroscopic cross sections.

SUBRØUTINE TRAFØ(IC,NE,ISM,S,XM,AL,A)

Purpose: Transformation of angular distributions for elastic neutron scattering from the c.m.-system into the laboratory system according to equ. (7.7)

Arguments:

IC	number of uniformly spaced cosine meshpoints of the angular distributions in the c.m.-system
NE	number of angular distributions undergoing transformation
ISM	maximum number of angular distributions
S(IC,NE)	angular distributions in the c.m.-system
A(IC)	uniformly spaced cosine meshpoints of the angular distributions in the c.m.-system with A(1) = -1, A(IC) = 1
AL	ALFA (see MAKRØ)

Results:

A(IC)	cosine meshpoints in the laboratory system
S(IC,NE)	angular distributions in the laboratory system

SUBRØUTINE INFØRM(ALFA,NEGR,ABN,R,IL,IM,INTT,INT,NST,NSTIS,IR,ISTT, K,NTK,NTT,NØUT)

Purpose: Printing of additional information if ISEL < 0

Arguments:

ALFA,NEGR,ABN, IL,IM,INTT,INT, NØUT	see MAKRØ
R(NEGR-1)	group lethargy widths
NST(6),NSTIS	see LECAL
IR	macro-group index
ISTT	number of energy meshpoints in the fine-mesh in the IR-th macro-group

K	number of discrete SGN-energies in the IR-th macro-group
NTK	pointer for micro-weighting
NTT	number of discrete energies of the micro-weighting spectrum in the IR-th macro-group if NTK ≠ 0

SUBRØUTINE PUNK(NGR,NEGR,ABN,NA,NE,NEN,ALFA,NK,NR,ISM,ISMP,ISN,E,R,ALLN)

Purpose: Generation of the basic energy grid uniformly spaced in lethargy

Arguments:

NGR	number of energy groups
NEGR	number of energy group boundaries
ABN(NEGR)	group boundaries
NA,NE	first and last group in the considered macro-group
NEN	number of angular distributions in the considered macro-group
ALFA,ALLN	see MAKRØ
NK	number of basic points in the outgroup scattering region
NR	maximum number of basic points in the ingroup scattering region; is reduced if the whole group is ingroup sent.reg.
ISM	maximum number of basic points plus discrete SGNC-energies per macro-group
R(NGR)	group lethargy widths

Results:

ISN	calculated number of basic points in the macro-group defined through NA,NE
E(ISN)	calculated basic points in this macro-group
ISMP	increment of ISM if ISM is too small

SUBRØUTINE LØØKO(XMAT,MASSE,CØM,*)

CØMMØN STØFF, ISTRUK, ISPA, NØUT

Purpose: Reading the atomic weight from KEDAK and relating it to the neutron mass as mass unit, calculation of the mass number and of the mean scattering cosine in the laboratory system for isotropic scattering in the c.m.-system

Arguments:

STØFF nucleus in KEDAK notation

Results:

XMAT atomic weight of the nucleus in STØFF in neutron mass units

MASSE mass number

CØM $\frac{2}{3 \cdot XMAT}$

Remark: LØØKO calls the Entry NDFLØC of the KEDAK routine NDF

SUBRØUTINE LØØKI(ISD,K,E,SGN,EØ,EE,NT,ISGT)

CØMMØN STØFF, ISTRUK, ISPA, NØUT

Purpose: Reading of SGN, MUEL and SGT from KEDAK

Arguments:

STØFF nucleus in KEDAK notation for which data shall be read from KEDAK

ISD maximum number of data which may be read with a single call

EØ, EE lower and upper boundary of the energy region for which data shall be read

NT data-type pointer (NT = 1: SGN are read; NT = 2: MUEL are read; NT = 3: SGT are read)

NØUT printed-output unit

Results:

K	number of data (SGN, MUEL or SGT) in [EØ, EE].
E(K)	discrete energies at which data are given
SGN(K)	data read from KEDAK (SGN, MUEL or SGT)
ISGT	interrupt indicator (see MAKRØ)
Remarks:	The conditions E(1) = EØ and E(K) = EE are met by linear interpolation or constant extrapolation. LØØK1 calls the Entries NDFLØC and NDFNXT of the KEDAK routine NDF.

SUBRØUTINE LØØK2(NEN,EA,ICØS,ICØSP,ISM,AR,SGNC)

CØMMØN STØFF, ISTRUK, ISPA, NØUT

Purpose: Reading of SGNC from KEDAK

Arguments:

STØFF	nucleus in KEDAK notation
NEN	number of discrete energies at which SGNC are given
EA(NEN)	discrete energies for which SGNC shall be read (they have been read before with LØØK3)
ICØS	maximum number of SGNC cosine meshpoints
ISM	maximum number of discrete SGNC-energies
NØUT	printed-output unit

Results:

ICØSP	increment of ICØS if ICØS has found to be too small during reading SGNC from KEDAK
AR(ICØS)	SGNC cosine meshpoints from KEDAK
SGNC(ICØS,NEN)	SGNC from KEDAK corresponding to the cosine mesh AR and the energy mesh EA
Remarks:	The cosine mesh must be the same for all energies. LØØK2 calls the entries NDFLØC and NDFNCT of the KEDAK routine NDF.

SUBRØUTINE LØØK3(NE,EA,ISØ,NGR,ABN,ISM,ISMP,LST,NEGR,ISEL,ISGNC)

CØMMØN STØFF, ISTRUK, ISPA, NØUT

Purpose: Reading from KEDAK the entire SGNC-energy mesh for one nucleus

Arguments:

STØFF,ISM,NØUT — see LØØK2

NGR,NEGR,ABN — see MAKRØ

Results:

ISEL — pointer for additional output

ISMP — estimated increment of ISM if there are more than ISM angular distributions on KEDAK for the considered nucleus

NE — number of angular distributions on KEDAK for the nucleus in question

EA(NE) — SGNC-energy mesh on KEDAK for the considered nucleus

LST(NGR) — LST(I) = number of energies EA(N) with ABN(I+1) $\leq$ EA(N) < ABN(I)

ISØ — see MAKRØ

ISGNC — interrupt indicator (compare ISGT in MAKRØ)

Remark: LØØK3 calls the Entry NDFLØC of the KEDAK routine NDF

SUBRØUTINE LECAL(MASSE,XMAT,ALFA,ISØT,LEG,NLE,NANF,NEND,NUEB,IL,IM,
NEGR,ABN,ICØS,AR,ISN,E,SGNC,NST,NSTIS,ISM,ISD,NECU,
ITA,NF,GR, FEKØE ,FU,EW,A,H,V,W,F,FEKØ)

Purpose: Control of the calculation of the $w_\ell(E \to g)$ according to equations (7.8) and (7.10)

Arguments:

MASSE — atomic mass number of the scattering nucleus

XMAT — atomic weight of the scattering nucleus in neutron mass units

ALFA — $((XMAT-1)/(XMAT+1))^2$

ISØT	anisotropy pointer (ISØT=1: the considered macro-group is within the energy region of anisotropic scattering in the c.m.-system, ISØT = 0 otherwise)
LEG(6)	sequence of calculated moments
NLE	upper Legendre index (input)
NANF,NEND	indices of the first and the last group in the macro-group for which scattering matrices etc. shall be calculated
NUEB	scattering width
IL,IM	indices of the first and the last group for which scattering matrices etc. shall be calculated
NEGR	number of energy group boundaries
ABN(NEGR)	energy group boundaries
ICØS	number of cosine meshpoints of the SGNC on KEDAK
AR(ICØS)	cosine meshpoints of the SGNC on KEDAK
ISM	number of basic points plus discrete SGNC-energies in the macro-group to be calculated
E(ISN)	basic points plus discrete SGNC-energies in the macro-group to be calculated (coarse mesh)
SGNC(ICØS,ISM)	angular distributions in the laboratory system
NST(6)	moment-dependent number of uniformly spaced cosine meshpoints for μ_o-integration when ISØT = 1
NSTIS	moment-independent number of uniformly spaced cosine meshpoints for μ_o-integration when ISØT = 0
ISM	maximum number of basic points and discrete SGNC-energies per macro-group
ISD	ISM plus maximum number of discrete SGN-energies per macro-group
NECU	maximum scattering width
ITA	pointer for the calculation of Legendre integrals by means of LEGINT (ITA = 0: Legendre integrals are calculated, ITA = 1: Legendre integrals have already been calculated)
NF	unit on which the $w_\ell(E \to g)$ are stored temporarily

Auxiliary arrays:
GR(NEGR), FEKØE(NEGR), FU(ICØS), EW(ISM), A(ISD), H(ISD), V(ISD), W(ISD), F(ISD), FEKØ(ISM,NECU)

Results: $w_\ell(E \to g)$ on unit NF

SUBRØUTINE LEGPØL(NST,A,N,NSTIS)

CØMMØN /INTEG/ X, F, D

Purpose: Calculation of pointwise Legendre polynomials

Arguments:

NST	number of uniformly spaced cosine meshpoints
N	order up to which Legendre polynomials shall be calculated
NSTIS	number of uniformly spaced cosine meshpoints if ISØT = 0 (here: maximum length of A)

Results:

A(NST)	uniformly spaced cosine meshpoints
X(NST)	uniformly spaced cosine meshpoints (double precision)
F(NST,N+1)	Legendre polynomials pointwise F(L,I) = P_{L-1}(A(I))
D	spacing of the A(I): D = A(I) - A(I-1), I = 2, NST

SUBRØUTINE LEGINT(N,NAK,XMAT,ITA)

CØMMØN /INTEG/ H, GRAL, D

Purpose: Calculation of Legendre integrals

$$B_n(\omega) = \frac{1}{2A} \int_{-1}^{\omega} d\mu_o \frac{\left(\mu_o + \sqrt{\mu_o^2 - 1 + A^2}\right)^2}{\sqrt{\mu_o^2 - 1 + A^2}} P_n(\mu_o)$$

$$n = 0,1,\ldots,5$$

Arguments:

N	upper Legendre index (is ignored; the $B_n(w)$ are always determined for N = 0, 1, 2, 3, 4, 5)
NAK	number of cosine meshpoints
XMAT	atomic weight in neutron mass units

Results:

H(NAK)	uniformly spaced cosine mesh-points, H(1) = -1, H(NAK) = 1
D	spacing of the H(I)
GRAL(6,NAK)	GRAL(L,I) = $2 \cdot B_{L-1}(H(I))$
ITA	pointer (ITA = 1 after calculation)

Remarks: For A = 1, 1 < A $\leq$ 30, A > 30 the above integral is treated numerically in different ways.

FUNCTIØN G(N, X, Y)

$$G(N, X, Y) = \frac{X^N - Y^N}{X - Y}$$

is determined according to

$$\frac{X^N - Y^N}{X - Y} = D^{N-1} + \binom{N}{1} D^{N-2}\ Y + \binom{N}{2} D^{N-3}\ Y^2 + \ldots + \binom{N}{N-1} Y^{N-1}$$

where

$$D = X - Y$$

SUBRØUTINE LEGIST(L,NST,IA,IB,NEGR,GR,E)

CØMMØN /INTEG/ X, GRAL, D

Purpose: Calculation of partial Legendre coefficients when scattering is isotropic in the c.m.-system according to equ. (7.8)-multiplication with 2π is performed in LECAL:

$$E(I) = \frac{1}{4\pi} \int_{GR(I+1)}^{GR(I)} d\mu_o \frac{d\bar{\mu}_o}{d\mu_o} P_{L-1}(\mu_o)$$

using the previously in LEGINT determined integrals

$$GRAL(L,I) = 2 \int_{-1}^{X(I)} d\mu_o \frac{d\bar{\mu}_o}{d\mu_o} P_{L-1}(\mu_o)$$

Arguments:

L	Legendre degree plus 1
NST	number of uniformly spaced cosine meshpoints
X(NST)	cosine mesh from LEGINT
D	spacing of the X(I)
GRAL(6,NST)	see above
NEGR	length of array E
IA,IB	boundary indices within which the E(I) shall be determined
(GR(I),I=IA,IB)	cosine integration boundaries

Results:

E(NEGR)	(E(I), I=IA,IB-1) = partial Legendre coefficients (see above) E(NEGR) = total Legendre coefficient $= \sum_{I=IA}^{IB-1} E(I)$

SUBRØUTINE LEGANS (L,NST,F,IA,IB,NEGR,GR,E,PØLY,A)

CØMMØN /INTEG/ X,PØL,D

Purpose: Calculation of partial Legendre coefficients when scattering is anisotropic in the c.m.-system according to equ. (7.10)-multiplication with 2π is performed in LECAL:

$$E(I) = \int_{GR(I+1)}^{GR(I)} d\mu_o \; w(E,\mu_o) \; P_{L-1}(\mu_o)$$

Arguments:

L,NST,D,NEGR, IA,IB,GR	see LEGIST
X(NST)	cosine mesh from LEGPØL
F(NST)	pointwise angular distribution corresponding with the X(I)
PØL(6,NST)	Legendre polynomials pointwise from LEGPØL corresponding with the X(I)

Auxiliary arrays:

PØLY(NST), A(NST)

Results:

E(NEGR)	(E(I),I=IA,IB-1) = partial Legendre coefficients (s.above) E(NEGR) = total Legendre coefficient $= \sum_{I=IA}^{IB-1} E(I)$

SUBRØUTINE GRUPIN(MASSE,XMAT,ALFA,CØM,ISØT,PM,LEG,NLE,NANF,NEND,NUEB,IL,
IM,NGR,NEGR,ABN,ISN,EH,K,H,F,M,G,EN,NTT,ET,ST,MAZ,KSPE,
KSPEK,ESP,SPEK,NSPEK,LSPEK,ISM,ISD,NECU,ISCØ,ISEC,NF,
E,EW,GR,WA,U,V,W,ISTT,RSP,ELSIG,NGT,NGG,EG,SG,SGTØT)

Purpose: Preparing of weighted energy integration

Arguments:

MASSE,XMAT,ALFA, ISØT,LEG,NLE,NANF, NEND,NUEB,IL,IM, NEGR,ABN,ISN,ISM, ISD,NECU,NF	} see LECAL
CØM	mean scattering cosine when scattering is isotropic in the c.m.-system = 2/(3·XMAT)
PM	fraction of MUEL in the corrected first moment (normally 1.)
NGR	number of energy groups
EH(ISN)	basic points plus discrete SGNC-energies in the macro-group to be calculated
K	number of SGN

H(K) discrete SGN-energies

F(K) SGN corresponding with the H(I)

M number of MUEL

G(M) discrete MUEL-energies

EN(M) MUEL corresponding with the G(I)

NTT,ET(NTT),ST(NTT),
MAZ(2),KSPE,KSPEK,NSPEK,
LSPEK,ESP(KSPEK),SPEK(KSPEK), } see subroutine SPRAL

NTT,ET(NTT),ST(NTT),MZ(2),
KS,NS,NP,NL,E,S } , correspondingly

NGT pointer for the calculation of ψ_ℓ-weighted total group cross sections (= 1: calculation, = 0: no calculation)

NGG number of given total cross section values in the macro-group considered

EG(NGG) total cross section energy points

SG(NGG) total cross sections corresponding to EG

ISCØ dimension of WA (see below and FLUMMI)

ISEC dimension of U (see below and FLUMMI)

Auxiliary arrays:

E(ISD), EW(ISM), GR(NEGR), WA(ISCØ), U(ISEC), V(ISD), W(ISD)

Results:

ISTT number of energy meshpoints in the fine energy grid consisting of the basic points (from PUNK), the discrete SGNC-energies, the discrete SGN- and MUEL-energies

RSP(6,NGR) energy group integrals of the weighting spectra

$$RSP(L,N) = \int_N dE\ \psi_{L-1}(E)$$

ELSIG(6,NUEB,NGR) elastic scattering transfer cross sections

$$ELSIG(L,I,N) = \sigma_{L-1}^{N\to II}$$

$$= \int_N dE\ \sigma(E)\ w_{L-1}(E\to II)\psi_{L-1}(E) / \int_N dE \psi_{L-1}(E)$$

where II = N + I-1

SGTØT(6,NGR) total group cross sections (if NGT = 1)

$$SGTØT(L,N) = \sigma^{N}_{t,L-1}$$

$$= \int_{N} dE\ \sigma_t(E)\psi_{L-1}(E) / \int_{N} dE\ \psi_{L-1}(E)$$

SUBRØUTINE IPØLIN(M,A,B,N,X,Y,HR)

Purpose: Linear interpolation

Arguments:

M number of given points

A(M),B(M) given points

N number of given new abszissae

X(N) given new abszissae where X(1) = A(1), X(N) = A(M)

Auxiliary array:

HR(M)

Results:

Y(N) new ordinates corresponding with the X(I)

SUBROUTINE SPRAL(KS,NS,MZ,E,S,NTT,ET,ST,L,IKK,EN,H,G,VAL,NP,NL,NLE)

Purpose: Calculation of integrals

$$\int_{g} dE\ H(E)\ \psi_{\ell}(E), \text{ where } H(E) = \begin{cases} \sigma(E)w_{\ell}(E\to h) \\ \sigma_t(E) \\ 1 \end{cases}$$

Arguments:

KS pointer for macro-weighting
(= 0 :1/E-weighting, = 1: weighting with a pointwise spectrum)

NS number of energy points of the macro-weighting spectrum if KS = 1; = 0 otherwise

MZ(2)	pointers for the weighting of the higher moments (MZ(1) = 0; same macro-weighting for all moments, = 1: special macro-weighting for each moment; MZ(2): same as MZ(1) but for micro-weighting
NP	field dimension (= NS if KS = 1, = 1 otherwise)
NLE	order of the last Legendre-moment to calculated ($1 \leq NLE \leq 5$)
NL	field dimension (= NS if MZ(1) = 0, = NP·(NLE+1) if MZ(1) = 1)
E(NS)	macro-spectrum energy points overlapping group g if KS = 1, no meaning otherwise
S(NL)	macro-spectrum values corresponding to E if KS = 1, no meaning otherwise
NTT	field dimension and pointer for micro-weighting (= 1: no micro-weighting, > 1: micro-weighting with NTT energy points)
ET(NTT)	energy points for micro-weighting overlapping group g
ST(NTT)	total macroscopic cross sections for micro-weighting corresponding to ET
L	Legendre-order for which cross sections shall be calculated plus 1 (L = ℓ+1)
IKK	number of energy points in the fine energy grid
EN(IKK)	energy points in the fine energy grid for group g, boundaries included
H(IKK)	values of the function H in the fine energy grid (see Purpose) corresponding to EN

Auxiliary array:

G(IKK)

Result:

VAL	$\int_g dE\ H(E)\ \psi_\ell(E)$, H see Purpose

Remarks: In case of fine weighting with $1/\Sigma_t^{\ell+1}$ the energy grid for integration consists of the fine grid and the points at which the Σ_t's are given. The behaviour of the cross sections to be integrated, the macro-weighting spectrum and the $1/\Sigma^{\ell+1}$-values is assumed to be linear between adjoining points of this grid.

FUNCTIØN PHI(E) = 1/E

SUBRØUTINE MUKØN(ELSIG,ELTØT,NLE,NECU,NUEB,IL,IM,NGR,MASSE)

Purpose: Determination of σ^{NN}, $S_L^{NN\to II}$ and $\bar{\mu}^{NN}$ from $\sigma_L^{NN\to II}$ according to (7.1), (7.2) and (7.3):

$$\sigma^{NN} = \sum_{II \geq NN} \sigma_o^{NN\to II},$$

$$S_L^{NN\to II} = \sigma_L^{NN\to II}/\sigma^{NN},\ L = 0,1,\ldots,NLE,$$

$$\bar{\mu}^{NN} = \sum_{II \geq NN} S_1^{NN\to II}$$

Arguments:

NLE — Legendre degree up to which scattering matrices are calculated

NUEB — scattering width

IL,IM — first and last calculated energy group

ELSIG(6,NUEB,NGR) — ELSIG(L,I,NN) = $\sigma_{L-1}^{NN\to NN+I-1}$ (see GRUPIN)

where NN = IL,...,IM
I = 1,...,NUEB
L = 1,2,...,NLE+1

Results:

ELSIG(6,NUEB,NGR) — ELSIG(L,I,NN) = $S_{L-1}^{NN\to NN+I-1}$ (see above)

ELTØT(2,NGR) — ELTØT(1,NN) = σ^{NN}
ELTØT(2,NN) = $\bar{\mu}^{NN}$ (see above)

where NN = IL,...,IM
I = 1,...,NUEB,
L = 1,2,...,NLE+1

Remark: Comparisons with cases which can be treated analytically (atomic weight A > 1) whow that the matrixelements $S_{L-1}^{NN\to NN+I-1}$ are calculated here with a maximum absolute error

$\Delta S \approx 4 \cdot 10^{-4}$

Thus quantities smaller than 10^{-5} in absolut value are ignored and set equal to zero (except for hydrogen)

SUBRØUTINE PRINT(ELSIG,ELTØT,NLA,NLE,NECU,NUEB,ISEL,NGR,KSPEK,MAZ,NTK,
KIM,NGT,SGTØT,RSP,MASSE,NGS)

CØMMØN STØFF, ISTRUK, ISPA, NØUT, KPR, NEND, NANF

Purpose: Printing and reserving of final results

Arguments:

ELSIG,ELTØT	see MUKØN results
NGT,RSP,SGTØT,	see GRUPIN
NLE,NECU,NUEB, NGR	see MUKØN
MAZ,NTK,KIM	see FLUMMI
KSPEK	corresponds to KSPE in GRUPIN
NLA	first Legendre moment to be calculated (NLA = 0 always)
NANF,NEND	indices of the first and last group for which scattering matrices have been calculated
STØFF	nucleus for which scattering matrices have been calculated
ISEL	pointer for additional output
NØUT	printed-output unit
KPR	unit on which all MIGRØS-results are stored
MASSE	mass number of the nucleus in STØFF
NGS	index of the first group in which has been put SGN = SGT = 1 (only for heavy materials in case of /ISEL/ = 1 (input))

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8. The Calculation of the interval cross sections and the zero'th and higher moments of the normalized elastic transfer elements for the REMO-correction. Module 9.

8.1 Basic formulae and notations

a) The fine interval system for the REMO-Correction /1/.
The I-th group of the basic broad group system is divided into NFG(I) fine-groups, equidistant in lethargy. Any of these fine groups is divided into NFI(I) fine intervals, equidistant in energy. The fine interval width is denoted by ΔE.

b) The fine-interval averaged cross-sections are defined by:

$$\langle \sigma \rangle = \frac{\int_{\Delta E} dE\ \sigma(E)F(E)}{\int_{\Delta E} dE F(E)} \tag{8.1}$$

The REMO correction procedure requires the total σ_t and the elastic scattering cross-sections σ_e and the averaged cosine which is defined by

$$\langle \mu_e \rangle = \frac{\int_{\Delta E} dE\ \mu_e(E)\ \sigma_e(E)F(E)}{\int_{\Delta E} dE\ \sigma_e(E)F(E)} \tag{8.2}$$

c) The elastic scattering transfer probability matrix-elements are defined by

$$\langle {}_\ell P(E\to n) \rangle = \frac{\int_{\Delta E} dE\ \sigma_e(E)\ \pi_\ell(E\to n)F(E)}{\sum_n \int_{\Delta E} dE\ \sigma_e(E)\ \pi_o(E\to n)F(E)} \tag{8.3}$$

where

$$\pi_\ell(E\to n) = \frac{(A+1)^2}{4A} \cdot \frac{1}{E} \cdot \int_{\max(\alpha E, E_{n+1})}^{E_n} dE'\ \gamma(\mu_c)\ P_\ell(t) \tag{8.4}$$

where $P_\ell(t)$ are the Legendre polynomials.

A is the mass of the scatterer, and

$$\alpha = \left(\frac{A-1}{A+1}\right)^2 .$$

The scattering angle in the center-of-mass system

$$\mu_c = 1 - \frac{(A+1)^2}{2A} \cdot \left(1 - \frac{E'}{E}\right),$$

and that in the laboratory system,

$$t = \frac{A+1}{2}\sqrt{\frac{E'}{E}} - \frac{A-1}{2}\sqrt{\frac{E}{E'}} \quad .$$

$\gamma(\mu_c)$ = the angular distribution of the elastic scattering in the center of mass system. It should be normalized i.e.

$$\frac{1}{2}\int_{-1}^{+1} d\mu_c \; \gamma(\mu_c) = 1$$

($\gamma(\mu_c) \equiv 1$, for isotropic case)

It is practical to transform the integral (8.4) into

$$\pi_\ell(E \to n) = \frac{1}{2}\int_{\mu_{n+1}}^{\mu_n} d\mu_c \; \gamma(\mu_c) \; P_\ell(t(\mu_c)), \tag{8.5}$$

where

$$t(\mu_c) = 0.5\sqrt{1-(1-\mu_c)\frac{2A}{(A+1)^2}}\left\{A+1 - \frac{A-1}{1-(1-\mu_c)\frac{2A}{(A+1)^2}}\right\} \tag{8.6}$$

or after some calculations

$$t(\mu_c) = \frac{\mu_c + \frac{1}{A}}{\sqrt{\frac{1}{A^2} + \frac{2\mu_c}{A} + 1}} \tag{8.6-b}$$

Let the energy E fall into the group g. The neutron transfer may occur into the groups g, g+1, ... g+k, where $E_k > \alpha E > E_{k+1}$. As there is an unambiguous relation between the scattering angle μ_c and energy loss, a division of the angle interval $-1 \leq \mu_c \leq 1$ corresponds to the acceptor groups, i.e.

$$-1 \equiv \mu_{k+1} < \mu_k \ldots < \mu_1 < 1$$

Thus the neutrons scattered with angle $1 \geq \mu \geq \mu_1$ remain in the group g, and those with the angle $\mu_j \geq \mu \geq \mu_{j+1}$ will fall into the group g+j.

According to our experience, the calculation and the physical interpretation are the simplest when the integration is performed over the center-of-mass scattering angle.

8.2 Method of calculation

According to the formulae (8.1), (8.2), (8.3) and (8.5) the main task is to perform numerical integrations.

For (8.1) and (8.2) a simple trapezoidal rule is used. The meshpoints for the integration are derived from the KEDAK-data. All different energy points of the datatypes SGT, SGN and MUEL and the intervalboundaries are taken. The functional values are obtained by linear interpolation in the energy. For the integral (8.3) and (8.5) the Romberg integration method (see app. III in /2/) is used. The alternating sign of the Legendre polynomial P_ℓ and the "ill-behaviour" of the $\gamma(\mu_c)$ at some energy values require special consideration which are described in app. IV. of /2/.

Before the integral (8.3) is performed, the fine interval ΔE is to be divided into subintervals with the following mesh-points:

i All energy points for which elastic scattering cross-sections are given in the nuclear data file should be a mesh point.

ii If an energy value E_k/α falls into the fine interval, this also should be a mesh point. The Romberg integration procedure is performed for each subinterval.

8.3 The removal of possible inconsistencies between the average cosine calculated from the angular distribution and the average cosine available on KEDAK

There may two types of the above inconsistency exist:

a) The angular distributions of the scattered neutrons for the energy range in question are not given, but the retrieved average cosine μ_{ret} is different from 2/3A. In this case a linear anisotropy is assumed i.e. the following center of mass angular distribution is used

$$\gamma(\mu_c) = 1 + (\overline{\mu_{ret}} - \frac{2}{3A}) \frac{3}{1 - \frac{3}{5A^2}} \cdot \mu_c \qquad (8.7)$$

Formula (8.7) is always used for the calculations.

b) The nuclear data file gives center of mass angular distributions for the energy range in question, but the calculated average cosine differs from the retrieved one. This difference can be attributed to the uncertainties in the evaluated angular distribution as well as to the uncertainties in their interpolation. Consequently there exist only ad hoc methods for the removal of this inconsistency. We have applied the following simple treatment.

Let the Legendre expansion of the scattering probability in the labor system be.

$$w_s(\mu) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} \cdot b_{s,\ell} \cdot P_\ell(\mu), \; b_{s,o} = 1, \; b_{s,1} = \bar{\mu}_{ang} \qquad (8.8)$$

$\overline{\mu_{ang}}$ is the labor average cosine calculated from the given mass angular distribution. The above scattering probability is corrected with the retrieved average cosine i.e.

$$\bar{w}_s(\mu) = w_s(\mu) + \frac{3}{2} (\overline{\mu_{ret}} - \overline{\mu_{ang}}) P_1(\mu) \qquad (8.9)$$

and the correction to a transfer matrix element is

$$\Delta \pi_{\ell}(E \to n) = \frac{3}{2}(\bar{\mu}_{ret} - \bar{\mu}_{ang}) \int_{\mu_{n+1}}^{\mu_n} d\mu \; P_{\ell}(\mu) \; P_1(\mu) \qquad (8.10)$$

where (μ_n, μ_{n+1}) is the angle interval in the laboratory system belonging to the scattering from E into the group N.
Formula (8.10) is always used for the calculations.

8.4 Strategy of the extrapolation

It may occur that for a cross-section or angular distribution the energy interval given on the KEDAK library does not cover the whole energy range of the group system. In this case a message is printed out and the functional values are taken equal to the corresponding boundary value (horizontal extrapolation).

8.5 Description of the routines

In this chapter a brief description of the purpose and the argumentlists of the programmes of module 9 of MIGROS-3 will be given. The meaning of each variable of the argumentlists is explained once: the first time they occur.

Module 9 only has one working array (WØRK, IWØRK) for storing the results and other variables dynamically. The contents of this array is described in Table VIII.All the results are transfered within the system with the help of (WØRK, IWØRK)

8.5.1 List of the programmes[+)]

Name	Purpose
REMØ	main control program
REMP	Control program for groupwise calculation

[+)] (F) means FUNCTIØN, otherwise SUBRØUTINE

Name	Purpose
KEDDAT DATNUM KEDLEC NIVNUM	Data retrieval from the KEDAK Library
AUSGL	Correction of a groupwise energy mesh
MASSIN	Initialisation of mass dependent quantities
ENERG	Calculation of groupwise energy intervals
ØRDNI	Sorting the members of an array in increasing order
SEARCH	Organisation of the output of scalar group constants
SUCHM	Organisation of the output of transfer matrices
SINT	Calculation of scalar group constants
FXINT	Integration by trapezoidal rule
ISOFAL	Organisation of the groupwise calculation of elastic transfer probabilities
WAHRS	Organisation of the subdivision of an energy interval according to the principle in chapter 8.2
LMI	Calculation of the transferprobabilities
ANINT(F)	Calculation of the integral (8.5)
AMESH	Subdivision of an angle interval
IRDMES	Initialisation of the polynomial roots
INTEN	Interpolation of angular distributions
AKØR	Calculation of the average cosine correction for (8.9)
BCM(F)	Cosine of scattering angle in centre of mass system
PTL(F)	Calculation of Legendre polynomials
WINK(F)	Calculation of $\gamma(\mu)\sigma_s$
IPOL	Interpolation of angular distributions of elastically scattered neutrons
HIDR	Calculation of integral (8.5) for the hydrogen case
LININT	array-wise linear interpolation
FIPOL(F)	point-wise linear interpòlation
NØRM	Normalisation of angular distribution
SMØRN	Normalisation of transfer probabilities

Name	Purpose
ZWIN	Determination of the boundaries of an energy range
ICSOP(F)	Determination of the groupnumber of an energy point
IWØ(F)	Getting integer from an array
IWIN	Storing integer in an array
EGRENZ	Dummy routine
ANG	Calculation of formula (8.6-b)

8.5.1 Purpose and argumentlists of the routines

+ Module 9 is entered at the SUBROUTINE REMO (NG,ABN,NSP,F,E,ERR,NLA,NLE, NGRE,NFG,NFI,NJM,NUJM,ISEL,IWORK,WORK,L)

with

NG	The number of energy boundaries
ABN(I),I=1, NG	The energy group boundaries /eV/
NSP	The number of energy points for the neutron spectrum
F(I),I=1, NSP	The neutron spectrum
E(I),I=1, NSP	Energy points for the neutron spectrum
ERR	The error limit for the Romberg integration
NLA,NLE	The first and the last moment to be calculated
NGRE	The number of groups to be calculated
NFG(I),I=1,NGRE	The number of finegroups
NFI(I),I=1,NGRE	The number of fine-intervals per fine-group
NJM	The maximum number of mesh points for angle integration is 2**NJM+1
NUJM	The maximum number of mesh points for energy integration is 2**NUJM+1
ISEL	= 1: The formula (8.3) will be computed 0: The fomula to be obtained from (8.3), when $\sigma_s(E) = 1$, will be computed
IWORK(I),WORK(I)I=1,L	Work-array. IWØRK and WØRK must be the same array in the calling program
L	The length of the work-array

The routine REMO performs the following tasks:

- to determine and to store the controlinformation of TABLE VIII in the array WØRK. For this purpose the KEDDAT entries NIVNUM and DATNUM and the routine MASSIN are called.

- to retrieve the angular distributions in the energy range to be calculated from the KEDAK library with the KEDDAT entry KEDLEC.

- to determine the needed length and compare with the available length of the array WØRK.

- to call the subroutine REMP for the groupwise calculations.

+ SUBROUTINE REMP(ABN,IGR,NFI,FLUX,EFLUX,WØRK,IWØK,IS)

ABN and NFI are defined in REMØ.

IGR	is identical with NFG	} in REMØ
FLUX	is identical with F	
EFLUX	is identical with E	

IS is the lowest energy group for which angular distributions are available

In REMP the calculations are organised groupwise. The following tasks are carried out:

- to establish the energy group- and intervalstructure with the routine ENERG

- to retrieve the nuclear data from the nuclear library KEDAK for the data types SGT, SGN and MUEL with the routine KEDDAT.

- to determine the final energy meshpoints for the calculations from the available data for SGT, SGN and MUEL. All different energy points and the groupboundaries are taken. These points are sorted by the routine ØRDN1.

- to interpolate the datatypes SGT, SGN and MUEL for the final energy array with the routine LININT.

- to calculate the group averaged quantities of formula (8.1) and (8.2) with the routine SINT

- to call the organisation program for the transfer matrices ISOFAL

- to call the output organisation routines SEARCH and SUCHM

+ The retrieval of the data from the KEDAK library is organised by the routine KEDDAT with the special entries DATNUM, NIVNUM and KEDLEC

SUBRØUTINE KEDDAT (NAMIZ,NAMTYP,NW,NW1,FNW,NDAT,FA,FF,EP,*,*,*)

NAMIZ /8-bytes/	name of the material
NAMTYP /8-bytes/	data type name
NW	if there is a further name the sequential number of the required namecombination, otherwise without meaning.
NW1	if there is a further name then the number of retrieved name combination, otherwise without meaning.
FNW	if there is a further name then its value, otherwise without meaning.
NDAT	the number of retrieved data pairs.
FA(I),I=1,NDAT	argument values
FF(I),I=1,NDAT	function values
EP,EM	upper and lower energy boundary [ev], for which the cross-section values are to be retrieved.

ENTRY DATNUM (NAMIZ,NAMTYP,NDAT,NW,EP,EM,*,*,*)
This entry is used when only NDAT is to be determined.

ENTRY KEDLEC (NAMIZ,NAMTYP,NW1,EA,IAE,EPW,EMW,FA,FF,FAW,FFW,EP,EM,*,*,*)
This entry is used to retrieve angular distributions in the energy interval [EPW, EMW] [eV].
In this case EP, EM are not energy but cosine of the scattering angle.

EA(I),I=1,NW1 the energy points
IEA(I),I=1,NW1 the number of angle points per angular distribution
FAW(I),I=1,NW1xNDAT the angle points of angular distributions
FFW(I),I=1,NW1xNDAT the angular distributions (in one field,one by one)

ENTRY NIVNUM (NAMIZ,NAMTYP,NW1,EPW,EMW,EFR,*,*,*)
EFR is the energy for the first angular distribution. This entry is used for the determination of NW1 and EFR.

The dataretrieval from the KEDAK library is performed with the standard retrieval package NDF. If no KEDAK data is available for a material or a data type the RETURN 1 statement is carried out.
In the present version RETURN 2 and RETURN 3 are defined in the argument-lists, but are not used in the program.

Further the subroutine AUSGL is called by KEDDAT in order to correct the retrieved energy meshpoints.

+ SUBRØUTINE AUSGL(NDAT,EM,EP,FA,FF)

The arguments are explained in KEDDAT.
The input of AUSGL are NDAT datapoints with argument values FA and function values FF and the following properties:

$$FA(1) \leq EM$$

$$FA(NDAT) \geq EP$$

In AUSGL

$$FA(1) = EM$$

$$FA(NDAT) = EP$$

with corresponding interpolation of FF is carried out. In the case that

$$\left| \frac{FA(2) - FA(1)}{FA(1)} \right| \leq 10^{-6} ,$$ the point FA(2)

and

$$\left|\frac{FA(NDAT) - FA(NDAT-1)}{FA(NDAT)}\right| \leq 10^{-6}, \quad \text{the point FA(NDAT-1)}$$

are omitted to avoid difficulties during the RØMBERG integration.

+ SUBRØUTINE MASSIN(WØRK,ABN)

WORK and ABN are defined in REMØ.
The routine MASSIN gets the mass of the desired material from KEDAK and calculates often used mass dependent quantities and stores them into the array WØRK (see TABLE VIII).

Moreover in MASSIN a transformation of the roots of the Legendre polynomials is performed and the results are transferred to the subroutine AMESH with the help of the entry IRDMES.

+ SUBRØUTINE ENERG(NFG,NFI,EM,EP,E)

NFG and NFI are defined in REMØ
EM and EP are defined in KEDDAT
E REAL*8 array with results

ENERG is the centralized subroutine for the groupwise calculation of the group- and interval boundaries. The result has double precision.

+ SUBRØUTINE ØRDN1(KMAX,FELD)

KMAX number of values to be sorted
FELD(KMAX) array with input values

The routine ØRDN1 sorts the first KMAX members of the array FELD in increasing order .

+ SUBRØUTINE SEARCH(NFG,NFI,WØRK,IWØRK,FLUX,EFLUX,ENERG)

NFG,NFI,WØRK,IWØRK are defined in REMØ
FLUX is identical with F
EFLUX is identical with E
} in REMØ
ENERG REAL*8 array with group- and intervalboundaries

In the routine SEARCH the output of the scalar groupconstants $\langle\sigma_t\rangle$, $\langle\sigma_s\rangle$ and $\langle\mu_s\rangle$ is organized and performed groupwise.

+ SUBRØUTINE SUCHM(NFG,NFI,IWØRK,WØRK,MØM,ABN)

NFG,NFI,WØRK,IWØRK and ABN are defined in REMØ

MØM	Moment of the Legendre Polynomials, used for the storing formats.

The routine SUCHM organizes the output of the transfer probability matrices.

+ SUBRØUTINE SINT(NG,NI,FLUX,EFLUX,WØRK,N,N4,ENERG)

NG	is identical with NFG	in REMØ
NI	is identical with NFI	
FLUX	is identical with F	
EFLUX	is identical with E	
WØRK	is defined in REMØ	
ENERG	is defined in SEARCH	
N4	Index of WØRK of the actual energy mesh	
/N/	Index of WØRK of the functional values to be integrated by the trapezoidal rule.	
	if N > 0 Formula (8.1) is calculated	
	N < 0 Formula (8.2) is calculated	

+ FUNCTIØN FXINT(EP,EM,SGN,ES,FLUX,EFLUX,NSP,NDAT)

EP	Upper integration boundary	
EM	lower integration boundary	
SGN(I)	functional values of the integration	
ES(I)	energy mesh points of the integration	
FLUX	is identical with F	in REMØ
EFLUX	is identical with E	
NSP	is defined in REMØ	
NDAT	total number of datapoints in ES,SGN	

The function FXINT calculates the integral

$$\int_{EM}^{EP} dE\ \sigma(E)\ F(E)$$

by the trapezoidal rule.

+ SUBRØUTINE ISØFAL(ABN,IGR2,NFII,FLUX,EFLUX,WØRK,ENERG)

ABN and WØRK	are defined in REMØ	
IGR2	is identical with NFG(I)	in REMØ
NFII	is identical with NFI(I)	
FLUX	is identical with F	
EFLUX	is identical with E	
ENERG	is defined in SEARCH	

The routine ISØFAL organises the calculation of the transfer probability matrices.

+ SUBRØUTINE WAHRS(EP,EM,IMAX,PI,ABN,NM1,NUJM,FLUX,EFLUX,TE,WØRK,EZ)

ABN,NUJM,WØRK	are defined in REMØ	
EP,EM	are defined in KEDDAT	
FLUX	is identical with F	in REMØ
EFLUX	is identical with E	
IMAX	maximum group change + 1	
NM1 NLE+1	(NLE defined in REMØ)	
PI(NM1,IMAX)	auxiliary arrays	
TE(NM1,IMAX,NUJM)		
EZ	array with energy meshpoints	

The routine WAHRS subdivides the energy interval (EM,EP) for the calculation of the integral (8.3) by the RØMBERG method.
Partial results are calculated and stored.

+ SUBRØUTINE LMI(EP,EM,E1,E2,SG1,SG2,AMU1,AMU2,IMAX,ABN,TE,NM1,NUJ,NUJM,
FLUX,EFLUX,WØRK,PER,IMAM,PL)

ABN,NUJ,NUJM,WØRK	are defined in REMØ	
FLUX	is identical with F	in REMØ
EFLUX	is identical with E	in REMØ
TE,NM1	are defined in WAHRS	
EP	upper energy boundary	$E2 \leq EM < EP \leq E1$
EM	lower energy boundary	$E2 \leq EM < EP \leq E1$
E1	upper meshpoint with	
SG1	elastic scattering cross section at anergy E1	
AMU1	average cosine at energy E1	
E2	as above for the lower meshpoint	
SG2	as above for the lower meshpoint	
AMU2	as above for the lower meshpoint	
IMAX	the maximum group change by a scattering in the interval (EM,EP)	
IMAM	is identical with IMAX in WAHRS	
PER(NM1,IMAM)	auxiliary arrays	
PL(NM1,IMAM) REAL*8	auxiliary arrays	

The routine LMI calculates transfer probabilities from the energy interval (EM,EP).

+ DØUBLE PRECISION FUNCTIØN ANINT(BU,BL,K,SG,XL,AZ,ICØS,WØRK,T,NJM)

The function ANINT calculates the integral (8.5) by the RØMBERG method.

BU	corresponds with	μ_n
BL	" "	μ_{n+1}
K	" "	k
XL(I)	" "	μ_c
SG(I)	" "	$\gamma(\mu_c)$
ICØS	number of meshpoints of XL and SG	
AZ	is calculated in LMI $(\bar{\mu}_{ret} - \frac{2}{3A}) \frac{3}{(1-\frac{3}{5A^2})}$	Part of formula (8.7)
WØRK, NJM	are defined in REMØ	
T(NJM)	auxiliary array	

+ SUBRØUTINE AMESH(B1,B2,Z,J2,NX,NL)

B1	is identical with BU	in ANINT
B2	is identical with BL	
Z	array with the zeros of Legendre polynomials	
J2	starting index of the zeros of the NL Legendre polynomial	
NX	starting index for the zeros of the (NL+1) Legendre polynomial	
NL	moment of the Legendre polynomial	

The subroutine AMESH prepares the division of the angle interval (B1,B2) according to the roots of Legendre polynomial of the order NL. The entry IRDMES(AC) initialises the array AC with preprocessed data from the roots of the first five Legendre polynomials. These initialisation takes place in the routine MASSIN.

+ SUBRØUTINE INTEN(E,SG,SGNC,EA,ICØS)

E	Energy for which the angular distribution is to be interpolated
SG	array with results
SGNC(ICØS,1)	angular distributions
EA	energy mesh points of the distributions
ICØS	number of angles

The routine INTEN performs a linear interpolation of the angular distributions at the energy E.

+ FUNCTIØN AKØR(B1,BL,K,AM)

The function AKØR calculates analytically the integral of formula (8.10).

$$AKØR = \frac{3}{2}\int_{\mu_{n+1}}^{\mu_n} d\mu \; P_\ell(\mu)\; P_1(\mu)$$

B1	corresponds with μ_n
BL	" " μ_{n+1}
K	" " ℓ
AM	is the mass of the scatterer.

+ FUNCTIØN BCM(EI,EO,WØRK)

EI	the energy of the neutron before scattering
EO	the energy of the neutron after scattering
WØRK	is defined in REMØ
BCM	gives the cosine of the scattering angle in the center of mass system

+ DØUBLE PRECISIØN FUNCTIØN PTL(N,XX)

N		Order of the Legendre polynomial
XX	REAL*8	Argument of the Legendre polynomial
PTL	REAL*8	Value of the Legendre polynomial

+ FUNCTIØN WINK(XL,SG,KJ,ICØS,AZ,AM)

XL,SG,ICØS,AZ	are defined in ANINT
KJ	control number for the anisotropy identical with IWØRK(23) see TABLE VIII
	KJ = 0 no angular distributions on KEDAK in the actual energy group
	KJ ≠ 0 angular distributions from KEDAK
AM	is identical with μ
WINK	$\gamma(\mu)$ of formula (8.5)

+ SUBRØUTINE IPØL(M,A,B,X,Y,T)

M	number of datapoints
A(M)	array with angles
B(M)	array with functional values
X	angle for which the interpolation is to be done
Y	result of the interpolation
T(M)	auxiliary array

The routine IPØL is a slightly modified version of the SUBRØUTINE IPOLIN by H. Wiese in chapter 7 of /2/. IPØL performs the pointwise interpolation of angular distributions of elastically scattered neutrons.

+ SUBRØUTINE HIDR(BU,BL,K,A,+)

BU,BL,K	are defined in ANINT	
A	result of the integral (8.5) for the material hydrogen	

Only a RETURN 1 is performed in the program.

The integral (8.5) is calculated analytically in the case of hydrogen.

+ SUBRØUTINE LININT(N,X1,Y1,M,X2,Y2)

N	number of datapoints	input
X1(N)	arguments	input
Y1(N)	functional values	input
M	number of datapoints	input
X2(M)	arguments	input
Y2(M)	functional values	output

Starting from the input N,X1,Y1 for the M arguments of array X2 the functional values are calculated by linear interpolation and stored into the array Y2.

+ FUNCTIØN FIPØL (XA,XB,XC,YA,YC)

$$FIPØL = \frac{YA\ (XC-CB) + YB(XB-XA)}{(XC-XA)}$$

FIPØL is the centralized function for pointwise linear interpolation.

+ SUBRØUTINE NØRM(J2,J1,SC,WØRK)

WØRK	is defined in REMØ
SC	array with angular distributions
J2	first angular distribution to be normalized
J1	last angular distribution to be normalized

The routine NØRM normalizes angular distributions in the array SC. If the normalisation integral cannot be calculated with the desired accuracy and the allowed number of points, the control number for anisotropy KJ=IWØRK (23) is set equal two. In this case in ANINT the angle meshpoints from KEDAK instead from AMESH are taken.

+ SUBRØUTINE SMØRN(PI,N,IM,WØRK)

WØRK	is defined in REMØ
PI(N,IM)	array with transfer matrix elements, when SMØRN is entered.
N	NLE+1 (NLE defined in REMØ)
IM	maximum group change + 1

In the routine SMØRN the calculated transfer matrices are normalized in order to get the transfer probabilities.

+ SUBRØUTINE ZWIN(KL,EP,EM,ES,J2,J1)

EP	upper energy
EM	lower energy
KL	number of energy meshpoints
ES(KL)	array with energy meshpoints
J2	largest index of the array ES fulfilling the condition ES(J2) $\leq$ EM
J1	smallest index of the array ES fulfilling the condition ES(J1) $\geq$ EP

+ FUNCTIØN ICSØP(E,ABN)

ABN	is defined in REMØ
E	energy point
ICSØP	groupnumber of the system ABN for the energy E

+ FUNCTIØN IWØ(L,IWØRK)

IWØRK	is defined in REMØ
L	index
IWØ	IWØRK(L)

+ SUBRØUTINE IWIN(L,N,IWØRK)

IWØRK	is defined in REMØ
L	index
N	number

The routine IWIN performs the statement IWØRK(L) = N.

+ SUBRØUTINE EGRENZ(E,ABN,IK,IV,WØRK)

This subroutine was intended for the inelastic scattering case. In the module 9 for the REMØ correction EGRENZ is a dummy routine.

+ DØUBLE PRECISIØN FUNCTIØN ANG(XX,GAM)

XX	Corresponds with μ_c
GAM	Corresponds with $\frac{1}{A}$
ANG	the result of equation (8.6-b)

TABLE VIII

Control information in the array (WØRK,IWØRK)

Word	Content	Comment
1	Address of EA/1/	Energy meshpoints for angular distribution
2	Address of XL/1/	Angle mesh points
3	Address of SGNC/1/	Angular distributions
4	I	The number of the actual calculated group
5	Address of SGN/1/	Elastic scattering or total cross-section
6	Address of AMU/1/	Retrieved average cosine
7	Address of ES/1/	Energy mesh points for cross-sections
8	ISEL	See input description
9	Address of SG/1/	Auxiliary array defined in ANINT
10	Address of TE/1/	Auxiliary array defined in WAHRS
11	Address of PER/1/	Auxiliary array defined in LMI
12	Address of SP/1/	Array for the storage of results
13	Address of BUF/1/	Buffer-array for output
14	NG	See input description
15	NSP	" " "
16	NLA	" " "
17	NLE	" " "
18	IMAX	Maximum group change+1
19	NJM	See input description
20	NUJM	" " "
21	ICOS	Number of angle mesh points
22	Address of the actual first free word of SP	
23	KJ	Control number of the anisotropy (see routine WINK)
24	NJ	2**NJ+1 number of mesh points to be required for angular integration
25	NDAT	Number of cross section points
26	NIV	Number of energy points for angular distribution
27	ERR	Error for RØMBERG integration procedure
28	A	
29	$((A+1)/(A-1))^2$	

TABLE VIII (cont.)

Word	Content	Comment
30	$(A+1)^2/2A$	
31	$\log\left(\left(\frac{A+1}{A-1}\right)^2\right)$	
32	Q =-0.1	
33	Address of T/1/	REAL*8 Auxiliary array defined in ANINT
34	Address of PL/1/	REAL*8 Auxiliary array defined in LMI
35	Address of E/1/	REAL*8 array with groupwise energy boundaries defined in ENERG
36	NMAX	The maximum number of datapoints of one of the datatypes SGT,SGN or MUEL within an energy group

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MIGRØS-2. A Program written in FØRTRAN for the Calculation of Microscopic Group Constants from Nuclear Data.

KFK 1784 (1973)

9. The calculation of average group cross sections for infinite dilution and of energy resonance self-shielding factors from energy pointwise data. Module 3 (FSTRUK).[+)]

9.1 Introduction

The calculation of the group constants defined in the following has originally done by a module written by B. Krieg and described in /1/. The results of this module showed in general good agreement with results obtained from other sources. But in some cases discrepancies (about 10 %) occurred.The reason for this effect was a not sufficient dense storage of the energy points of the cross sections on the used library.

By this presupposition of a sufficient dense energy grid, it was possible, that the structure of a pointwise given weighting function has been overlooked by the program, or that by using the trapezoidal rule, the numerical value of an integral has been calculated with unsufficient accuracy.

Number and largeness of the discrepancies increased, when due to limited storage the use of a common energy grid on KEDAK (/2/ and /3/) for all cross sections types of the form Q = F(E), could not longer be hold. Because the program has relied upon this assumption, only the energy points of a specified cross section type have been used as integration base. This can induce big errors, if another cross section type, which is participating in the function to be integrated, has - within the integration range - a different energy grid with great fluctuations of the cross section values.

Due to the reasons given in the preceding we have decided to revise this module 3. Attempts in this direction showed, that it would be more effective to reprogram this module and by doing this also to use new methods in solving the problems.

[+)] This chapter has been written completely new, because the program, described by this chapter, has also been rewritten. Compared with the old program the program described here is using other methods in solving the problem. Yet the formulaes defining the physical quantities, are identical to those given by B. Krieg, H. Huschke in /1/.

In the following, first the physical quantities to be calculated are defined. Afterwards a description of the program is given.

9.2 Definition of the quantities calculated by the program

Starting with pointwise data the program FSTRUK calculates energetic self shielding factors and average group cross sections for infinite dilution. Flux and current weighting is used.

For simplification of the formulaes the following definitions are used. If E_ℓ and E_h are two energy group boundaries with $E_\ell < E_h$, then we define

$$< y(E) > \equiv \frac{1}{E_h - E_\ell} \int_{E_\ell}^{E_h} y(E)dE \qquad (1)$$

We also define

$$\begin{aligned} x &= \text{type of neutron reaction } (n,x) \\ g &= \text{number of the energy group} \\ \sigma_o &= \text{background cross section} \end{aligned} \qquad (2)$$

All these definitions are related to a specified isotope. But for simplification we have neglected the corresponding index.

Flux weighted resonance self shielding factor are calculated for

capture (reaction (n,c) = total absorption-fission, type name FC[+)] for fissionable resp. FA for non fissionable materials),

elastic scattering (reaction (n,e), type name FN)

and

fission (reaction (n,f), type name FF):

[+)] These type names FC, FA, FN,... are used in the print output of the program and in the general parts of this report.

$$f_{x,g}(\sigma_o) = \frac{\sigma_{x,g}(\sigma_o)}{\sigma_{x,g}(\sigma_o \to \infty)} \tag{3}$$

with

$$\sigma_{x,g}(\sigma_o) = \frac{\left\langle \frac{\sigma_x(E) \cdot F(E)}{\sigma_t(E) + \sigma_o} \right\rangle}{\left\langle \frac{F(E)}{\sigma_t(E) + \sigma_o} \right\rangle} \tag{4}$$

F(E) means tne weighting function, $\sigma_t(E)$ the total microscopic cross section and $\sigma_x(E)$ - according to the desired self shielding factor - the microscopic capture cross section σ_c (resp. σ_a), the microscopic elastic scattering cross section σ_e, or the microscopic fission cross section σ_f. If the term σ_x in the formulaes (3) and (4) is replaced by $\sigma_e(E) \cdot \bar{\mu}_e(E)$, then the flux weighted self shielding factor FNO1[+)] is produced with

$$1,o f_{e,g}(\sigma_o) = \frac{\{\sigma_e \bar{\mu}_e\}\ (\sigma_o)}{\{\sigma_e \bar{\mu}_e\}\ (\sigma_o \to \infty)} \tag{5}$$

with

$$\{\sigma_e \bar{\mu}_e\}\ (\sigma_o) = \frac{\left\langle \frac{\sigma_e(E) \cdot \bar{\mu}_e(E) \cdot F(E)}{\sigma_t(E) + \sigma_o} \right\rangle}{\left\langle \frac{F(E)}{\sigma_t(E) + \sigma_o} \right\rangle} \tag{6}$$

+) See footnote on page 9.5

$\bar{\mu}_e(E)$ means the average cosine for elastic scattering.

The terms in the denominator in formulaes (3) and (5) are the group cross sections for infinite dilution. For σ_o toward infinity in the formulaes (4) and (6) - with respect to formulae (1) - we get

$$\lim_{\sigma_o \to \infty} \sigma_{x,g}(\sigma_o) = \sigma^{\infty}_{x,g} = \frac{\langle \sigma_x(E) \cdot F(E) \rangle}{\langle F(E) \rangle} \qquad (7)$$

and

$$\lim_{\sigma_o \to \infty} \{\sigma_e \bar{\mu}_e\}_g(\sigma_o) = \{\sigma_e \bar{\mu}_e\}^{\infty}_g = \frac{\langle \sigma_e(E) \bar{\mu}_e(E) \cdot F(E) \rangle}{\langle F(E) \rangle} \qquad (8)$$ +)

Replacing x in formulae (7) by c, e or f we get the following quantities:

x = c (capture) SIGMA A for non fissionable materials
SIGMA C for fissionable materials

x = e (elastic scattering) SIGMA N

x = f (fission) SIGMA F

The denomination of the quantity calculated in formulae (8) is SIGMA NO1.

All self shielding factors defined until now have been flux weighted. For the elastic scattering and the total reactions additionally the following current weighted quantities are calculated:

$${}_1f_{t,g}(\sigma_o) = \frac{{}_1\sigma_{t,g}(\sigma_o)}{{}_1\sigma_{t,g}(\sigma_{o \to \infty})} \qquad (9)$$ +)

and

$${}_1f_{e,g}(\sigma_o) = \frac{{}_1\{\sigma_e \bar{\mu}_e\}_g(\sigma_o)}{{}_1\{\sigma_e \bar{\mu}_e\}_g(\sigma_{o \to \infty})} \qquad (10)$$ +)

+) See footnote on page 9.5

The terms $_1\sigma_{t,g}(\sigma_o)$ and $_1\{\sigma_e\bar{\mu}_e\}(\sigma_o)$ are defined by the following expressions:

$$ {}_1\sigma_{t,g}(\sigma_o) = \frac{\left\langle \frac{\sigma_t(E) \cdot F(E)}{(\sigma_t(E) + \sigma_o)^2} \right\rangle}{\left\langle \frac{F(E)}{(\sigma_t(E) + \sigma_o)^2} \right\rangle} \qquad (11) $$

and

$$ {}_1\{\sigma_e\bar{\mu}_e\}_g(\sigma_o) = \frac{\left\langle \frac{\sigma_e(E) \cdot \bar{\mu}_e(E) \cdot F(E)}{(\sigma_t(E) + \sigma_o)^2} \right\rangle}{\left\langle \frac{F(E)}{(\sigma_t(E) + \sigma_o)^2} \right\rangle} \qquad (12) $$

The quantity defined in formulae (9) will be found in the program output headed with FT1, whereas the quantity defined in formulae (10) will be found under the heading FN1. Doing the limit for σ_o toward infinity in the formulaes (11) respectively (12) we get expressions similar to those in formulaes (7) and (8).

$$ {}_1\sigma^{\infty}_{t,g} = \lim_{\sigma_o \to \infty} {}_1\sigma_{t,g}(\sigma_o) = \frac{\langle \sigma_t(E) \cdot F(E) \rangle}{\langle F(E) \rangle} \qquad (13) $$

and

$$ {}_1\{\sigma_e\bar{\mu}_e\}^{\infty}_g = \lim_{\sigma_o \to \infty} {}_1\{\sigma_e\bar{\mu}_e\}_g = \frac{\langle \sigma_e(E) \cdot \bar{\mu}_e(E) \cdot F(E) \rangle}{\langle F(E) \rangle} \qquad (14) $$

+) The quantities in formulaes (5) and (8) respectively (10) and (14) are used, together with other quantities, to determine the transport cross section. For consistent transport and diffusion calculations the current weighting (see formulaes 10 and 14) should be used. But remember that for average cross sections for infinite dilution there is no difference between flux or current weighting.
The quantities in formulaes (9) and (13) are used to calculate the total current weighted cross section.

This current weighted average group cross sections for infinite dilution are named in the program with SIGMA T1 ($_1\sigma^{\infty}_{t,g}$) respectively SIGMA N1 ($_1\{\sigma_e\bar{\mu}_e\}^{\infty}_g$). If we compare formulae (13) with formulae (7), and formulae (14) with formulae (8), we see, that there is no difference for the average cross sections for infinite dilution between flux and current weighting. Therefore the following statement is valid:

$$\text{SIGMA N1} = {}_1\{\sigma_e\bar{\mu}_e\}^{\infty}_g = \{\sigma_e\bar{\mu}_e\}^{\infty}_g = \text{SIGMA NO1} \tag{15}$$

9.3 Numerical calculation of the integrals

A central task of FSTRUK is to calculate the integral defined in formulae (1). Therefore we will describe in this section, how we have solved the problem to determine the numerical value of

$$\int_{E_\ell}^{E_h} y(E)dE \tag{16}$$

One can see in the preceding section 9.2 that y(E) is normally composed out of several functions. For example y(E) may be $\sigma_e(E)\cdot\bar{\mu}_e(E)\cdot F(E)$ or $\frac{\sigma_t(E)\cdot F(E)}{(\sigma_t(E)+\sigma_o)^2}$ or simply F(E). The cross sections ($\sigma_e(E)$, $\sigma_t(E)$,...) are given pointwise (see KEDAK /2/ and /3/), whereas F(E) may be given as an analytical expression or also pointwise. The cross sections can - according to KEDAK conventions - predicted by linear interpolation between two adjacent energy values. We assume that this is also the case for the pointwise given weighting function.

If we take a specific cross sections (or the pointwise weighting function), then it follows that this quantity can be represented in the interval $[E_\ell, E_h]$ by a set of straight line equations $y = a_i \cdot E + b_i$ with a_i and b_i defined in the interval $[E_i, E_{i+1}]$. E_i and E_{i+1} are adjacent energy points at which the specific cross sections (or the pointwise weighting function) are stored resp. given. The formation of the composite function y(E) out of the partial functions is best shown in an example. Assuming E_ℓ = 1 eV, E_h = 2.15 eV (group 23 in the ABN-group set) and $y(E) = \sigma^1(E) \cdot \sigma^2(E)$. The two cross section types σ^1 and σ^2 are given at the following energy points:

σ^1: E_i^1 = 1.0 eV, 1.2 eV, 1.5 eV, 2.0 eV, 2.5 eV.

σ^2: E_i^2 = 0.8 eV, 1.2 eV, 1.4 eV, 1.6 eV, 1.8 eV, 2.0 eV, 2.2 eV.

We calculate for both cross section types the a_i and b_i:

cross section type: σ^1		
Interval [eV]	i	a, b
1.0-1.2	1	a_1^1, b_1^1
1.2-1.5	2	a_2^1, b_2^1
1.5-2.0	3	a_3^1, b_3^1
2.0-2.15	4	a_4^1, b_4^1

cross section type: σ^2		
Interval [eV]	i	a, b
1.0-1.2	1	a_1^2, b_1^2
1.2-1.4	2	a_2^2, b_2^2
1.4-1.6	3	a_3^2, b_3^2
1.6-1.8	4	a_4^2, b_4^2
1.8-2.0	5	a_5^2, b_5^2
2.0-2.15	6	a_6^2, b_6^2

If there are no energy points stored corresponding to the lower or upper group boundary, the next point near the boundary (next means less at the beginning and greater at the end) is taken to calculate the a_i and b_i. It is evident that this a_i and b_i are also valid in the minor interval until the group boundary.

To get the function y(E) all the energy values of the various participating cross sections are taken and a new energy grid is composed. Equal or nearly equal[+)] values are taken only once. In the case of nearly equal values the minor one is taken.

In the new energy grid we can now define the function y(E). In our example it is a quadratical polynomial, as shown in the following table:

Interval [eV]	y(E)
1.0 - 1.2	$(a_1^1 \cdot E + b_1^1) \cdot (a_1^2 \cdot E + b_1^2)$
1.2 - 1.4	$(a_2^1 \cdot E + b_2^1) \cdot (a_2^2 \cdot E + b_2^2)$
1.4 - 1.5	$(a_2^1 \cdot E + b_2^1) \cdot (a_3^2 \cdot E + b_3^2)$
1.5 - 1.6	$(a_3^1 \cdot E + b_3^1) \cdot (a_3^2 \cdot E + b_3^2)$
1.6 - 1.8	$(a_3^1 \cdot E + b_3^1) \cdot (a_4^2 \cdot E + b_4^2)$
1.8 - 2.0	$(a_3^1 \cdot E + b_3^1) \cdot (a_5^2 \cdot E + b_5^2)$
2.0 - 2.15	$(a_4^1 \cdot E + b_4^1) \cdot (a_6^2 \cdot E + b_6^2)$

If we generalize this method, we can define y(E) for all cases (appearing in the preceding chapter) over an energy grid, contructed in the same manner as in the example. By this subdividing of the integration range we can transform the integral (16) as shown in the following:

+) Nearly equal will be defined in the following.

$$\int_{E_\ell}^{E_h} y(E)dE = \int_{E_1}^{E_2} y_1(E)dE + \int_{E_2}^{E_3} y_2(E)dE + \ldots\ldots$$

$$+ \int_{E_{n-1}}^{E_n} y_{n-1}(E)dE \qquad (17)$$

with

$$E_1 = E_\ell,\ E_n = E_h;\quad E_i < E_{i+1} \text{ for } i = 1,2,\ldots,\ n-1;$$

$$\left[\overline{E_\ell},\ E_h\right] = \left[\overline{E_1},\ E_2\right] + \left[\overline{E_2},\ E_3\right] + \ldots + \left[\overline{E_{n-1}},\ E_n\right]$$

Each of this subintegrals

$$\int_{E_i}^{E_{i+1}} y_i(E)dE \qquad (18)$$

can now be calculated in a very simple way, because a rule to calculate $y_i(E)$ exists for each value of E in the interval $\left[\overline{E_i},\ E_{i+1}\right]$. By summation of the subintegrals, we will get the total integral. The subintegrals can be calculated by numerical methods or, if the expression of the weighting function is known, also analytically. Before this will be shown in part 9.4 and 9.5, we must first define the expression "nearly equal". Due to numerical reasons it is not desirable to deal with very small intervals. Therefore points with very close energy distance are regarded as one point, and only the lower value is taken. Two points E_a and E_b are "nearly equal", if they fulfill the condition

$$\frac{|E_a - E_b|}{\max(|E_a|,\ |E_b|)} \leq \varepsilon \qquad (19)$$

max means the maximum value. The value of ε depends from the number representation accuracy of the specified computer. In the version running on the IBM/370 model 168 of the GfK, ε has the value 1.0E-6.

9.4 Romberg integration

For the calculation of the integrals (18) we have choosen the trapezoidal rule in connection with the Romberg extrapolation method (/4/). A modified subroutine of the SSP (Scientific Subroutine Package) from IBM (/5/) has been used.

We assume, that the Romberg method is known. If not, a description can be found e.g. in /4/ or in the numerical mathematics literature. Because of our assumption we will only describe special features of the used method.

For each bisection of the integration interval an approximation of the integral is calculated. These approximations are compared. The process will stop, if the changes will be small enough. The process will also stop, if the changes, which normally become smaller, will increase, whereby one times an increase will be tolerated. By this, we avoid an endless running of the program due to rounding errors.
The tests on the desired accuracy or on the occurance of rounding errors will be switched on normally after some bisections of the integration interval. The number of this bisections depends on the size of the interval. For very small ones all tests will start after the first bisection. By this method we avoid unnecessary calculation expense.

The results of the integration can be divided into three classes:

class 1: desired integration error has been reached.
Tests have been started after the first bisection.

class 2: desired integration error has been reached.
Tests have been started after some (defined in the routine) bisections. This is the normal case.

class 3: desired integration error has not been reached because of rounding errors.

The Romberg integration is controlled by the values of the variables given in BLOC 31 (see input description 2.1.1). The iteration is stopped if the absolute relative difference is less or equal EPSROM. In the case of a termination of the process, before the error has reached the value EPSROM, a printout in the routine is done, if this actual error is DRINWA-times greater than EPSROM. If BLOC 31 is not given in the input, the values EPSROM = 5.0E-5 and DRINWA = 5.0 are used.

9.5 Analytical integration

If the analytical representation for the weighting function F(E) is known, we can try to solve the integrals (18) by an analytic expression. This is done in the program for two weighting functions: first for the pointwise given weighting function, which can be represented as straight lines, and second for the function F(E) = 1/E. Regarding the equations in 9.2 we can see that the general form for $y_i(E)$ is

$$y_i(E) = \frac{h_3E^3 + h_2E^2 + h_1E + h_o}{(r_1E + r_o)^n} \qquad n = 0,1,2 \qquad (20)$$

for the pointwise given weighting function and

$$y_i(E) = \frac{h_2\,E^2 + h_iE + h_o}{E\,(r_1\,E + r_o)^n} \qquad n = 0,1,2 \qquad (21)$$

for the 1/E-weighting. The terms h_3, h_2, h_1, h_o, r_1 and r_o are determined by the a and b of the contributing functions and by σ_o

The integration of these functions is not very difficult. But it generates very extended expressions.For example, if using $y_i(E)$ from formulae (20) with n = 2 and the prepositions r_1 and r_o not equal zero, and $(r_1E + r_o)$ not changing sign in the integration range, we get:

$$\int_{E_i}^{E_{i+1}} y_i(E)dE = \int_{E_i}^{E_{i+1}} \frac{h_3E^3 + h_2E^2 + h_1E + h_o}{(r_1E + r_o)^2}\, dE$$

$$= \left[\frac{h_3}{r_1^4} \left(\frac{1}{2}(r_1E + r_o)^2 - 3\, r_o(r_1E + r_o) \right.\right.$$

$$\left. + 3\, r_o^2 \cdot \log(r_1E + r_o) + \frac{r_o^3}{r_1E + r_o} \right)$$

$$+ \frac{h_2}{r_1^3} \left((r_1E + r_o) - 2\, r_o \log(r_1E + r_o) - \frac{r_o^2}{r_1E + r_o} \right)$$

$$+ \frac{h_1}{r_1^2} \left(\frac{r_1}{r_1E + r_o} + \log(r_1E + r_o) \right)$$

$$\left. - \frac{h_o}{r_1} \frac{1}{r_1E + r_o} \right] \Bigg|_{E_i}^{E_{i+1}}$$

Integrating the other functions we get similar expressions. But it will be shown in the following that it is in some cases numerically very difficult to evaluate these expressions.

9.6 Output of the program for non fissionable and fissionable materials

The output of the program is different whether the material is fissionable or not. A material is regarded as fissionable by the program, if the cross section type σ_f can be found in the data base KEDAK. In the other case the material is regarded as non fissionable.

For non fissionable materials the following quantities are calculated by the program:

SIGMA A, SIGMA N, SIGMA NO1, SIGMA N1, SIGMA T1,
FA, FN, FNO1, FN1, FT1

For fissionable materials the following quantities are produced:

SIGMA C, SIGMA N, SIGMA F, SIGMA NO1, SIGMA N1, SIGMA T1
FC, FN, FF, FNO1, FN1, FT1.

(The meaning of the names can be found in 9.2.)

The self shielding factors are calculated in both cases for all defined σ_o-values.

9.7 Replacing the program built in weighting function 1/E

If the weighting function is not given pointwise, or if it is demanded in the control input, MIGROS-3 uses a built-in function, which generates 1/E. This function must be given in single precision (name PHI) and in double precision (name DPHI) (see 1.4.2). Normally the single precision function is used in MIGROS-3. But the program FSTRUK described here, demands a double precision function. Therefore if one desires to change this function, one has to add a single and double version of this function in a compile-, link- and go-step. This job must have the following job control cards:

```
// (job card)
/* (Setup-card (s) for the disk containing the KEDAK library and eventually
   other disks.)
// EXEC FHCLG,LIB=NUSYS
//C.SYSIN DD *
    (new functions PHI and DPHI)
/*
//L.SYSIN DD *
 INCLUDE LOAD(MIGROS3)
 INCLUDE OBJ(MIGROS3)
/*
          (Necessary DD-cards and control input for
           the go-step.)
//
```

9.8 Selection of different weighting functions and integration modes independent of the group boundaries

In the program FSTRUK the user can subdivide the whole energy range, given by the energy groups, into subranges, in which he can define the integration mode and the weighting function. These subranges, which are independent from the energy group boundaries, must cover the whole energy range. In the now running version of the program up to five subranges are possible. This number can be increased by changing the variables MAXEBR, MIBER and increasing the array dimensions of ENBER, NWFUN and CONWFU.

In the present version of the program the following weighting functions and integration modes can be choosen: If there is no pointwise weighting function given in the input, one can select either the program built-in function DPHI (resp. PHI) - or a linked function -, or the function CONWFU(I)/E, with CONWFU(I) given in the input. If a pointwise weighting function is existent, one can additionally choose this possibility. There are two integration modes: numerical and analytical as defined in 9.4 and 9.5. But due to numerical difficulties in the evaluation of the analytically calculated integrals in some cases (especially for great σ_o-values and high energies), we recommend to use only the numerical (Romberg) integration.

The option described in this chapter is controlled by the variables given in BLOC 33 of the input description 2.1.1. If this BLOC is not given one energy range is used, in which numerical (Romberg) integration is made. If there exists a pointwise given weighting function, this will be used. If no pointwise function is available, the program built in or program linked function DPHI is used.

9.9 Error processing and test printoutput

The program generates and prints messages, warnings and errormessages, which are self explaining. Some errors will cause a termination of the program FSTRUK, e.g. negative total cross sections.

The message

+++WARNING NDF. 3: THE DATA FOR ... 30190 ARE NOT INCLUDED IN THE KEDAK LIBRARY

has no meaning in our case and can be ignored. Due to program technical reasons it can not be suppressed. In production runs not all messages, which are generated, will be printed out. But it may be useful, to have more messages printed out in test cases in order to find errors. How to switch on this option, which is normally only used by programmers to correct errors, can be seen in the input description 2.1.1 in the BLOC 32.

9.10 Short description of the subroutines of the FSTRUK-segment

In the following all subroutines of the FSTRUK-segment will be described. All the descriptions will have the following scheme:

problem solved by the routine
definition with argument list (and entry names if existant)
explanation of the quantities in the list
used common blocks (with an explanation of the quantities)
called subprograms (except those, which are FORTRAN-supplied procedures or subprograms like IBCOM).

In the explanation lists of the arguments and of the common variables the following abbreviations will be used:

in the mode column :

- I for variables which values must be defined before calling the subroutine or must be set in the common by a previous program.
- O for variables which are set in the subroutine (or in programs called by the subroutine) and used outside (and within) the subroutine.
- L for arrays (or variables) which are only used for placing some storage for the disposal of the subroutine and have only the meaning of local quantities.

IO for a combination of I and O

\- for quantities, which are not referenced in the subprogram, or non of the given classifications is true.

in the type column :

R4 for REAL*4 quantities

R8 for REAL*8 quantities

I4 for INTEGER*4 quantities

L4 for LOGICAL*4 quantities

B4 for 4 Byte quantities of any type. The actual type will be determined by additional information.

F8 for functions supplying REAL*8 values.

In the dimension column the maximal dimension of arrays will be given. For scalar quantities the word "scalar" is used.

9.10.1 Subroutine FSTRUK

Problem solved:

Calculation of energy resonance self shielding factors and of average group cross sections for infinite dilution from energy pointwise data.

Definition:

```
SUBROUTINE FSTRUK (MI,SIGO,NE,ENG,NFE,RFFE,EFE,
                   NENBER,ENBER,NWFUN,CONWFU,
                   EPSROM,DRINWA,
                   ITEST,IZPUMS,ITUMS,
                   ISPATE,
                   MIBER,GIBER,MIBERP,IIBER,CIBER,
                   FFAKT,
                   MABWF,ABWF,MABWFP,
                   MXINT,XINT,MXINTP,
                   MABQ1,ABQ1,MABQ1P,
```

MABQ2,ABQ2,MABQ2P,
MABQ3,ABQ3,MABQ3P,
KMROM,AUXROM,KMROMP,
RF,MRF,RFL,MRFP)

Explanation of the quantities in the list:

name	mode	type	dimension	remarks
MI	I	I4	scalar	number of σ_o-values
SIGO	I	R4	(MI)	σ_o-values [barn]
NE	I	I4	scalar	number of group boundaries
ENG	I	R4	(NE)	group boundaries [eV]
NFE	I	I4	scalar	number of energy points of the weighting spectrum
REFE	I	R4	(NFE)	energy points of the weighting spectrum [eV]
EFE	I	R4	(NFE)	weighting function values at the energy points of the field REFE
NENBER	I	I4	scalar	number of ranges of different weighting functions and integration modes (see BLOC 33 of the input)
ENBER	I	R4	(NENBER)	range boundaries (see BLOC 33)
NWFUN	I	I4	(NENBER)	selection of weighting functions and integration modes (see BLOC 33 of the input)
CONWFU	I	R4	(NENBER)	factor(s) in the weighting function CONWFU(I)/E (see BLOC 33 of the input)
EPSROM	I	R4	scalar	termination accuracy in Romberg integration (see BLOC 31 of the input)
DRINWA	I	R4	scalar	control of error printout in Romberg integration (see BLOC 31 of the input)
ITEST	I	I4	scalar	control of printout of messages, warnings and error messages (see BLOC 32 of the input)

name	mode	type	dimension	remarks
IZPUMS	I	I4	scalar	control of changing ITEST-conditions during the calculations (see BLOC 32 of the input)
ITUMS	I	I4	scalar	new value of "ITEST", when having changed due to IZPUMS. (see BLOC 32 of the input)
ISPATE	IO	I4	scalar	should be 0 for non fissionable and 1 for fissionable materials. But it can be redefined in the FSTRUK-segment.
MIBER	I	I4	scalar	maximum number + 1 of ranges of different weighting functions and integration modes for one group.
GIBER	L	R4	(MIBER)	range boundaries for one group. (see MIBER)
MIBERP	O	I4	scalar	necessary increase of MIBER if MIBERP is greater zero. MIBERP is always greater or equal zero.
IIBER	L	I4	(MIBER)	selection of weighting functions and integration modes within one specified group
CIBER	L	R4	(MIBER)	factor(s) in the weighting function CIBER(I)/E within one group
FFAKT	L	R4	(MI,6)	local storage for self shielding factors for one specified group
MABWF	I	I4	scalar	used for dimensioning of array ABWF
ABWF	L	R4	(MABWF,4)	representation of the pointwise given weighting function as parts of straight lines
MABWFP	O	I4	scalar	necessary increase of MABWF if MABWFP is greater than zero
MXINT	I	I4	scalar	used for dimensioning of array XINT
XINT	L	R4	(MXINT)	integration points within one group or within subintervals in this group
MXINTP	O	I4	scalar	necessary increase of MXINT if MXINTP is greater than zero
MABQ1	I	I4	scalar	used for dimensioning of array ABQ1
ABQ1	L	R4	(MABQ1,4)	representation of the cross section types σ_t, σ_a, σ_e or σ_f as parts of straight lines.

name	mode	type	dimension	remarks
MABQ1P	O	I4	scalar	necessary increase of MABQ1 if MABQ1P is greater zero
MABQ2	I	I4	scalar	used for dimensioning of array ABQ2
ABQ2	L	R4	(MABQ2,4)	representation of the cross section type μ_e as parts of straight lines.
MABQ2P	O	I4	scalar	necessary increase of MABQ2 if MABQ2P is greater zero
MABQ3	I	I4	scalar	used for dimensioning of array ABQ3
ABQ3	L	R4	(MABQ3,4)	representation of the cross section type σ_t as parts of straight lines
MABQ3P	O	I4	scalar	necessary increase of MABQ3 if MABQ3P is greater zero
KMROM	I	I4	scalar	KMROM-1 = maximum number of bisections in Romberg integration.
AUXROM	L	R8	(KMROM)	array used in Romberg integration
KMROMP	O	I4	scalar	necessary increase of KMROM if KMROMP is greater zero
RF	L	R4	(MI,MRF)	auxiliary array for storing σ_o-dependent-integral results
MRF	I	I4	scalar	must have the value 7 for non fissionable and the value 8 for fissionable materials. If it has not the correct value, MRFP is set bo 1, ISPATE is set to the correct value and a RETURN to the calling program is done.
RFL	L	R4	(MI,MRF)	local storing of RF-values
MRFP	O	I4	scalar	normal O. Is set to 1, if MRF (and ISPATE) has had a wrong value (see MRF description).

Used common blocks (with an explanation of the quantities):

name of the common block: BLANK COMMON					
name	mode	type	dimension	word	remarks
MAT	I	R8	scalar	1	name of the material
MR3	-	I4	(2)	3	dummy array. Not used in FSTRUK
NOUTP	I	I4	scalar	5	unit number for print output
JA	-	I4	scalar	6	external storage number for the output of the results. Not used in this subroutine.
NANF	I	I4	scalar	7	number of the first energy group
NEND	I	I4	scalar	8	number of the last energy group
KL	IO	I4	scalar	9	at the end of each module, KL must be enlarged by one.

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
TEST1	O	L4	scalar	1	control of test printout
TEST2	O	L4	scalar	2	control of test printout
TEST3	O	L4	scalar	3	control of test printout
LERMSG	O	L4	scalar	4	control of σ_o-dependent test and error printout
GLSCH	O	R4	scalar	5	two numbers a and b are considered as equal, if $\frac{\lvert a-b\rvert}{\max(\lvert a\rvert,\lvert b\rvert)} \leq$ GLSCH or if a = b = 0.
MNFTYP	O	I4	scalar	6	maximum value of NFTYP
NFTYP	O	I4	scalar	7	mode of integration and type of the weighting function

name of the common block: CFSTRU (continued)					
name	mode	type	dimension	word	remarks
ITYP	O	I4	scalar	8	type of the function to be integrated
ITYPFU	O	I4	scalar	9	subtype of the function to be integrated
UGR	O	R4	scalar	10	lower limit of the integration range
OGR	O	R4	scalar	11	upper limit of the integration range
CONST	O	R4	scalar	12	constant in the weighting function CONST/E
NR1	-	I4	(8)	13	dummy array. Not used in FSTRUK.
BSIGO	O	R4	scalar	21	actuell σ_o-value

name of the common block: CFSDUR					
name	mode	type	dimension	word	remarks
IDUR	IO	I4	scalar	1	number of groups for which calculations have been done in a previous subroutine-call.

Called subprograms:

FSGRAL
FSQUER
FSTRUO
FSTRU1
FSTRU2
FSTRU3
FSTRU4
FSTRU5
FSWRS9
FSWROO
FSWRO1 } (entries of FSWROO)
FSWRO2 }
FSWRO3 }
FSWRO4 }
FSXIIN (entry of FSXINT)
FSXINT

9.10.2 Subroutine FSTRUO

Problem solved:

Test and printout of some quantities.

Definition:

```
SUBROUTINE FSTRUO(NE,ENG,NANF,NEND,
                  NFE,REFE,EFE,
                  NENBER,ENBER,NWFUN,CONWFU,
                  EPSROM,KMROM,DRINWA,
                  ISPATE,
                  MIBER,MABWF,MXINT,
                  MABQ1,MABQ2,MABQ3,
                  MRF,MRFP,*,*)
```

Explanation of the quantities in the argument list:

name	mode	type	dimension	remarks
NE	I	I4	scalar	see 9.10.1 (argument list)
ENG	I	R4	(NE)	" "
NANF	IO	I4	scalar	" "
NEND	IO	I4	scalar	" "
NFE	I	I4	scalar	" "
REFE	I	R4	(NFE)	" "
EFE	I	R4	(NFE)	" "
NENBER	I	I4	scalar	" "
ENBER	I	R4	(NENBER)	" "
NWFUN	I	I4	(NENBER)	" "
CONWFU	I	R4	(NENBER)	" "
EPSROM	I	R4	scalar	" "
KMROM	I	I4	scalar	" "
DRINWA	I	R4	scalar	" "
ISPATE	IO	I4	scalar	" "
MIBER	I	I4	scalar	" "

name	mode	type	dimension	remarks
MABWF	I	I4	scalar	see 9.10.1 (argument list)
MXINT	I	I4	scalar	" "
MABQ1	I	I4	scalar	" "
MABQ2	I	I4	scalar	" "
MABQ3	I	I4	scalar	" "
MRF	I	I4	scalar	" "
MRFP	O	I4	scalar	" "
*	-	-	-	RETURN1 is done in the case of serious errors
*	-	-	-	RETURN2 is done, if MRFP is set to 1 in the subroutine

Used common blocks (with an explanation of the quantities):

```
BLANK COMMON  MAT,NR1(2),NO
COMMON/CFSTRU/ TEST1,TEST2,TEST3,LERMSG,
               GLSCH,MNFTYP,NFTYP
COMMON/CFSDUR/IDUR
```

All quantities are explained in 9.10.1. (NO is NOUTP, NR1(2) is a dummy array). The mode is I for all variables, with the exception of NFTYP, which has the mode IO.

Called subprograms:

FSTOLE
FSWRO0
FSWRO1
FSWRO2
FSWRO3
FSWRO5
FSWRO6
FSWRO7
} (entries of FSWRO0)
NDFLOC

9.10.3 Subroutine FSTRU1

Problem solved:

Test of the existance of the cross section types σ_a, σ_e, σ_t and $\bar{\mu}_e$.

Definition:

```
SUBROUTINE FSTRU1(*)
```

Explanation of the arguments:

RETURN1 is done if at least one of the cross section types σ_a, σ_e, σ_t or $\bar{\mu}_e$ is not existant.

Used common blocks (with an explanation of the quantities):

```
BLANK COMMON  MAT
COMMON/CFSTRU/TEST1,TEST2,TEST3,LERMSG
```

All the quantities are explained in 9.10.1 with all quantities having the mode I.

Called subprograms:

```
FSWR00
FSWR04      (entry of FSWR00)
NDFLOC
```

9.10.4 Subroutine FSTRU2

Problem solved:

Printing some values for the actual energy group. Setting and printing of integration ranges, integration modes and weighting functions within this group.

Definition:

```
SUBROUTINE FSTRU2(IGR,NE,ENG,NIBER,MIBER,
                  GIBER,MIBERP,IIBER,CIBER,
                  NENBER,ENBER,NWFUN,CONWFU,
                  *)
```

Explanation of the arguments:

name	mode	type	dimension	remarks
IGR	I	I4	scalar	actual group number
NE	I	I4	scalar	see 9.10.1 (argument list)
ENG	I	R4	(NE)	" "
NIBER	O	I4	scalar	number+1 of the integration rangres within the energy group
MIBER	I	I4	scalar	see 9.10.1 (argument list)
GIBER	O	R4	(MIBER)	" "
MIBERP	O	I4	scalar	" "
IIBER	O	I4	(MIBER)	" "
CIBER	O	R4	(MIBER)	" "
NENBER	I	I4	scalar	" "
ENBER	I	R4	(NENBER)	" "
NWFUN	I	I4	(NENBER)	" "
CONWFU	I	R4	(NENBER)	" "
*	-	-	-	RETURN1 is done for MIBERP > 0

Used common blocks (with an explanation of the quantities):

```
BLANK COMMON  MAT,NR1(2),NO
COMMON/CFSTRU/ TEST1,TEST2,TEST3,LERMSG,GLSCH
```

All quantities are explained in 9.10.1. NR1(2) is a dummy array. All quantities have the mode I.

Called subprograms:

```
FSTOLE
FSWR00
FSWR03      (entry of FSWR00)
```

9.10.5 Subroutine FSTRU3

Problem solved:

Representation of the pointwise given weighting function by parts of straight lines.

Definition:

```
SUBROUTINE FSTRU3(NFE,REFE,EFE,
                  NABWF,MABWF,ABWF,MABWFP,
                  *,*)
```

Explanation of the arguments:

name	mode	type	dimension	remarks
NFE	I	I4	scalar	see 9.10.1 (argument list)
REFE	I	R4	(NFE)	" "
EFE	I	R4	(NFE)	" "
NABWF	O	I4	scalar	number + 1 of straight line parts
MABWF	I	I4	scalar	see 9.10.1 (argument list)
ABWF	O	R4	(MABWF,4)	" "
MABWFP	O	I4	scalar	" "
*	-	-	-	RETURN 1 is done if MABWF has been too small. MABWFP > 0 gives the necessary increase.
*	-	-	-	RETURN 2 is done, if the energy range of the weighting spectrum does not cover the integration range.

Used common blocks (with an explanation of the quantities):

```
BLANK COMMON  NR1(4),NO
COMMON/CFSTRU/ TEST1,TEST2,TEST3,LERMSG,GLSCH,
               NR2(4),UGR,OGR
```

All quantities are explained in 9.10.1. NR1 and NR2 are dummy array. NO is NOUTP. The mode is I for all quantities.

Called subprograms:

FSTOLE
FSWRO2
FSWRO3 } (entries of FSWROO)
FSWRO7

9.10.6 Subroutine FSTRU4

Problem solved:
Groupwise calculation of self shielding factors and average cross sections for infinite dilution out of the integral values. Output of the calculated quantities.

Definition:

```
SUBROUTINE FSTRU4(ENG,NE,IGR,FFAKT,
                  MI,SIGO,
                  RPHI,RABS,RELA,RTOT,RFISS,RELFL,
                  RF,MRF,ISPATE)
```

Explanation of the arguments:

name	mode	type	dimension	remarks
ENG	I	R4	(NE)	see 9.10.1 (argument list)
NE	I	I4	scalar	" "
IGR	I	I4	scalar	actual group number
FFAKT	L	R4	(MI,6)	local storage of groupwise self shielding factors
MI	I	I4	scalar	number of σ_o-values
SIGO	I	R4	(MI)	σ_o-values
RPHI	I	R4	scalar	result of $\int_{UGR}^{OGR} F(E)dE$ (F(E) = weighting function)

name	mode	type	dimension	remarks
RABS	I	R4	scalar	result of $\int_{UGR}^{OGR} \sigma_a(E) \cdot F(E) \cdot dE$
RELA	I	R4	scalar	result of $\int_{UGR}^{OGR} \sigma_e(E) \cdot F(E) \cdot dE$
RTOT	I	R4	scalar	result of $\int_{UGR}^{OGR} \sigma_t(E) \cdot F(E) \cdot dE$
RFISS	I	R4	scalar	result of $\int_{UGR}^{OGR} \sigma_f(E) \cdot F(E) \cdot dE$
RELFL	I	R4	scalar	result of $\int_{UGR}^{OGR} \sigma_e(E) \cdot F(E) \cdot dE$
RF	I	R4	(MI,MRF)	results of integrations necessary for the calculation of the self shielding factors
MRF	I	I4	scalar	see 9.10.1 (argument list)
ISPATE	I	I4	scalar	" "

Used common blocks (with an explanation of the quantities):

```
BLANK COMMON  MAT,NR1(2),NOUTP,JA,NANF,NEND
COMMON/CFSTRU/  TEST1,TEST2,TEST3,LERMSG
COMMON/CFSDUR/  IDUR
```

All quantities are explained in 9.10.1. NR1 is a dummy array. All quantities have the mode I.

Called subprograms:

FSSNGL
FSWR00
FSWR01
FSWR02
FSWRP3
FSWR06
} (entries of FSWR00)

9.10.7 Function FSSNGL

Problem solved:

Truncation of the REAL*8 number A to the REAL*4 value FSSNGL. If necessary rounding up is done.

Definition:

```
FUNCTION  FSSNGL(A)
```

Explanation of the argument:

name	mode	type	dimension	remarks
A	I	R8	scalar	value to be truncated

Used common blocks:

No common blocks are used.

Called subprograms:

No subprograms are called.

9.10.8 Subroutine FSTRU5

Problem solved:

The contents of the array A1 is stored into the array A2.

Definition:

```
SUBROUTINE FSTRU5(A1,NA1,MA1,
                  A2,NA2,MA2,MA2P,*)
```

Explanation of the arguments:

name	mode	type	dimension	remarks
A1	I	R4	(MA1)	array of which the contents are stored in A2
NA1	I	I4	scalar	number of elements of A1 to be stored in A2
MA1	I	I4	scalar	maximum dimension of array A1
A2	O	R4	(MA2)	array which is receiving the contents of A1
NA2	O	I4	scalar	after RETURN NA2 has the same value as NA1
MA2	I	I4	scalar	maximum dimension of array A2
MA2P	O	I4	scalar	is set to NA1-MA2 if NA1 is greater than MA2
*	-	-	-	RETURN 1 is done if NA1 is greater than MA2

Used common blocks:

None

Called subprograms:

None

9.10.9 Subroutine FSQUER

Problem solved:

Retrieval of the cross sections for a specified energy group. Calculation of the straight line parameters.

Definition:

```
SUBROUTINE FSQUER(TYP,UGR,OGR
                  NAB,MAB,AB,MABP,
                  *,*)
```

Explanation of the arguments:

name	mode	type	dimension	remarks
TYP	I	R8	scalar	name of the cross section type
UGR	I	R4	scalar	lower energy limit
OGR	I	R4	scalar	upper energy limit
NAB	O	I4	scalar	number + 1 of straight line parameters
MAB	I	I4	scalar	maximal possible value for NAB
AB	O	R4	(MAB,4)	straight line parameters
MABP	O	I4	scalar	necessary increase of MAB if MABP is greater than zero
*	-	-	-	RETURN 1 is made, if the array AB has been too small
*	-	-	-	RETURN 2 is made for serious errors of the KEDAK-data

Used common blocks (with an explanation of the quantities):

```
BLANK COMMON  MAT,NR1(2),NO
COMMON/CFSTRU/  TEST1,TEST2,TEST3,LERMSG,GLSCH
```

All quantities are explained in 9.10.1. NR1 is a dummy array. NO is NOUTP. The mode for all quantities is I.

Called subprograms:

FSTOLE
FSWRO0
FSWRO2
FSWRO3
FSWRO4
FSWRO5
FSWRO6
FSWRO7
NDFLOC

(FSWRO2 … FSWRO7: entries of FSWRO0)

9.10.10 Subroutine FSWROO

Problem solved:

Control of printing messages, warnings, and error messages.

Definition:

```
SUBROUTINE   FSWROO(N)
ENTRY        FSWRO1(N,IV1)
ENTRY        FSWRO2(N,IV1,IV2)
ENTRY        FSWRO3(N,IV1,IV2,IV3)
ENTRY        FSWRO4(N,IV1,IV2,IV3,IV4)
ENTRY        FSWRO5(N,IV1,IV2,IV3,IV4,IV5)
ENTRY        FSWRO6(N,IV1,IV2,IV3,IV4,IV5,IV6)
ENTRY        FSWRO7(N,IV1,IV2,IV3,IV4,IV5,IV6,IV7)
ENTRY        FSWRO8(N,IV1,IV2,IV3,IV4,IV5,IV6,IV7,IV8)
ENTRY        FSWRO9(N,IV1,IV2,IV3,IV4,IV5,IV6,IV7,IV8,IV9)
```

Explanation of the arguments:

name	mode	type	dimension	remarks
N	I	I4	scalar	selection of the message, warning or error message.
IV1 to IV9	I	B4	scalar	additional information given to the printing routines. The type of IV1 to IV9 depends on the number N .

Used common blocks (with an explanation of the quantities):

name of the common block: BLANK COMMON					
name	mode	type	dimension	word	remarks
NR1	-	I4	(4)	1	dummy array. Not used in FSWROO .
NO	I	I4	scalar	5	print output unit number .

name of the common block: CFSTRF					
name	mode	type	dimension	word	remarks
FELARR	O	I4	(NGMAX,3)	1	storage of the message, warning and error numbers that have been appeared
NGMAX	O	I4	scalar	55	maximal possible first index in FELARR (= 18)

Called subprograms:

FSWRS1

FSWRS2

FSWRS3

9.10.11 Subroutine FSWRS1

Problem solved:

Printout of messages.

Definition:

```
SUBROUTINE FSWRS1(NI,IV1,IV2,IV3,
                  IV4,IV5,IV6,
                  IV7,IV8,IV9,*)
```

Explanation of the arguments:

name	mode	type	dimension	remarks
NI	I	I4	scalar	see 9.10.10 (argument list) argument N.
IV1 to IV9	I	B4	scalar	see 9.10.10 (argument list) .
*	-	-	-	RETURN 1 is done, if NI has an invalid value.

Used common blocks (with an explanation of the quantities):

name of the common block: BLANK COMMON					
name	mode	type	dimension	word	remarks
NR1	-	I4	(4)	1	dummy array. Not used in FSWRS1
NO	I	I4	scalar	5	print output unit number

Called subprograms:

None.

9.10.12 Subroutine FSWRS2

Problem solved:
Printout of warnings.

Definition:

```
SUBROUTINE FSWRS2(NI,IV1,IV2,IV3,
                  IV4,IV5,IV6,
                  IV7,IV8,IV9,*)
```

Explanation of the arguments:

name	mode	type	dimension	remarks
NI	I	I4	scalar	see 9.10.10 (argument list) argument N
IV1 to IV9	I	B4	scalar	see 9.10.10 (argument list)
*	-	-	-	RETURN 1 is done, if NI has an invalid value

Used common blocks (with an explanation of the quantities):

BLANK COMMON NR1(4),NO

name of the common block: BLANK COMMON					
name	mode	type	dimension	word	remarks
NR1	-	I4	(4)	1	dummy array. Not used in FSWRS2
NO	I	I4	scalar	5	print output unit number

Called subprograms: None.

9.10.13 Subroutine FSWRS3

Problem solved:

Printout of error messages.

Definition:

```
SUBROUTINE FSWRS3(NI,IV1,IV2,IV3,
                  IV4,IV5,IV6,
                  IV7,IV8,IV9,*)
```

Explanation of the arguments:

name	mode	type	dimension	remarks
NI	I	I4	scalar	see 9.10.10 (argument list) argument N
IV1 to IV9	I	B4	scalar	see 9.10.10 (argument list)
*	-	-	-	RETURN 1 is done, if NI has an invalid value

Used common blocks (with an explanation of the quantities):

BLANK COMMON NR1(4), NO

name of the common block: BLANK COMMON					
name	mode	type	dimension	word	remarks
NR1	-	I4	(4)	1	dummy array. Not used in FSWRS3
NO	I	I4	scalar	5	print output unit number

Called subprograms:

None.

9.10.14 Subroutine FSWRS9

Problem solved:
Printout of the array FELARR (see 9.10.10 explanation of the quantities in the common blocks).

Definition:

SUBROUTINE FSWRS9

Used common blocks (with an explanation of the quantities):

name of the common block: BLANK COMMON					
name	mode	type	dimension	word	remarks
NR1	-	I4	(4)	1	dummy array. Not used in FSWRS9
NO	I	I4	scalar	5	print output unit number

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
TEST1	I	L4	scalar	1	see 9.10.1 (common blocks)
TEST2	I	L4	scalar	2	" "
TEST3	I	L4	scalar	3	" "
LERMSG	I	L4	scalar	4	" "

name of the common block: CFSTRF					
name	mode	type	dimension	word	remarks
FELARR	I	I4	(NGMAX,3)	1	see 9.10.10 (common blocks)
NGMAX	I	I4	scalar	55	" "

Called subprograms:

A8FORM
RAMANF } (entries of A8FORM)
RAMEND }

9.10.15 Function FSTOLE

Problem solved:

Test of $\frac{|A-B|}{\max(|A|,|B|)} \leq$ GLSCH. If true FSTOLE is set to.TRUE., else ist is set to .FALSE.

Definition:

```
LOGICAL FUNCTION FSTOLE(A,B,GLSCH)
```

Explanation of the arguments:

name	mode	type	dimension	remarks
A	I	R4	scalar	first number
B	I	R4	scalar	second number
GLSCH	I	R4	scalar	see problem solved

Used common blocks:

None

Called subprograms:

None

9.10.16 Subroutine FSXINT

Problem solved:

Construction of the energy grid used as integration basis.

Definition:

```
SUBROUTINE FSXINT(NXINT,MXINT,XINT,MXINTP,
                  NV,V,ID1,ID2,*)
ENTRY FSXIIN(NXINT,MXINT,XINT,UGR,OGR)
```

(UGR and OGR are stored in XINT. The rest of the array is set equal -1.0).

Explanation of the arguments:

name	mode	type	dimension	remarks
NXINT	O	I4	scalar	number of energy points
MXINT	I	I4	scalar	dimension of XINT
XINT	O	R4	(MXINT)	energy grid
MXINTP	O	I4	scalar	see 9.10.1 (argument list)
NV	I	I4	scalar	number of points in V
V	I	R4	(ID1,ID2)	V(I,1) = points to be inserted in XINT, if the condition UGR $\leq$ V(I,1) $\leq$ OGR is fulfilled
ID1	I	I4	scalar	used for dimensioning V
ID2	I	I4	scalar	used for dimensioning V
*	-	-	-	RETURN 1 is done, if the array XINT is too small
UGR	I	R4	scalar	lower energy group (or integration range) boundary
OGR	I	R4	scalar	upper energy group (or integration range) boundary

Used common blocks (with an explanation of the quantities:

```
BLANK COMMON NR1(4),NO
COMMON/CFSTRU/ TEST1,TEST2,TEST3,LERMSG,GLSCH
```

All quantities are explained in 9.10.1. They have all the mode I.
NR1 is a dummy array, NO is NOUTP.

Called subprograms:

FSTOLE
FSWRO3 (entry of FSWROO)

9.10.17 Subroutine FSGRAL

Problem solved:

Control of the integration of the functions

PHI(E), F1(E)·PHI(E), F1(E)·F2(E)·PHI(E),

$$\frac{1}{F3(E)} * PHI(E), \quad \frac{1}{(F3(E))} * PHI(E),$$

$$\frac{F1(E)}{F3(E)} * PHI(E), \quad \frac{F1(E)}{(F3(E))^2} \cdot PHI(E),$$

$$\frac{F1(E) * F2(E)}{F3(E)} * PHI(E), \quad \frac{F1(E) * F2(E)}{(F3(E))^2} * PHI(E)$$

Definition:

```
SUBROUTINE FSGRAL(RESULT,NXINT,XINT,
                  NABWF,ABWF,MABWF,
                  NABQ1,ABQ1,MABQ1,
                  NABQ2,ABQ2,MABQ2,
                  NABQ3,ABQ3,MABQ3,
                  KMROM,AUXROM,KMROMP,EPSROM,DRINWA,
                  IFAR,LFAR,LFARA,
                  FARIN,FARAN,IFUNAR,*,*)
```

Explanation of the arguments:

name	mode	type	dimension	remarks
RESULT	O	R8	scalar	result of the integration
NXINT	I	I4	scalar	see 9.10.16 (argument list)
XINT	I	R4	(NXINT)	" "

name	mode	type	dimension	remarks
NABWF	I	I4	scalar	see 9.10.5 (argument list)
ABWF	I	R4	(MABWF,4)	" "
MABWF	I	I4	scalar	" "
NABQ1	I	I4	scalar	number of data in ABQ1
ABQ1	I	R4	(MABQ1,4)	see 9.10.1 (argument list)
MABQ1	I	I4	scalar	" "
NABQ2	I	I4	scalar	number of data in ABQ2
ABQ2	I	R4	(MABQ2,4)	see 9.10.1 (argument list)
MABQ2	I	I4	scalar	" "
NABQ3	I	I4	scalar	number of data in ABQ3
ABQ3	I	R4	(MABQ3,4)	see 9.10.1 (argument list)
MABQ3	I	I4	scalar	" "
KMROM	I	I4	scalar	" "
AUXROM	L	R8	(KMROM)	" "
KMROMP	O	I4	scalar	" "
EPSROM	I	R4	scalar	" "
DRINWA	I	R4	scalar	" "
IFAR	I	I4	scalar	local index for exact attachement of error appearance in a loop
LFAR	IO	L4	(2,3)	used for collected error printout
LFARA	IO	L4	(2,3)	" " " " "
FARIN	O	R4	(2,3,2)	storage of energy range for collected error printout
FARAN	O	R4	(2,3)	storage of σ_o for collected error printout
IFUNAR	O	I4	(2,3)	additional information for collected error printout
*	-	-	-	RETURN 1 is done, if AUXROM is too small
*	-	-	-	RETURN 2 is done, if there are σ_t cross section values less or equal zero

Used common blocks (with an explanation of the quantities):

name of the common block: BLANK COMMON					
name	mode	type	dimension	word	remarks
NR1	-	I4	(4)	1	dummy array. Not used in FSGRAL
NO	I	I4	scalar	5	print output unit number

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
TEST1	I	L4	scalar	1	see 9.10.1 (common blocks)
TEST2	I	L4	scalar	2	" "
TEST3	I	L4	scalar	3	" "
LERMSG	I	L4	scalar	4	" "
GLSCH	I	R4	scalar	5	" "
MNFTYP	I	I4	scalar	6	" "
NFTYP	I	I4	scalar	7	" "
ITYP	I	I4	scalar	8	" "
ITYPFU	I	I4	scalar	9	" "
NR2	-	I4	(3)	10	dummy array. Not used in FSGRAL
AW	O	R4	scalar	13	straight line parameter for weighting function
BW	O	R4	scalar	14	straight line parameter for weighting function
A1	O	R4	scalar	15	straight line parameter for σ_t, σ_a, σ_e or σ_f
B1	O	R4	scalar	16	straight line parameter for σ_t, σ_a, σ_e or σ_f
A2	O	R4	scalar	17	straight line parameter for $\bar{\mu}_e$
B2	O	R4	scalar	18	" " " "
A3	O	R4	scalar	19	straight line parameter for σ_t
B3	O	R4	scalar	20	" " " "

name of the common block: CFSTRU (continuation)					
name	mode	type	dimension	word	remarks
BSIGO	I	R4	scalar	21	actual σ_o-value
XIA	O	R4	scalar	22	lower limit of subinterval for the integration
XIE	O	R4	scalar	23	upper limit of subinterval for the integration
L	O	I4	scalar	24	points to the respective formulae for analytic integration
Y	L	R8	scalar	25	result for [XIA,XIE] integration of the functions
NDIMP	O	I4	scalar	27	if > 0 necessary increase for KMROM
DRUCKL	L	L4	scalar	28	control of printing in the case of errors

Called subprograms:

DPHI
FSANO2
FSANO3
FSANO4
FSANO5
FSANO6
FSANO7
FSANO8
FSANO9
FSEXIN
FSGRA1
FSGRA2
FSGRA3
FSNUO1
FSNUO2
FSNUO3
FSNUO4
FSNUO5
FSNUO6
FSNUO7
FSNUO8
FSNUO9
FSROMB
FSROMI (entry of FSROMB)
FSTOLE
FSWROO
FSWRO1
FSWRO3 } (entries of FSWROO)
FSWRO4
FSWRO9

9.10.18 Function FSNUO1

Problem solved:

Calculation of the function (with double precision)

AW • X + BW

(AW • X + BW is the representation of the pointwise given weighting function).

Definition:

REAL FUNCTION FSNUO1 * 8(X)

Explanation of the argument:

name	mode	type	dimension	remarks
X	I	R8	scalar	energy value for which the function is to be calculated

Used common blocks (with explanations of the quantities):

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
NR1	-	I4	(12)	1	dummy array. Not used in FSNUO1
AW	I	R4	scalar	13	straight line parameter for the weighting function
BW	I	R4	scalar	14	straight line parameter for the weighting function

Called subprograms:

None

9.10.19 Function FSNUO2

Problem solved:

Calculation of the function (with double precision)

(AW • X + BW) • (A1 • X + B1)

(AW • X + BW is the representation of the pointwise given weighting function).

Definition:

```
REAL FUNCTION FSNUO2 * 8(X)
```

Explanation of the argument:

name	mode	type	dimension	remarks
X	I	R8	scalar	energy value for which the function is to be calculated

Used common blocks (with explanations of the quantities):

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
NR1	-	I4	(12)	1	dummy array. Not used in FSNUO2
AW	I	R4	scalar	13	straight line parameter for the weighting function
BW	I	R4	scalar	14	straight line parameter for the weighting function
A1	I	R4	scalar	15	straight line parameter for σ_t, σ_a, σ_e or σ_f
B1	I	R4	scalar	16	straight line parameter for σ_t, σ_a, σ_e or σ_f

Called subprograms:

None

9.10.20 Function FSNUO3

Problem solved:

Calculation of the function (with double precision)

(AW • X + BW) • (A1 • X + B1) • (A2 • X + B2)

(AW • X + BW is the representation of the pointwise given weighting function)

Definition:

```
REAL FUNCTION FSNUO3 * 8(X)
```

Explanation of the argument:

name	mode	type	dimension	remarks
X	I	R8	scalar	energy value for which the function is to be calculated

Used common blocks (with explanations of the quantities):

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
NR1	-	I4	(12)	1	dummy array. Not used in FSNUO3
AW	I	R4	scalar	13	straight line parameter for the weighting function
BW	I	R4	scalar	14	straight line parameter for the weighting function
A1	I	R4	scalar	15	straight line parameter for σ_t, σ_a, σ_e or σ_f
B1	I	R4	scalar	16	straight line parameter for σ_t, σ_a, σ_e or σ_f
A2	I	R4	scalar	17	straight line parameter for $\bar{\mu}_e$
B2	I	R4	scalar	18	straight line parameter for $\bar{\mu}_e$

Called subprograms:

None

9.10.21 Function FSNUO4

Problem solved:

Calculation of the function (with double precision)

$$(AW \cdot X + BW) \cdot \frac{1}{A3 \cdot X + B3 + BSIGO}$$

(AW · X + BW is the representation of the pointwise given weighting function).

Definition:

REAL FUNCTION FSNUO4 * 8(X)

Explanation of the argument:

name	mode	type	dimension	remarks
X	I	R8	scalar	energy value for which the function is to be calculated

Used common blocks (with explanations of the quantities):

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
NR1	-	I4	(12)	1	dummy array. Not used in FSNUO4
AW	I	R4	scalar	13	straight line parameter for the weighting function
BW	I	R4	scalar	14	straight line parameter for the weighting function
NR2	-	I4	(4)	15	dummy array. Not used in FSNUO4
A3	I	R4	scalar	19	straight line parameter for σ_t
B3	I	R4	scalar	20	" " " " "
BSIGO	I	R4	scalar	21	σ_o-value

Called subprograms:

None

9.10.22 Function FSNUO5

Problem solved:

Calculation of the function (with double precision)

$$(AW \cdot X + BW) \cdot \frac{1}{(A3 \cdot X + B3 + BSIGO)^2}$$

(AW · X + BW is the representation of the pointwise given weighting function).

Definition:

```
REAL FUNCTION FSNUO5 * 8(X)
```

Explanation of the argument:

name	mode	type	dimension	remarks
X	I	R8	scalar	energy value for which the function is to be calculated

Used common blocks (with explanations of the quantities):

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
NR1	-	I4	(12)	1	dummy array. Not used in FSNUO5
AW	I	R4	scalar	13	straight line parameter for the weighting function
BW	I	R4	scalar	14	straight line parameter for the weighting function
NR2	-	I4	(4)	15	dummy array. Not used in FSNUO5.
A3	I	R4	scalar	19	straight line parameter for σ_t
B3	I	R4	scalar	20	" " " " "
BSIGO	I	R4	scalar	21	σ_o-value

Called subprograms:

None

9.10.23 Function FSNU06

Problem solved:

Calculation of the function (with double precision)

$$(AW \cdot X + BW) \cdot \frac{(A1 \cdot X + B1)}{(A3 \cdot X + B3 + BSIGO)}$$

(AW · X + BW is the representation of the pointwise given weighting function).

Definition:

```
REAL FUNCTION FSNU06 * 8(X)
```

Explanation of the argument:

name	mode	type	dimension	remarks
X	I	R8	scalar	energy value for which the function is to be calculated

Used common blocks (with explanations of the quantities):

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
NR1	-	I4	(12)	1	dummy array. Not used in FSNU06
AW	I	R4	scalar	13	straight line parameter for the weighting function
BW	I	R4	scalar	14	straight line parameter for the weighting function
A1	I	R4	scalar	15	straight line parameter for σ_t, σ_a, σ_e or σ_f
B1	I	R4	scalar	16	straight line parameter for σ_t, σ_a, σ_e or σ_f
NR2	-	I4	(2)	17	dummy array. Not used in FSNU06
A3	I	R4	scalar	19	straight line parameter for σ_t
B3	I	R4	scalar	20	" " " " "
BSIGO	I	R4	scalar	21	σ_o-value .

Called subprograms:

None

9.10.24 Function FSNUO7

Problem solved:

Calculation of the function (with double precision)

$$(AW \cdot X + BW) \cdot \frac{A1 \cdot X + B1}{(A3 \cdot X + B3 + BSIGO)^2}$$

(AW · X + BW is the representation of the pointwise given weighting function).

Definition:

```
REAL FUNCTION FSNUO7 * 8(X)
```

Explanation of the argument:

name	mode	type	dimension	remarks
X	I	R8	scalar	energy value for which the function is to be calculated

Used common blocks (with explanations of the quantities):

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
NR1	-	I4	(12)	1	dummy array. Not used in FSNUO7
AW	I	R4	scalar	13	straight line parameter for the weighting function
BW	I	R4	scalar	14	straight line parameter for the weighting function
A1	I	R4	scalar	15	straight line parameter for σ_t, σ_a, σ_e or σ_f
B1	I	R4	scalar	16	straight line parameter for σ_t, σ_a, σ_e or σ_f
NR2	-	I4	(2)	17	dummy array. Not used in FSNUO6
A3	I	R4	scalar	19	straight line parameter for σ_t
B3	I	R4	scalar	20	" " " " "
BSIGO	I	R4	scalar	21	σ_o-value

Called subprograms:

None

9.10.25 Function FSNUO8

Problem solved:

Calculation of the function (with double precision)

$$(AW \cdot X + BW) \cdot \frac{(A1 \cdot X + B1) \cdot (A2 \cdot X + B2)}{(A3 \cdot X + B3 + BSIGO)}$$

(AW · X + BW is the representation of the pointwise given weighting function)

Definition:

```
REAL FUNCTION  FSNUO8 * 8(X)
```

Explanation of the argument:

name	mode	type	dimension	remarks
X	I	R8	scalar	energy value for which the function is to be calculated

Used common blocks (with explanations of the quantities):

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
NR1	-	I4	(12)	1	dummy array. Not used in FSNUO8
AW	I	R4	scalar	13	straight line parameter for the weighting function
BW	I	R4	scalar	14	straight line parameter for the weighting function
A1	I	R4	scalar	15	straight line parameter for σ_t, σ_a, σ_e or σ_f
B1	I	R4	scalar	16	straight line parameter for σ_t, σ_a, σ_e or σ_f
A2	I	R4	scalar	17	straight line parameter for $\bar{\mu}_e$
B2	I	R4	scalar	18	" " " " "
A3	I	R4	scalar	19	straight line parameter for σ_t
B3	I	R4	scalar	20	" " " " "
BSIGO	I	R4	scalar	21	σ_o-value

Called subprograms

None

9.10.26 Function FSNU09

Problem solved:

Calculation of the function (with double precision)

$$(AW \cdot X + BW) \cdot \frac{(A1 \cdot X + B1) \cdot (A2 \cdot X + B2)}{(A3 \cdot X + B3 + BSIGO)^2}$$

(AW · X + BW is the representation of the pointwise given weighting function)

Definition:

```
REAL FUNCTION  FSNU09 * 8(X)
```

Explanation of the argument:

name	mode	type	dimension	remarks
X	I	R8	scalar	energy value for which the function is to be calculated

Used common blocks (with explanations of the quantities):

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
NR1	-	I4	(12)	1	dummy array. Not used in FSNU09
AW	I	R4	scalar	13	straight line parameter for the weighting function
BW	I	R4	scalar	14	straight line parameter for the weighting function
A1	I	R4	scalar	15	straight line parameter for σ_t, σ_a, σ_e or σ_f
B1	I	R4	scalar	16	straight line parameter for σ_t, σ_a, σ_e or σ_f
A2	I	R4	scalar	17	straight line parameter for $\bar{\mu}_e$
B2	I	R4	scalar	18	" " " " "
A3	I	R4	scalar	19	straight line parameter for σ_t
B3	I	R4	scalar	20	" " " " "
BSIGO	I	R4	scalar	21	σ_o-value

Called subprograms:

None

9.10.27 Function DPHI

Problem solved:

Calculation of the function (with double precision)

$$1/E$$

Definition:

REAL FUNCTION DPHI * 8(E)

Explanation of the argument:

name	mode	type	dimension	remarks
E	I	R8	scalar	energy value for which the function is to be calculated

Used common blocks:

None

Called subprograms:

None

9.10.28 Function FSANO2

Problem solved:

Calculation of the function (with double precision)

DPHI + (A1 • X + B1)

(DPHI(X) is the program built in weighting function)

Definition:

REAL FUNCTION FSANO2 * 8(X)

Explanation of the argument:

name	mode	type	dimension	remarks
X	I	R8	scalar	energy value for which the function is to be calculated

Used common blocks (with explanations of the quantities):

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
NR1	-	I4	(14)	1	dummy array. Not used in FSANO2
A1	I	R4	scalar	15	straight line parameter for σ_t, σ_a, σ_e or σ_f
B1	I	R4	scalar	16	straight line parameter for σ_t, σ_a, σ_e or σ_f

Called subprograms:

None

9.10.29 Function FSANO3

Problem solved:

Calculation of the function (with double precision)

DPHI · (A1 · X + B1) · (A2 · X + B2)

(DPHI(X) is the program built in weighting function)

Definition:

```
REAL FUNCTION FSANO3 * 8(X)
```

Explanation of the argument:

name	mode	type	dimension	remarks
X	I	R8	scalar	energy value for which the function is to be calculated

Used common blocks (with explanations of the quantities):

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
NR1	-	I4	(14)	1	dummy array. Not used in FSANO3
A1	I	R4	scalar	15	straight line parameter for σ_t, σ_a, σ_e or σ_f
B1	I	R4	scalar	16	straight line parameter for σ_t, σ_a, σ_e or σ_f
A2	I	R4	scalar	17	straight line parameter for $\bar{\mu}_e$
B2	I	R4	scalar	18	" " " " "

Called subprograms:

None

9.10.30 Function FSANO4

Problem solved:

Calculation of the function (with double precision)

$$DPHI \cdot \frac{1}{(A3 \cdot X + B3 + BSIGO)}$$

(DPHI(X) is the program built in weighting function)

Definition:

```
REAL FUNCTION FSANO4 * 8(X)
```

Explanation of the argument:

name	mode	type	dimension	remarks
X	I	R8	scalar	energy value for which the function is to be calculated

Used common blocks (with explanations of the quantities):

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
NR1	-	I4	(18)	1	dummy array. Not used In FSANO4
A3	I	R4	scalar	19	straight line parameter for σ_t
B3	I	R4	scalar	20	" " " " "
BSIGO	I	R4	scalar	21	σ_o-value

Called subprograms:

None

9.10.31 Function FSANO5

Problem solved:

Calculation of the function (with double precision)

$$DPHI \cdot \frac{1}{(A3 \cdot X + B3 + BSIGO)^2}$$

(DPHI(X) is the program built in weighting function)

Definition:

```
REAL FUNCTION  FSANO5 *8(X)
```

Explanation of the argument:

name	mode	type	dimension	remarks
X	I	R8	scalar	energy value for which the function is to be calculated

Used common blocks (with explanations of the quantities):

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
NR1	-	I4	(18)	1	dummy array. Not used in FSANO5
A3	I	R4	scalar	19	straight line parameter for σ_t
B3	I	R4	scalar	20	" " " " "
BSIGO	I	R4	scalar	21	σ_o-value

Called subprograms:

None

9.10.32 Function FSANO6

Problem solved:

Calculation of the function (with double precision)

$$DPHI \cdot \frac{A1 \cdot X + B1}{(A3 \cdot X + B3 + BSIGO)}$$

(DPHI(X) is the program built in weighting function)

Definition:

REAL FUNCTION FSANO6 * 8(X)

Explanation of the argument:

name	mode	type	dimension	remarks
X	I	R8	scalar	energy value for which the function is to be calculated

Used common blocks (with explanations of the quantities):

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
NR1	-	I4	(14)	1	dummy array. Not used in FSANO6
A1	I	R4	scalar	15	straight line parameter for σ_t, σ_a, σ_e or σ_f
B1	I	R4	scalar	16	straight line parameter for σ_t, σ_a, σ_e or σ_f
NR2	-	I4	(2)	17	dummy array. Not used in FSANO7
A3	I	R4	scalar	19	straight line parameter for σ_t
B3	I	R4	scalar	20	" " " " "
BSIGO	I	R4	scalar	21	σ_o-value

Called subprograms:

None

9.10.33 Function FSANO7

Problem solved:

Calculation of the function (with double precision)

$$DPHI \cdot \frac{A1 \cdot X + B1}{(A3 \cdot X + B3 + BSIGO)^2}$$

(DPHI(X) is the program built in weighting function)

Definition:

```
REAL FUNCTION FSANO7 * 8(X)
```

Explanation of the argument:

name	mode	type	dimension	remarks
X	I	R8	scalar	energy value for which the function is to be calculated

Used common blocks (with explanations of the quantities):

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
NR1	-	I4	(14)	1	dummy array. Not used in FSANO7
A1	I	R4	scalar	15	straight line parameter for σ_t, σ_a, σ_e or σ_f
B1	I	R4	scalar	16	straight line parameter for σ_t, σ_a, σ_e or σ_f
NR2	-	I4	(2)	17	dummy array. Not used in FSANO7
A3	I	R4	scalar	19	straight line parameter for σ_t
B3	I	R4	scalar	20	" " " " "
BSIGO	I	R4	scalar	21	σ_o-value

Called subprograms:

None

9.10.34 Function FSANO8

Problem solved:

Calculation of the function (with double precision)

$$DPHI \cdot \frac{(A1 \cdot X + B1) \cdot (A2 \cdot X + B2)}{(A3 \cdot X + B3 + BSIGO)}$$

(DPHI(X) is the program built in weighting function)

Definition:

REAL FUNCTION FSANO8 * 8(X)

Explanation of the argument:

name	mode	type	dimension	remarks
X	I	R8	scalar	energy value for which the function is to be calculated

Used common blocks (with explanations of the quantities):

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
NR1	-	I4	(14)	1	dummy array. Not used in FSANO8 .
A1	I	R4	scalar	15	straight line parameter for σ_t, σ_a, σ_e or σ_f
B1	I	R4	scalar	16	straight line parameter for σ_t, σ_a, σ_e or σ_f .
A2	I	R4	scalar	17	straight line parameter for $\bar{\mu}_e$.
B2	I	R4	scalar	18	" " " " "
A3	I	R4	scalar	19	straight line parameter for σ_t
B3	I	R4	scalar	20	" " " " "
BSIGO	I	R4	scalar	21	σ_o-value

Called subprograms:

None

9.10.35 Function FSANO9

Problem solved:

Calculation of the function (with double precision)

$$DPHI \cdot \frac{(A1 \cdot X + B1) \cdot (A2 \cdot X + B2)}{(A3 \cdot X + B3 + BSIGO)^2}$$

(DPHI(X) is the program built in weighting function)

Definition:

```
REAL FUNCTION FSANO9 * 8(X)
```

Explanation of the argument:

name	mode	type	dimension	remarks
X	I	R8	scalar	energy value for which the function is to be calculated

Used common blocks (with explanations of the quantities):

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
NR1	-	I4	(14)	1	dummy array. Not used in FSANO9
A1	I	R4	scalar	15	straight line parameter for σ_t, σ_a, σ_e or σ_f
B1	I	R4	scalar	16	straight line parameter for σ_t, σ_a, σ_e or σ_f
A2	I	R4	scalar	17	straight line parameter for $\bar{\mu}_e$
B2	I	R4	scalar	18	" " " " "
A3	I	R4	scalar	19	straight line parameter for σ_t
B3	I	R4	scalar	20	" " " " "
BSIGO	I	R4	scalar	21	σ_o-value

Called subprograms:

None

9.10.36 Subroutine FSEXIN

Problem solved:

Analytical integration of the functions described in 9.10.18 to 9.10.26 and 9.10.27 to 9.10.34 with DPHI(X) = $\frac{1.0}{X}$.

Definition:

SUBROUTINE FSEXIN

Used common blocks (with explanations of the quantities):

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
NR1	-	I4	(11)	1	dummy array. Not used in FSEXIN
CONST	I	R4	scalar	12	see 9.10.1 (common blocks)
AW	I	R4	scalar	13	see 9.10.17 (common blocks)
BW	I	R4	scalar	14	" "
A1	I	R4	scalar	15	" "
B1	I	R4	scalar	16	" "
A2	I	R4	scalar	17	" "
B2	I	R4	scalar	18	" "
A3	I	R4	scalar	19	" ""
B3	I	R4	scalar	20	" "
BSIGO	I	R4	scalar	21	" "
XIA	I	R4	scalar	22	" "
XIE	I	R4	scalar	23	" "
L	I	I4	scalar	24	" "
Y	O	R8	scalar	25	" "

Called subprograms:

FSLOMQ

FSWRO3 (entry of FSWROO)

9.10.37 Function FSLOMQ

Problem solved:

With $Q = F \cdot (XIE - XIA)/(1 + F \cdot XIA)$ the function calculates - with double precision - $\log(1 + Q) - Q + 0.5 \cdot Q^2$ by using an expansion into series. The value is calculated with an relative error less or equal 10^{-15}.

Definition:

```
REAL FUNCTION  FSLOMQ * 8(XIE,XIA,F)
```

Explanation of the arguments:

name	mode	type	dimension	remarks
XIE	I	R8	scalar	see problem solved
XIA	I	R8	scalar	" " "
F	I	R8	scalar	" " "

Used common blocks (with explanations of the quantities):

name of the common block: BLANK COMMON					
name	mode	type	dimension	word	remarks
NR1	-	I4	(4)	1	dummy array. Not used in FSLOMQ
NO	I	I4	scalar	5	print output unit number

Called subprograms:

FSWR03 (entry of FSWR00)

9.10.38 Function FSGRA1

Problem solved:

Checks if all straight line parameter ranges cover the integration sub-interval.

Definition:

LOGICAL FUNCTION FSGRA1(AB,IAB,MAB,XIA,XIE)

Explanation of the arguments:

name	mode	type	dimension	remarks
AB	I	R4	(MAB,4)	straight line parameters
IAB	I	I4	scalar	pointer to the actual straight line parameter set
MAB	I	I4	scalar	used for dimensioning AB
XIA	I	R4	scalar	lower limit of integration sub-interval
XIE	I	R4	scalar	upper limit of integration sub-interval

Used common blocks (with explanations of the quantities):

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
NR1	-	I4	(4)	1	dummy array. Not used in FSGRA1
GLSCH	I	R4	scalar	5	see 9.10.1 (common blocks)

Called subroutines:

FSTOLE

9.10.39 Subroutine FSGRA2

Problem solved:

Localisation of the actual straight line parameters. Testing if cross sections are zero or less than zero or if they are changing the sign.

Definition:

```
SUBROUTINE FSGRA2(IFUN,AB,IAB,MAB,NAB,
                  XIA,XIE,XIEE,SPRUO,SPRU3,
                  IFAR,LFAR,LFARA,
                  FARIN,FARAN,IFUNAR,
                  NUDUR)
```

Explanation of the arguments:

name	mode	type	dimension	remarks
IFUN	I	I4	scalar	selection of (A1,B1),(A2,B2) or (A3,B3)
AB	I	R4	(MAB,4)	straight line parameters
IAB	IO	I4	scalar	pointer to the actual straight line parameter set
MAB	I	I4	scalar	used for dimensioning AB
NAB	I	I4	scalar	maximum value of IAB
XIA	I	R4	scalar	lower subinterval limit
XIE	I	R4	scalar	upper subinterval limit
XIEE	IO	R4	scalar	XIEE $\geq$ XIE. energy value until which - starting at XIA - the cross section is zero or has any error
SPRUO	IO	L4	scalar	test control. Switch for some tests
SPRU3	O	L4	scalar	is set .TRUE. if a cross section has been equal zero in the interval [XIA,XIE]
IFAR	I	I4	scalar	see 9.10.17 (argument list)
LFAR	IO	L4	(2,3)	" "

name	mode	type	dimension	remarks
LFARA	O	L4	(2,3)	see 9.10.17 (argument list)
FARIN	IO	R4	(2,3,2)	" "
FARAN	O	R4	(2,3)	" "
IFUNAR	IO	I4	(2,3)	" "
NUDUR	I	L4	scalar	Switch for changing sign test

Used common blocks (with explanations of the quantities):

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
NR1	-	I4	(3)	1	dummy array. Not used in FSGRA2
LERMSG	I	L4	scalar	4	see 9.10.1 (common blocks)
GLSCH	I	R4	scalar	5	" "
NR2	-	I4	(2)	6	dummy array. Not used in FSGRA2
ITYP	I	I4	scalar	8	see 9.10.1 (common blocks)
ITYPFU	I	I4	scalar	9	" "
NR3	-	I4	(5)	10	dummy array. Not used in FSGRA2
A1	O	R4	scalar	15	see 9.10.17 (common blocks)
B1	O	R4	scalar	16	" "
A2	O	R4	scalar	17	" "
B2	O	R4	scalar	18	" "
A3	O	R4	scalar	19	" "
B3	O	R4	scalar	20	" "
BSIGO	I	R4	scalar	21	" "

Called subprograms:

FSGRA1
FSTOLE
FSWRO2 }
FSWRO3 } (entries of FSWROO)
FSWRO4 }

9.10.40 Subroutine FSGRA3

Problem solved:

Localisation of the desired straight line parameters for the interval [XIA,XIE]

Definition:

```
SUBROUTINE FSGRA3(AB,IAB,MAB,NAB,
                  XIA,XIE)
```

Explanation of the arguments:

name	mode	type	dimension	remarks
AB	I	R4	(MAB,4)	see 9.10.38 (argument list)
IAB	IO	I4	scalar	" "
MAB	I	I4	scalar	" "
NAB	I	I4	scalar	maximum value of IAB
XIA	I	R4	scalar	see 9.10.38 (argument list)
XIE	I	R4	scalar	" "

Used Common blocks (with explanations of the quantities):

```
COMMON/CFSTRU/NR1(4),GLSCH
```

All quantities are explained in 9.10.38. All have the same mode.

Called subprograms:

```
FSGRA1
FSWR03          (entry of FSWR00)
```

9.10.41 Subroutine FSROMB

Problem solved:

Numerical integration with the Romberg method (see /4/).

Definition:

```
SUBROUTINE FSROMB(FCT,*)

ENTRY FSROMI(EPS,NDIM,DRINWA,YF,
             YFEPS,AUX)
```

(Passes the argument addresses to the subroutine)

Explanation of the arguments:

name	mode	type	dimension	remarks
FCT	I	F8	-	name of the function to be integrated
*	-	-	-	RETURN1 is done if the wished accuracy could not be reached within NDIM-1 bisections
EPS	I	R4	scalar	desired integration accuracy
NDIM	I	I4	scalar	NDIM-1 = possible number of bisections
DRINWA	I	R4	scalar	see 9.10.1 (argument list)
YF	IO	R4	(3)	results added for the different classes (see 9.4)
YFEPS	IO	R4	(3)	maximum relative integration error for the results of each class
AUX	L(O)	R4	(NDIM)	auxiliary array (see /4/)

Used common blocks (with explanations of the quantities):

name of the common block: BLANK COMMON					
name	mode	type	dimension	word	remarks
NR1	-	I4	(4)	1	dummy array. Not used in FSROMB
NO	I	I4	scalar	5	print output unit

Used common blocks (with explanations of the quantities):

name of the common block: CFSTRU					
name	mode	type	dimension	word	remarks
TEST1	I	L4	scalar	1	see 9.10.1 (common blocks)
TEST2	I	L4	scalar	2	" "
TEST3	I	L4	scalar	3	" "
LERMSG	I	L4	scalar	4	" "
GLSCH	I	R4	scalar	5	" "
NR2	-	I4	(2)	6	dummy array. Not used in FSROMB
ITYP	I	I4	scalar	8	see 9.10.1 (common blocks)
ITYPFU	I	I4	scalar	9	" "
NR3	-	I4	(11)	10	dummy array. Not used in FSROMB
BSIGO	I	R4	scalar	21	σ_o-value
XL	I	R4	scalar	22	lower integration limit
XH	I	R4	scalar	23	upper integration limit
NR4	-	I4	(1)	24	dummy array. Not used in FSROMB
Y	O	R8	scalar	25	result of the integration
NDIMP	O	I4	scalar	27	if > 0 necessary increase of NDIM
DRUCK	O	L4	scalar	28	is set to .TRUE., if an error printing has been done in the routine

Called subprograms:

FCT (see argument list)

FSWROO

FSWRO3 (entry of FSWROO)

9.10.42 Block_Data

Problem solved:

Initialisation of IDUR in COMMON/CFSDUR/.

9.10.43 Subroutine A8FORM

Problem solved:

Printing of text with "big" letters.

Definition:

The compiled program is stored in a system library as object code (see /6/).

9.10.44 Subroutine NDF

Problem solved:

Retrieval of KEDAK-data. (see /3/, /2/)

Definition:

The program is used in all parts of MIGROS-3. The definition may be found in /3/.

9.11 References

/1/ H. Huschke, B. Krieg

MIGROS-2: A Program Written in FORTRAN for the Calculation of Microscopic Group Constants from Nuclear Data.

Institut für Neutronenphysik und Reaktortechnik,
Projekt Schneller Brüter,
Gesellschaft für Kernforschung mbH., Karlsruhe

KFK 1784, Juni 1973

/2/ B. Goel, B. Krieg

Status of the Nuclear Data Library KEDAK-3 October 1975.

Institut für Neutronenphysik und Reaktortechnik
Gesellschaft für Kernforschung mbH., Karlsruhe

KFK 2234, NEANDC(E) 171 "U" , Dezember 1975

/3/ B. Krieg

Handling and Service Programs for the Karlsruhe Nuclear Data File KEDAK.
Part I: Management and Retrieval Programs

Institut für Neutronenphysik und Reaktortechnik
Gesellschaft für Kernforschung mbH., Karlsruhe

KFK 1725, Juni 1973

/4/ S. Filippi

Das Verfahren von Romberg-Stiefel-Bauer als Spezialfall des allgemeinen Prinzips von Richardson.

Mathematik-Technik-Wirtschaft. Band 11, Nr. 2, Seiten 49-54. 1964

/5/ IBM
System/360 Scientific Subroutine Package.
Version III. Programmer's Manual.
Program Number 360A-CM-03X.

GH20-0205-4., August 1970

/6/ O. Eggenberger

A8FORM. Ausdruck von Texten in Großformat.

not published, 1970

10. The calculation of group constants in the thermal group. Module 10

10.1 This module is extended against the version in MIGROS-2 by the calculation of the average total cross section, Besides this three new types are entered into the program for formal reasons, $PROBSGI_{th}$, $SGNCO_{th}$ and CHI (definition see below). These types are used to facilitate the input for a GRUBA /1/ insertion run.

10.2 It is assumed, that the thermal energy range is covered by one energy group. For the cross sections except the elastic scattering cross section a 1/v-law is assumed, and for the weighting function a Maxwell distribution at T = 293.6K corresponding to kT = 0.0253 eV. The thermal group cross sections for types with a 1/v behaviour are then given by (/2/)

$$\bar{k\sigma}_{x,th} = \frac{\sqrt{\pi}}{2} \cdot {}^{k}\sigma_{x}(0.0253\ \text{eV}) \qquad (10.1)$$

k = isotope
x = neutron reaction (n,x) except (n,n) process
th = thermal

The thermal group cross sections are calculated by formula (10.1) for all types x of neutron reactions, except those for elastic scattering. Furthermore the following group constants are calculated:

- the average elastic scattering cross section

$$\bar{k\sigma}_{n,th} = {}^{k}\sigma_{n}(0.0253\ \text{eV}) \qquad (10.2)$$

- the average cosine of the elastic scattering

$$\bar{k\mu}_{e,th} = {}^{k}\mu_{e}(0.0253\ \text{eV}) \qquad (10.3)$$

- the average number of secondary neutrons per fission

$$\bar{k\nu}_{th} = {}^{k}\nu(0.0253\ \text{eV}) \qquad (10.4)$$

- the average α-value

$$\bar{k}_{\alpha_{th}} = \frac{\bar{k}_{\sigma_{\gamma,th}}}{\bar{k}_{\sigma_{f,th}}} \qquad \gamma = \text{radiative capture}, \; f = \text{fission} \tag{10.5}$$

- the average η-value

$$\bar{k}_{\eta_{th}} = \frac{\bar{k}_{\nu_{th}}}{1+\bar{k}_{\alpha_{th}}} \tag{10.6}$$

The assembled group constants are calculated as follows:

- the average capture cross section

$$\bar{k}_{\sigma_{c,th}} = \bar{k}_{\sigma_{a,th}} - \bar{k}_{\sigma_{f,th}} \quad *) \tag{10.7}$$

- the average total cross section

$$\bar{k}_{\sigma_{t,th}} = \bar{k}_{\sigma_{n,th}} + \bar{k}_{\sigma_{a,th}} + \bar{k}_{\sigma_{i,th}} + \bar{k}_{\sigma_{2n,th}} \tag{10.8}$$

For obtaining consistence with the data included in the GRUBA-library, it is necessary to set the following types in this module:

- the inelastic scattering matrice in the thermal group

$$\text{PROBSGI}_{th} = 1. \tag{10.9}$$

- the elastic scattering matrice in the thermal group

$$\text{SGNCO}_{th} = 1. \tag{10.10}$$

- in the case of a fissile isotope the fission spectrum in the thermal group

$$\text{CHI} = 0. \tag{10.11}$$

10.3 The following subroutine is necessary:

THERM (NE, NTY, TYP)

---

*) Definition of the absorption cross-section σ_a (KEDAK-type SGA)

$\sigma_a = \sigma_\gamma + \sigma_f + \sigma_p + \sigma_d + \sigma_\alpha$ (see /3/)

The following parameters are defined by the control program:

NE : number of energy group limits
NTY : number of cross section types
TYP(NTY) : one-dimensional field containing the cross section types.

References

/1/ D. Woll
Aufbau und Verwaltung der Gruppenkonstantenbibliothek GRUBA
KFK 1815, 1973

/2/ K.H. Beckurts, K. Wirtz
Neutron Physics, Springer Verlag Berlin, Göttingen, Heidelberg, New York, 1964, pages 98 - 100

/3/ B. Goel, B. Krieg
Status of the Nuclear Data Library KEDAK-3
October 1975
KFK 2234, NEANDC(E) 171 >>U<<, 1975

11. The calculation of the weighted average 1/v values. Module 8

11.1 The difference between the program version in MIGROS-2 and in MIGROS-3 is a more exact method of integration. In the case of a pointwise given weighting function the MIGROS-2 version uses only the energy points of the weighting function and the energy group limits as integration points. The MIGROS-3 version starts with the same energy points and calculates the numerator and the denominator of formula 11.2. Then the distance between the integration points is bisected and the numerator and the denominator is calculated once more. This technique is continued until the relative deviation of the numerator integral calculated with n and 2*n energy points and of the denominator integral calculated with n and 2*n energy points is less than or equal to a given error limit ε. In the case of a weighting function given as analytic function the numerator and the denominator integral is calculated starting with 10 equidistant energy points in the respective energy group. Then the number of energy points is doubled and the calculation is done once more. This technique is stopped if the error limit is reached as explained above.

11.2 The average 1/v values are defined as

$$\left(\frac{1}{v}\right)_g = \frac{\int_{(g)} \frac{1}{v} \cdot F(E)dE}{\int_{(g)} F(E)dE} \qquad (11.1)$$

11.3 The numerical integration is performed by the following formula: (trapezoidal rule)

$$\left(\frac{1}{v}\right)_g = c \cdot \frac{\sum_{i=1}^{n} \left\{\frac{F(E_i)}{\sqrt{E_i}} + \frac{F(E_{i+1})}{\sqrt{E_{i+1}}}\right\} \cdot \{E_{i+1} - E_i\}}{\sum_{i=1}^{n} \{F(E_i) + F(E_{i+1})\} \cdot \{E_{i+1} - E_i\}} \qquad (11.2)$$

i : index of the integration points

E_i : integration points in energy group g

$F(E_i)$: weighting function

n : number of integration points in energy group g

c : constant = $7.229286 \cdot 10^{-7}$

In the thermal group the 1/v value is set equal to $\frac{1}{2}\sqrt{\pi} \cdot \frac{c}{\sqrt{0.0253}}$.

11.4 The following subroutine is used:

EDV (NE, ENG, NSP, E, F, EPS, V, NEF, ST, FI, IW)

The following parameters must be defined:

NE	number of energy group boundaries
ENG(NE)	energy group boundaries in [eV]
NSP	number of energy points of the weighting function
E(NSP)	energy points of the weighting function in [eV]
F(NSP)	weighting function at the energy points E(NSP)
EPS	permissible integration error
NEF	dimension of the working fields ST and FI

V(NE), ST(NEF) and FI(NEF) are one-dimensional working fields, IW is a control word internally used .

12. The calculation of the fission spectrum. Module 7

12.1 The program version included in MIGROS-2 calculates the Watt-Cranberg fission spectrum using the KEDAK data type CHICR,/2/, which contains the corresponding parameters. For some isotopes the data type CHICR is not available on the KEDAK library. In such cases the module version included in MIGROS-3 calculates the Maxwellian spectrum using the KEDAK type SEDF, /2/, with the argument K=2 meaning that a Maxwell model is used and the first functional value p=1 meaning the fraction of the spectrum to the total energy distribution. Note, that if the highest energy group boundary is greater than or equal to 10.E6 eV this boundary is set equal to 20.E6 eV because otherwise $\sum_{i=1}^{NE} \chi_i$ is not close enough to 1. (Summation is carried out over all energy groups.)

12.2 Calculation of the Watt-Cranberg spectrum

$$\chi(E) = \frac{\exp\{-\frac{E_f}{T}\}}{\sqrt{\pi \cdot E_f \cdot T}} \cdot \exp\{-\frac{E}{T}\} \cdot \sinh\{\frac{2}{T}\sqrt{E \cdot E_f}\} \qquad (12.1)$$

E energy in MeV,

E_f fragment kinetic energy per nucleon in MeV,

T Watt fragment nuclear "temperature" in MeV.

The fission spectrum in energy group g is defined as

$$\chi_g = \int_{(g)} \chi(E)\, dE \qquad (12.2)$$

E_g upper group limit in MeV,

E_{g+1} lower group limit in MeV.

Using formula (12.1) one gets

$$\chi_g = \frac{1}{2\cdot\sqrt{\pi}} \sqrt{\frac{T}{E_f}} \cdot \{\exp(-x_{g+1}^2) - \exp(-x_g^2) - \exp(-y_{g+1}^2) + \exp(-y_g^2)\} - \frac{1}{2}\{\mathrm{erf}(x_{g+1}) - \mathrm{erf}(x_g) + \mathrm{erf}(y_{g+1}) - \mathrm{erf}(y_g)\} \qquad (12.3)$$

with

$$x_g = \sqrt{\frac{E_g}{T}} - \sqrt{\frac{E_f}{T}} \; ; \quad x_{g+1} = \sqrt{\frac{E_{g+1}}{T}} - \sqrt{\frac{E_f}{T}}$$

$$y_g = \sqrt{\frac{E_g}{T}} + \sqrt{\frac{E_f}{T}} \; ; \quad y_{g+1} = \sqrt{\frac{E_{g+1}}{T}} + \sqrt{\frac{E_f}{T}}$$

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} \, dt$$

12.3 Calculation of the Maxwellian spectrum

The assumption for the calculation of the Maxwell spectrum is the existence of the KEDAK data type SEDF, /2/, containing the nuclear temperatures Θ at the fission energies E_o. The Maxwellian spectrum is given by formula (12.4) which was taken from /1/.

$$\chi(E) = 2/(\Theta \cdot \sqrt{\pi\Theta}) \cdot \sqrt{E} \cdot \exp\left(-\frac{E}{\Theta}\right) \qquad (12.4)$$

The fission spectrum in energy group g is defined as

$$\chi_g = \int_{(g)} \chi(E) \, dE \qquad (12.5)$$

Using formula (12.4) one gets

$$\chi_g = \mathrm{erf}\left(\sqrt{\frac{E_g}{\Theta}}\right) - \mathrm{erf}\left(\sqrt{\frac{E_{g+1}}{\Theta}}\right) - \left\{ \sqrt{\frac{E_g}{\Theta}} \cdot e^{-\frac{E_g}{\Theta}} - \sqrt{\frac{E_{g+1}}{\Theta}} \cdot e^{-\frac{E_{g+1}}{\Theta}} \right\} \cdot \frac{2}{\sqrt{\pi}} \qquad (12.6)$$

For $\frac{E_g}{\Theta} <$ 1.E-3 a polynomial expansion is taken.

Θ is taken or interpolated from KEDAK at the median fission energy E_o = 165 keV for a typical SNR neutron energy distribution $\phi(E)$

$$\int_0^{E_o} \nu(E) \cdot \sigma_f(E) \cdot \phi(E) \, dE = \int_{E_o}^{\infty} \nu(E) \cdot \sigma_f(E) \cdot \phi(E) \, dE \qquad (12.7)$$

$$= \frac{1}{2} \int_0^{\infty} \nu(E) \cdot \sigma_f(E) \cdot \phi(E) \, dE$$

12.4 The following subroutine is necessary

SUBROUTINE SPALT(NE,ENG,X)

The following parameters are defined by the control program:

NE number of energy group limits,

ENG(NE) one-dimensional field containing the energy group limits in [eV].

The following parameter is defined by the subroutine SPALT:

X(NE) one-dimensional field containing the fission spectrum.

The subroutine SPALT calls subroutine CHIINM which calculates the value of the Maxwellian spectrum in one energy group

SUBROUTINE CHIINM (E1,E2,TETA,X2)

The following parameters are defined by SPALT:

E1 lower energy group limit,

E2 higher energy group limit,

TETA nuclear temperature at the fission energy 165 keV.

The following parameter is defined by subroutine CHIINM

X2 value of the Maxwellian fission spectrum in the energy region from E1 to E2.

References

/1/ E. Kiefhaber, D. Thiem

The Influence of Fission Neutron Spectra on Integral Nuclear Quantities of Fast Reactors

KFK 1651, März 1972, page 1

/2/ B. Krieg

KEDAK Basic Management

KFK 2387 II 2.9 (1977)

Acknowledgements

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Appendix A. Sample Problem

1. Job Control Cards

```
//INRO17MI  JOB  (0017,101,P6M1B),KRIEG,CLASS=A,TIME=11,REGION=370K
/*SETUP DEVICE=2314,ID=GFK050
/*FORMAT PR,DDNAME=SYSMSG,FORMS=REPRO
/*FORMAT PR,DDNAME=FT06F001,FORMS=REPRO
// EXEC PGM=MIGROS3
//STEPLIB  DD  DSN=LOAD.NUSYS,VOL=SER=KAPROS,UNIT=3330,DISP=SHR
//FT08F001  DD  UNIT=SYSDA,SPACE=(TRK,2)
//FT06F001  DD  SYSOUT=A,
// DCB=(RECFM=FBA,LRECL=133,BLKSIZE=1995),SPACE=(TRK,25)
//FT01F001  DD  UNIT=2314,VOL=SER=GFK050,DSN=KEDAK3,DISP=SHR
//FT03F001  DD  UNIT=SYSDA,SPACE=(TRK,20)
//FT10F001  DD  UNIT=SYSDA,SPACE=(TRK,200)
//FT05F001  DD *
```

2. Input

```
@U 235â  1
@ELCC@  3
8   1 18 18  2 14 14  4 14 14  5 5 4  5 1 1  7 25 1  8 25 1  10 26 26
@ENDE â  111
@C  16@  0
@BLOCâ  3
5   3 4 4  6 3 3  6 12 12  9 3 3  9 12 12
@ENDE @  111
@ENDE â  112
```

3. Overlay Cards

```
OVERLAY MIGRCS
INSERT EING,FREEFO
OVERLAY MIGRCS
INSERT FGEM,WIRQ,WIRQU,STCSS,PSIXI,EXPPX
OVERLAY MIGRCS
INSERT FSTAT,QUER,TAB,SIGC,PHASE,E22,CMIT,CELTA,EPSI,GAMN,GAMG,GAFM
INSERT POL,SUCH
OVERLAY MIGRCS
INSERT FSTRUK,FSTCLE,CFSTRU,CFSTRF,FSWRCO,FSWRS1,FSWRS2,FSWRS3,CFSMEL
OVERLAY FSTRU1
INSERT FSQUER,FSTRU2,FSTRU3,FSTRU4,FSTRU5,FSSNCL
INSERT FSXINT,FSGRAL,FSGRA1,FSGRA2,FSGRA3
OVERLAY FSTRU3
INSERT FSEXIN,FSLCMQ
OVERLAY FSTRU3
INSERT FSRCMB
OVERLAY FSTRU4
INSERT FSNUC1,FSNUC2,FSNUC3,FSNLC4,FSNUC5,FSNUC6,FSNUC7,FSNUC8,FSNLC9
OVERLAY FSTRU4
INSERT FSANC2,FSANC3,FSANC4,FSANC5,FSANC6,FSANC7,FSANC8,FSANC9
OVERLAY FSTRU1
INSERT FSTRUC
OVERLAY FSTRU1
INSERT FSTRU1
OVERLAY FSTRU1
INSERT FSWRS9,A8FORM
OVERLAY MIGRCS
INSERT SUND,FL,GRUP
OVERLAY MIGRCS
INSERT CRONEN,CUTS,FIPCLA,SCAT,SINPCL,FIPCLC
OVERLAY ONE
INSERT SCATD,AKED,TRA
OVERLAY A
INSERT DACRG
OVERLAY B
INSERT NOREAD
OVERLAY B
INSERT SPECT1
OVERLAY A
INSERT SICRG,SGINT,XINPCL
OVERLAY ONE
INSERT SCATC
OVERLAY A
INSERT ENCRG,CRD1
OVERLAY A
INSERT RENUCA
OVERLAY A
INSERT REPRCE
OVERLAY A
INSERT SIMPSI,FINT,PROB,EXD,THETA,CNFAK,TEMF
OVERLAY MIGRCS
```

```
INSERT FLUMMI,SUM,IPCLA,PUSUM,INTEG
OVERLAY A
INSERT MIXSGT,ADD
OVERLAY A
INSERT MUKON,PRINT
OVERLAY A
INSERT TRAFL,INFORM,PUNK
OVERLAY A
INSERT MAKRO,LOOKO,LOOK1,LOOK2,LOOK3
OVERLAY A
INSERT LEGAL,LEGPOL,LEGINT,LEGIST,LEGANS,G
OVERLAY A
INSERT GRUPIN,IPOLIN,SPRAL
OVERLAY MIGROS
INSERT SPALT,CHIINM
OVERLAY MIGROS
INSERT EDV
OVERLAY MIGROS
INSERT KEMC,KEMP,AMESH,IWIN,IWC,ZWIN,EGRENZ,ICSCP,ENERG,FIPCL,IPCL
OVERLAY A
INSERT KEODAT,AUSGL,CRDN1,LININT,SLCHM,SINT,FXINT,SEARCH,MASSIN
OVERLAY A
INSERT ISOFAL,SMCRN,WAHRS,LMI,BCM,ANINT,NCRM,INTEN,PTL,WINK,FICR,AKCR
OVERLAY MIGROS
INSERT THERM
ENTRY MAIN
NAME MIGROS3(R)
```

On the following pages A4 to A29 the output of the results is given. The input description, that also was printed out by the job has been omitted here. It corresponds to the input description given on pages 2.2 to 2.17.

```
STAND DER KERNDATENBIBLIOTHEK VOM     261076
@U 235@   1                                                                 *
@BLOC@   2                                                                  *
8    1 18 18  2 14 14  4 14 14  5 5 4  5 1 1  7 25 1  8 25 1  10 26 26     *
@ENDE @   111                                                               *
@C  16@   0                                                                 *
@BLOC@   2                                                                  *
5    3 4 4  6 3 3  6 12 12  9 3 3  9 12 12                                  *
@ENDE @   111                                                               *
@ENDE @   112                                                               *
```

```
M I G R O S - 3  TASK FOR MATERIAL  U 235
*****************************************
```

FOR THE WEIGHTING SPECTRUM THE FUNCTION PHI(E) OR DPHI(E) WILL BE USED.

DATE 22.11.76   TIME 18.01.51

IN MODULE 1   33310 WORDS ARE NOT USED IN THE REGION FIELD

PROGRAMM KENNZIFFER 1
PROGRAMM ZUR BERECHNUNG VON RESONANZSELBSTABSCHIRMFAKTOREN VON AUFGELOESTEN RESONANZPARAMETERN

MATERIAL	TEMPERATUR	GRUPPE	GRENZEN	
U 235	300.00	18	0.4650E+02	0.1000E+03

SIGMA G	SIGMA N	SIGMA F	SIGMAN1	SIGMAT1
0.23170120E+02	0.12886469E+02	0.28999680E+02	0.12886469E+02	0.65056259E+02

SIGMA 0	FG	FN	FF	FN1	FT1
0.0	0.42532988E+00	0.94356949E+00	0.44212914E+00	0.92716968E+00	0.36945707E+00
0.10000000E+02	0.49302417E+00	0.94963223E+00	0.50933707E+00	0.93204403E+00	0.42256057E+00
0.10000000E+03	0.71646893E+00	0.97010434E+00	0.72497588E+00	0.95298940E+00	0.62977850E+00
0.10000000E+04	0.93765211E+00	0.99268764E+00	0.93856294E+00	0.98639333E+00	0.90295374E+00
0.10000000E+05	0.99288553E+00	0.99910206E+00	0.99322623E+00	0.99829018E+00	0.98853195E+00
0.10000000E+06	0.99945521E+00	0.99989605E+00	0.99976951E+00	0.99979395E+00	0.99880898E+00
0.10000000E+07	0.99989414E+00	0.99999082E+00	0.99990296E+00	0.99998218E+00	0.99986422E+00

MATERIAL	TEMPERATUR	GRUPPE	GRENZEN	
U 235	900.00	18	0.4650E+02	0.1000E+03

SIGMA G	SIGMA N	SIGMA F	SIGMAN1	SIGMAT1
0.23157272E+02	0.12888164E+02	0.28985733E+02	0.12888164E+02	0.65031158E+02

SIGMA 0	FG	FN	FF	FN1	FT1
0.0	0.52090794E+00	0.95318604E+00	0.53101712E+00	0.93434250E+00	0.42303497E+00
0.10000000E+02	0.58767426E+00	0.95869917E+00	0.59581017E+00	0.93998843E+00	0.48589534E+00
0.10000000E+03	0.79037625E+00	0.97749454E+00	0.79024559E+00	0.96224260E+00	0.70428258E+00
0.10000000E+04	0.95936489E+00	0.99520826E+00	0.95805335E+00	0.99085903E+00	0.93382698E+00
0.10000000E+05	0.99556696E+00	0.99944174E+00	0.99552155E+00	0.99892360E+00	0.99259353E+00
0.10000000E+06	0.99967504E+00	0.99994004E+00	0.99981242E+00	0.99987465E+00	0.99924034E+00
0.10000000E+07	0.99994498E+00	0.99999851E+00	0.99993896E+00	0.99999207E+00	0.99990743E+00

MATERIAL	TEMPERATUR	GRUPPE	GRENZEN	
U 235	2100.00	18	0.4650E+02	0.1000E+03

SIGMA G	SIGMA N	SIGMA F	SIGMAN1	SIGMAT1
0.23122330E+02	0.12889277E+02	0.28932922E+02	0.12889277E+02	0.64944519E+02

SIGMA 0	FG	FN	FF	FN1	FT1
0.0	0.60590488E+00	0.96047390E+00	0.60755364E+00	0.93858165E+00	0.48321068E+00
0.10000000E+02	0.66609097E+00	0.96593255E+00	0.66553569E+00	0.94607395E+00	0.54955190E+00
0.10000000E+03	0.84069175E+00	0.98270690E+00	0.83474588E+00	0.96963567E+00	0.76128662E+00
0.10000000E+04	0.97142029E+00	0.99664253E+00	0.96915907E+00	0.99349582E+00	0.95181471E+00
0.10000000E+05	0.99692833E+00	0.99961740E+00	0.99674857E+00	0.99926466E+00	0.99474430E+00
0.10000000E+06	0.99976003E+00	0.99995834E+00	0.99984288E+00	0.99991411E+00	0.99947912E+00
0.10000000E+07	0.99996543E+00	0.99999750E+00	0.99997044E+00	0.99999344E+00	0.99994189E+00

IN MODULE 1 407.16 SECONDS CPU-TIME ARE USED

DATE 22.11.76 TIME 18.36.14

IN MODULE 2 37692 WORDS ARE NOT USED IN THE REGION FIELD

PROGRAMM KENNZIFFER 2
PROGRAMM ZUR BERECHNUNG VON RESONANZSELBSTABSCHIRMFAKTOREN VON STATISTISCHEN RESONANZPARAMETERN

NUMBER OF SERIES,TAKEN INTO ACCOUNT IS IT= 6

MATERIAL	TEMPERATUR	GRUPPE	GRENZEN	
U 235	300.00	14	C.1000E+04	C.2150E+04

SIGMA G	SIGMA N	SIGMA F	SIGMAN1	SIGMAT1
0.29596672E+01	0.12280684E+02	0.66533985E+01	0.12280684E+02	0.21893692E+02

SIGMA 0	FG	FN	FF	FN1	FT1
0.0	0.80614358E+00	C.98495656E+00	0.81168741E+00	0.97353542E+00	0.81270683E+00
C.1000C0C0E+02	0.86417347E+00	0.98894918E+00	0.86897EC6E+00	0.98050916E+00	0.87385619E+00
C.1CCCCCCCE+C3	0.96114337E+CC	C.99656564E+0C	0.96302EC7E+00	0.99361336F+00	0.96461695E+00
C.10000000E+04	0.99510652E+C0	C.99955565E+0C	0.9953821SE+00	0.99911815E+00	0.99540108E+00
C.1CCCCCC0E+C5	0.99949622E+CC	C.99994898E+00	0.99953932E+00	0.99990731E+0C	C.99952239E+00
0.10000000E+06	0.99995041E+00	0.99999088E+CC	0.9999565E+C0	0.99999350E+00	0.99995458E+00
C.10000C0CF+07	0.10000000E+01	0.10000000E+01	0.10000CC0E+01	0.10000000E+01	0.10000C00E+01

MATERIAL	TEMPERATUR	GRUPPE	GRENZEN	
U 235	900.00	14	0.1000E+04	C.2150E+04

SIGMA G	SIGMA N	SIGMA F	SIGMAN1	SIGMAT1
0.29596672E+01	0.12280684E+02	C.66533985E+01	C.12280684E+02	0.21893692E+02

SIGMA 0	FG	FN	FF	FN1	FT1
0.0	0.84466672E+00	C.98803872E+00	0.84577483E+00	0.97611034E+00	0.82758224E+00
C.1000C0C0E+02	0.89723802E+C0	C.99168956E+00	0.89840829E+00	0.98360044E+00	0.89160442E+00
0.1000C000E+03	0.97411436E+00	C.99772322E+0C	0.9746C175E+C0	C.99553901E+00	0.97473818E+00
C.1000C0C0E+04	0.99691331E+00	0.99972248E+00	0.99699957E+00	0.99944031E+00	0.99701816E+00
C.10000000E+05	0.99968135E+00	C.99996656E+00	0.99970567E+00	0.99994159E+00	0.99969399E+00
C.1CCC0000E+06	0.99996889E+00	0.99999362E+00	0.9999747SE+00	0.99999452E+C0	0.99997002E+00
C.100CCCCCE+07	0.10000000E+C1	0.100C0000E+01	0.10000CC0F+01	0.10000000E+01	0.10000000E+01

MATERIAL	TEMPERATUR	GRUPPE	GRENZEN	
U 235	2100.0C	14	0.1000E+04	0.2150F+04

SIGMA G	SIGMA N	SIGMA F	SIGMAN1	SIGMAT1
0.29596672E+01	0.12280684E+02	0.66533985E+01	0.12280684E+C2	0.21893692E+02

SIGMA 0	FG	FN	FF	FN1	FT1
C.0	0.87722653E+C0	C.99058086E+00	0.87678689F+00	0.97935218E+00	0.8499C674E+00
0.10000000E+02	0.92158425E+00	C.9936862CE+00	0.9215167EE+C0	0.98657191E+00	0.91042733F+00
C.1000C0C0E+03	0.98162389E+00	0.99839264E+00	0.98168224E+00	0.99675894E+00	0.98138368E+00
C.100CC0CCE+04	0.99786872E+C0	C.99980968E+00	0.99788657F+C0	0.99961442E+00	0.99791342E+00
C.10000000E+05	0.99978042E+00	C.9995761CE+0C	0.99979612E+00	0.99996030E+00	0.99978566E+00
C.1CCCCCC0E+06	0.99997687E+CC	C.99999410E+00	0.9999984C9F+00	0.99999613E+00	0.99997997E+00
C.100000C0E+07	0.10000000E+C1	C.1000000CE+01	0.1C000CCCE+C1	0.10000000E+01	0.10000000E+01

IN MODULE 2 155.39 SECONDS CPU-TIME ARE USED

DATE 22.11.76 TIME 18.44.55

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IN MODULE  4   34781 WORDS ARE NOT USED IN THE REGION FIELD


PROGRAMM KENNZIFFER 4
PROGRAMM ZUR BERECHNUNG VON GRUPPENWIRKUNGSQUERSCHNITTEN BEI UNENDLICHER VERDUENNUNG


***MESSAGE 4. 2 : STORAGE NOT SUFFICIENT TO CALCULATE  NUEL

IN MODULE  4    0.31 SECONDS CPU-TIME ARE USED


IN MODULE  4   34771 WORDS ARE NOT USED IN THE REGION FIELD


PROGRAMM KENNZIFFER 4
PROGRAMM ZUR BERECHNUNG VON GRUPPENWIRKUNGSQUERSCHNITTEN BEI UNENDLICHER VERDUENNUNG


***MESSAGE 4. 1 : BEGIN OF THE INTEGRATION AT  0.10000000E+04 EV

 U 235    NUEL        GRUPPE 14 BIS 14
  0.28608791E-02


***MESSAGE 4. 1 : BEGIN OF THE INTEGRATION AT  0.10000000E+04 EV

 U 235    NUE         GRUPPE 14 BIS 14
  0.24232779E+01


***MESSAGE 4. 1 : BEGIN OF THE INTEGRATION AT  0.10000000E+04 EV

 U 235    SGA         GRUPPE 14 BIS 14
  0.10925330E+02


***MESSAGE 4. 1 : BEGIN OF THE INTEGRATION AT  0.10000000E+04 EV

 U 235    SGF         GRUPPE 14 BIS 14
  0.74818325E+01

 U 235    SGC         GRUPPE 14 BIS 14
  0.34434577E+01


***MESSAGE 4. 1 : BEGIN OF THE INTEGRATION AT  0.10000000E+04 EV

 U 235    SGI         GRUPPE 14 BIS 14
  0.0
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***MESSAGE 4. 1 : BEGIN OF THE INTEGRATION AT  0.10000000E+04 EV

 U 235    SGN        GRUPPE 14 BIS 14
  0.14350866E+02

***MESSAGE 4. 1 : BEGIN OF THE INTEGRATION AT  0.10000000E+04 EV

 U 235    SG2N       GRUPPE 14 BIS 14
  0.0

***MESSAGE 4. 1 : BEGIN OF THE INTEGRATION AT  0.10000000E+04 EV

 U 235    SGT        GRUPPE 14 BIS 14
  0.25274826E+02

IN MODULE  4    3.14 SECONDS CPU-TIME ARE USED

DATE 22.11.76    TIME 18.45.03



PROGRAMM KENNZIFFER 5

PROGRAMM ZUR BERECHNUNG VON TRANSFERMATRIZEN FUER
  INELASTISCHE STREUUNG, (N,2N) - UND (N,3N) - PROZESSE


PROBSGI


PROGRAMM ZUR BERECHNUNG INELASTISCHER STREUMATRIZEN
VON DISKRETEN ANREGUNGSNIVEAUS.


***WARNING NOF. 2 : THE FURTHER NAME   0.20000190E+07 IS GREATER THAN THE GREATEST FURTHER NAME
INCLUDED IN THE KEDAK LIBRARY FOR U 235    SGIZ

***WARNING NOF. 2 : THE FURTHER NAME   0.20000190E+07 IS GREATER THAN THE GREATEST FURTHER NAME
INCLUDED IN THE KEDAK LIBRARY FOR U 235    SGIZ

***WARNING NOF. 2 : THE FURTHER NAME   0.20000190E+07 IS GREATER THAN THE GREATEST FURTHER NAME
INCLUDED IN THE KEDAK LIBRARY FOR U 235    SGIZ

***WARNING NOF. 2 : THE FURTHER NAME   0.20000190E+07 IS GREATER THAN THE GREATEST FURTHER NAME
INCLUDED IN THE KEDAK LIBRARY FOR U 235    SGIZ
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PROGRAMM ZUR BERECHNUNG INELASTISCHER STREUMATRIZEN
IM ENERGIEBEREICH KONTINUIERLICHER ANREGUNGSNIVEAUS DES RESTKERNS

***WARNING NDF. 3 : THE DATA FOR 920235 30051 ARE NOT INCLUDED IN THE KEDAK LIBRARY

***WARNING NDF. 3 : THE DATA FOR 920235 30051 ARE NOT INCLUDED IN THE KEDAK LIBRARY

***WARNING 5.00 : THE CROSS-SECTION-VALUES,GIVEN FOR THE MATERIAL U 235 ,TYPE SGI
***DO NOT COVER THE ENERGY-GROUP BETWEEN 0.140000E+07EV AND 0.250000E+07EV.THE LOWEST AND HIGHEST VALUES
***GIVEN ON KEDAK FOR THIS GROUP ARE 0.240000E+07EV AND 0.250000E+07EV.
***THE INTEGRATION IN THIS ENERGY-GROUP THEREFORE IS RESTRICTED.

***WARNING NDF. 3 : THE DATA FOR 920235 50053 ARE NOT INCLUDED IN THE KEDAK LIBRARY

***WARNING NDF. 3 : THE DATA FOR 920235 50053 ARE NOT INCLUDED IN THE KEDAK LIBRARY

NO INFORMATION ON THE NUCLEAR DATA LIBRARY FOR TYPE SEDIC OF MATERIALU 235 .AN EVAPORATION MODEL WITH
THETA=SQRT(E/(NUE*A)) IS USED.FOR THE NORMALIZATION THE THRESHOLD OF SGI IS TAKEN INTO ACCOUNT.
U= 0.20983E+05EV,A= 0.23504E+03NUE= 0.16000E+00

KZ= 3NAM=U 235 KD= 2

	5	6	7	8	9	10	11	12	13	14	15
5	2.764E-01	5.249E-01	1.677E-01	2.321E-02	5.944E-03	1.427E-03	3.504E-04	9.537E-05	2.963E-05	1.042E-05	4.154E-06
	16	17	18	19	20	21	22	23	24	25	26
	1.790E-06	7.911E-07	3.611E-07	1.672E-07	7.666E-08	3.557E-08	1.660E-08	7.635E-09	3.551E-09	1.659E-09	1.420E-09
	4	5	6	7	8	9	10	11	12	13	14
4	2.615E-02	1.532E-01	3.559E-01	2.793E-01	1.261E-01	4.469E-02	1.137E-02	2.609E-03	5.843E-04	1.289E-04	2.765E-05
	15	16	17	18	19	20	21	22	23	24	25
	6.003E-06	1.304E-06	2.781E-07	6.019E-08	1.306E-08	2.783E-09	6.021E-10	1.306E-10	2.783E-11	6.021E-12	1.306E-12
	26										
	3.551E-13										

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PROGRAMM KENNZIFFER 5

PROGRAMM ZUR BERECHNUNG VON TRANSFERMATRIZEN FUER
  INELASTISCHE STREUUNG, (N,2N) - UND (N,3N) - PROZESSE


PROBSG2N


KO=      0  NO TRANSFER MATRICES FOR TYPE  SMTOT2N IN THE  ENERGY REGION REQUIRED BY INPUT



IN MODULE  5   29730 WORDS ARE NOT USED IN THE REGION FIELD

IN MODULE  5    0.72 SECONDS CPU-TIME ARE USED

DATE 22.11.76    TIME 18.45.05
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PROGRAMM KENNZIFFER 5

PROGRAMM ZUR BERECHNUNG VON TRANSFERMATRIZEN FUER
  INELASTISCHE STREUUNG, (N,2N) - UND (N,3N) - PROZESSE


PROBSGI


PROGRAMM ZUR BERECHNUNG INELASTISCHER STREUMATRIZEN
VON DISKRETEN ANREGUNGSNIVEAUS.


***WARNING NOF. 2 : THE FURTHER NAME   0.20000190E+07 IS GREATER THAN THE GREATEST FURTHER NAME
INCLUDED IN THE KEDAK LIBRARY FOR U 235    SGIZ


***WARNING NOF. 2 : THE FURTHER NAME   0.20000190E+07 IS GREATER THAN THE GREATEST FURTHER NAME
INCLUDED IN THE KEDAK LIBRARY FOR U 235    SGIZ
 ***ERROR 5.04 : WITH INCIDENT NEUTRON ENERGIES OUT OF THE
ENERGY GROUPS REQUESTED IN THE INPUT INELASTIC SCATTERING
FROM DISCRETE LEVELS CANNOT OCCUR.
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PROGRAMM ZUR BERECHNUNG INELASTISCHER STREUMATRIZEN
IM ENERGIEBEREICH KONTINUIERLICHER ANREGUNGSNIVEAUS DES RESTKERNS


***WARNING NOF. 3 : THE DATA FOR   920235    30051 ARE NOT INCLUDED IN THE KEDAK LIBRARY


***WARNING NOF. 3 : THE DATA FOR   920235    50053 ARE NOT INCLUDED IN THE KEDAK LIBRARY


***WARNING NOF. 3 : THE DATA FOR   920235    50053 ARE NOT INCLUDED IN THE KEDAK LIBRARY

NO INFORMATION ON THE NUCLEAR DATA LIBRARY FOR TYPE SEDIC   OF MATERIALU 235   .AN EVAPORATION MODEL WITH
THETA=SQRT(E/(NUE*A)) IS USED.FOR THE NORMALIZATION THE THRESHOLD OF   SGI       IS TAKEN INTO ACCOUNT.
U= 0.20983E+05EV,A= 0.23504E+03NUE= 0.16000E+00

KZ=     3NAM=U 235   KD=     1
              1           2           3           4           5           6           7           8           9          10          11
    1   1.273E-05   1.658E-03   2.587E-02   1.609E-01   2.859E-01   3.045E-01   1.481E-01   5.197E-02   1.616E-02   3.838E-03   8.532E-04
             12          13          14          15          16          17          18          19          20          21          22
        1.882E-04   4.120E-05   8.817E-06   1.911E-06   4.150E-07   8.846E-08   1.914E-08   4.153E-09   8.849E-10   1.915E-10   4.153E-11
             23          24          25          26
        8.849E-12   1.915E-12   4.153E-13   1.129E-13


PROGRAMM KENNZIFFER 5

PROGRAMM ZUR BERECHNUNG VON TRANSFERMATRIZEN FUER
  INELASTISCHE STREUUNG, (N,2N) - UND (N,3N) - PROZESSE


PROBSG2N


***WARNING NOF. 3 : THE DATA FOR   920235    50163 ARE NOT INCLUDED IN THE KEDAK LIBRARY


***WARNING NOF. 3 : THE DATA FOR   920235    50163 ARE NOT INCLUDED IN THE KEDAK LIBRARY

NO INFORMATION ON THE NUCLEAR DATA LIBRARY FOR TYPE SED2N   OF MATERIALU 235   .AN EVAPORATION MODEL WITH
THETA=SQRT(E/(NUE*A)) IS USED.FOR THE NORMALIZATION THE THRESHOLD OF   SG2N      IS TAKEN INTO ACCOUNT.
U= 0.53000E+07EV,A= 0.23504E+03NUE= 0.16000E+00
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```
**WEIGHTED GROUP CROSS-SECTION = 0.493809E+00 FOR OUTSCATTERING - GROUP      1 U = 0.530000E+07KONT =      0

KZ=      3NAM=U 235   KD=      1
              1            2            3            4            5            6            7            8            9           10           11
    1       0.0       7.353E-04    2.331E-02    1.657E-01    2.969E-01    3.020E-01    1.424E-01    4.919E-02    1.517E-02    3.587E-03    7.958E-04
             12           13           14           15           16           17           18           19           20           21           22
           1.754E-04    3.838E-05    8.211E-06    1.780E-06    3.864E-07    8.237E-08    1.783E-08    3.867E-09    8.240E-10    1.783E-10    3.867E-11
             23           24           25           26
           8.240E-12    1.783E-12    3.867E-13    1.051E-13


IN MODULE  5   29730 WORDS ARE NOT USED IN THE REGION FIELD

IN MODULE  5    8.18 SECONDS CPU-TIME ARE USED

DATE 22.11.76    TIME 18.45.21


IN MODULE  7   37911 WORDS ARE NOT USED IN THE REGION FIELD


PROGRAMM KENNZIFFER 7
PROGRAMM ZUR BERECHNUNG DES SPALTSPEKTRUMS

IN THIS MODULE THE HIGHEST ENERGY GROUP BOUNDARY IS SET EQUAL TO 20.E6 EV


WATT - CRANBERG SPEKTRUM

 U 235      EINFALLSENERGIE =  0.0              VON GRUPPE 25 BIS  1
CHI 0
  0.10703226E-09  0.32318237E-09  0.99962683E-09  0.31642278E-08  0.98986028E-08  0.31139685E-07  0.99362580E-07
  0.31199164E-06  0.98314013E-06  0.31392719E-05  0.98584796E-05  0.31055431E-04  0.99062265E-04  0.31036930E-03
  0.97276480E-03  0.30689924E-02  0.93899146E-02  0.23881171E-01  0.61028179E-01  0.14057332E+00  0.20230591E+00
  0.26991755E+00  0.18339193E+00  0.88322282E-01  0.16692650E-01


IN MODULE  7    0.03 SECONDS CPU-TIME ARE USED

DATE 22.11.76    TIME 18.45.21
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IN MODULE  8   37511 WORDS ARE NOT USED IN THE REGION FIELD


EDV - A PROGRAM FOR THE CALCULATION OF THE 1/V AVERAGE GROUP VALUES

GRUPPE        1/V
   1    0.25221425E-09
   2    0.32105718E-09
   3    0.40761261E-09
   4    0.53069127E-09
   5    0.70539374E-09
   6    0.96682684E-09
   7    0.13673001E-08
   8    0.19336548E-08
   9    0.27883800E-08
  10    0.40953410E-08
  11    0.60131633E-08
  12    0.88176115E-08
  13    0.12950604E-07
  14    0.19015300E-07
  15    0.27883786E-07
  16    0.40953442E-07
  17    0.60131640E-07
  18    0.88176193E-07
  19    0.12950602E-06
  20    0.19015278E-06
  21    0.27883755E-06
  22    0.40953398E-06
  23    0.60131680E-06
  24    0.88176296E-06
  25    0.12950604E-05
  26    0.40279110E-05

IN MODULE  8     0.04 SECONDS CPU-TIME ARE USED

DATE 22.11.76     TIME 18.45.21


IN MODULE 10   37937 WORDS ARE NOT USED IN THE REGION FIELD


PROGRAMM KENNZIFFER 10
PROGRAMM ZUR BERECHNUNG DER THERMISCHEN QUERSCHNITTE

 U 235     MUEL              26
 0.28609300E-02
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L 235     NUE                26
C.24228992E+01

L 235     SGA                26
C.60553198E+03

L 235     SGF                26
C.51578394E+03

L 235     SGC                26
C.89748047E+02

L 235     SGI                26
C.0

L 235     SGN                26
C.16611298E+02

L 235     SG2N               26
C.0

L 235     SGT                26
C.62214307E+03

L 235     SGNCO              26
C.10000000E+01

L 235     PRCBSGI            26
C.10000000E+01

L 235     CHI                26
C.0

IN MODULE 10     0.04 SECONDS CPU-TIME ARE USED

DATE 22.11.76     TIME 18.45.22




M I G R O S - 3  TASK FOR MATERIAL  0  16
**********************************************


FOR THE WEIGHTING SPECTRUM THE FUNCTION PHI(E) OR DPHI(E) WILL BE USED.

DATE 22.11.76     TIME 18.45.26
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IN MODULE  3   17691 WORDS ARE NOT USED IN THE REGION FIELD



*** MESSAGE 3. 1  PROGRAMM-KENNZIFFER 2

                  PROGRAMM ZUR BERECHNUNG VON RESONANZSELBSTABSCHIRMFAKTOREN VON PUNKTWEISE GEGEBENEN
                  WIRKUNGSQUERSCHNITTEN FUER DAS MATERIAL C  16   .


***WARNING NOF. 3 : THE DATA FOR     80016     30190 ARE NOT INCLUDED IN THE KEDAK LIBRARY

THE CALCULATIONS WILL BE DONE FOR GROUP     4, WHICH HAS THE BOUNDARIES     1.400000E+06 EV  AND     2.500000E+06 EV.

THE MATERIAL IS  N O T   FISSIONABLE.

WARNING MESSAGES IN NUMERICAL INTEGRATION WILL BE PRINTED, IF THE ACTUAL RELATIVE ERROR
IS GREATER OR EQUAL THAN   5.000E+00 TIMES THE WISHED RELATIVE ERROR =   5.0000E-05.

THE FOLLOWING WEIGHTING SPECTRUM(S) IS (ARE) USED.
              ENERGY RANGE                      WEIGHTING SPECTRUM                    TYP OF INTEGRATION

              WHOLE RANGE                ORIGINAL FUNCTION DPHI=1.0D+0/E                  NUMERICAL

**********************************************************************************************************************
*0  16      GROUP=    4  LOWER BOUNDARY=  1.400000E+06 EV    UPPER BOUNDARY=  2.500000E+06 EV.                        *
*             FROM   1.400000E+06 EV  TO   2.500000E+06 EV  NUMERICAL  INTEGRATION IS USED. DPHI IS USED AS WEIGHTING SPECTRUM.*
**********************************************************************************************************************

                      SIGMA A          SIGMA N          SIGMA NG1        SIGMA N1         SIGMA T1

                   0.21283107E-07   0.17578802E+01   0.19009775E+00   0.19009775E+00   0.17578802E+01

     SIGO             FA               FN               FNG1             FN1              FT1

  0.0              0.96236938E+00   0.81353301E+00   0.96001279E+00   0.93244135E+00   0.60673928E+00
  0.10000000E+02   0.99562335E+00   0.97553360E+00   0.99076885E+00   0.98229152E+00   0.95218652E+00
  0.10000000E+03   0.99949831E+00   0.99704301E+00   0.99886262E+00   0.99773443E+00   0.99410820E+00
  0.10000000E+04   0.99994916E+00   0.99969763E+00   0.99988371E+00   0.99976742E+00   0.99939543E+00
  0.10000000E+05   0.99999499E+00   0.99996978E+00   0.99998844E+00   0.99997675E+00   0.99993950E+00
  0.10000000E+06   0.99999958E+00   0.99999708E+00   0.99999893E+00   0.99999779E+00   0.99999404E+00
  0.10000000E+07   0.10000000E+01   0.99999982E+00   0.10000000E+01   0.99999988E+00   0.99999952E+00

*** MESSAGE 3. 2  PROGRAM 3 HAS ENDED CORRECTLY. KL HAS THE VALUE=   2.

NO WARNING- OR ERROR-MESSAGES PRODUCED IN MODULE ESTRUK.


IN MODULE  3    2.07 SECONDS CPU-TIME ARE USED

DATE 22.11.76    TIME 18.45.29
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IN MODULE  6    9009 WORDS ARE NOT USED IN THE REGION FIELD


PROGRAMM KENNZIFFER 6
PROGRAMM ZUR BERECHNUNG ELASTISCHER STREUMATRIZEN


***WARNING NDF. 2 : THE FURTHER NAME   0.15830016E+08 IS GREATER THAN THE GREATEST FURTHER NAME
INCLUDED IN THE KEDAK LIBRARY FOR 0  16     SGNC

***WARNING NDF. 2 : THE FURTHER NAME   0.15830016E+08 IS GREATER THAN THE GREATEST FURTHER NAME
INCLUDED IN THE KEDAK LIBRARY FOR 0  16     SGNC

***MESSAGE 6.1 : WARNING NDF. 2 MAY BE IGNORED


                          SGNC0        ELASTISCHE STREUMATRIX  0. ORDNUNG FUER  0  16

    3.GRUPPE

 0.88355E+00
 0.11644E+00



                          SGNC1        ELASTISCHE STREUMATRIX  1. ORDNUNG FUER  0  16

    3.GRUPPE

 0.29722E+00
-0.27920E-01



                          SGNC2        ELASTISCHE STREUMATRIX  2. ORDNUNG FUER  0  16

    3.GRUPPE

 0.19122E+00
 0.96000E-03
```

SGNC3 ELASTISCHE STREUMATRIX 3. ORDNUNG FUER 0 16

3.GRUPPE

0.8682CE-01
-0.52200E-02

SGNC4 ELASTISCHE STREUMATRIX 4. ORDNUNG FUER 0 16

3.GRUPPE

0.16280E-01
-0.39000E-03

SGNC5 ELASTISCHE STREUMATRIX 5. ORDNUNG FUER 0 16

3.GRUPPE

-0.15300E-02
0.29000E-03

ERLAEUTERUNG
L-TE ORDNUNG, G-TE GRUPPE, I-TE ZEILE: MATRIXELEMENT L-TER ORDNUNG
FUER STREUUNG AUS DER G-TEN GRUPPE IN DIE (G+I-1)-TE GRUPPE, BEZOGEN
AUF DEN TOTALEN ELASTISCHEN QUERSCHNITT (TOTALES 0.MOMENT) DER
G-TEN GRUPPE

M A K R O W I C H T U N G F

ALLE MOMENTE WIE DAS 0. MOMENT MIT
F(E,1) (STANDARD F(E,1) = 1/E)

M I K R O W I C H T U N G FS (FEINSTRUKTUR)

ALLE MOMENTE MIT FS(E,1) = 1
(KEINE FEINSTRUKTURWICHTUNG)

G E S A M T W I C H T U N G F * FS

TOTALE ELASTISCHE GRUPPENSTREUQUERSCHNITTE SGN UND GRUPPENSTREUKOSINUS MUEL FUER 0 16

3.GRUPPE

2.04014E+CC
2.69300E-C1

ERLAEUTERUNG
G-TE GRUPPE, 1. ZEILE: TOTALER ELASTISCHER QUERSCHNITT DER G-TEN GRUPPE
G-TE GRUPPE, 2. ZEILE: MITTLERER STREUKOSINUS DER G-TEN GRUPPE

TOTALE GRUPPENQUERSCHNITTE SGT FUER 0 16

3.GRUPPE

2.04327E+CC
2.04327E+CC
2.04327E+CC
2.04327E+CC
2.04327E+CC
2.04327E+CC

ERLAEUTERUNG
G-TE GRUPPE, L-TE ZEILE: TOTALER QUERSCHNITT DER G-TEN GRUPPE, GEWICHTET WIE DAS (L-1)-TE MOMENT DER STREUMATRIX

NORMIERUNGSINTEGRALE BIS ZUM 5. MOMENT

3.GRUPPE

4.70007E-C1
4.70007E-01
4.70007E-01
4.70007E-C1
4.70007E-01
4.70007E-C1

ERLAELTERUNG
G-TE GRUPPE, L-TE ZEILE: (L-1)-TES MOMENT DES WICHTUNGSSPEKTRUMS
INTEGRIERT UEBER DIE G-TE GRUPPE

IN MODULE 6 43.42 SECONDS CPU-TIME ARE USED

DATE 22.11.76 TIME 18.47.03

IN MODULE 6 9009 WORDS ARE NOT USED IN THE REGION FIELD

PROGRAMM KENNZIFFER 6
PROGRAMM ZUR BERECHNUNG ELASTISCHER STREUMATRIZEN

***WARNING NDF. 2 : THE FURTHER NAME 0.15830016E+08 IS GREATER THAN THE GREATEST FURTHER NAME INCLUDED IN THE KEDAK LIBRARY FOR 0 16 SGNC

***WARNING NDF. 2 : THE FURTHER NAME 0.15830016E+08 IS GREATER THAN THE GREATEST FURTHER NAME INCLUDED IN THE KEDAK LIBRARY FOR 0 16 SGNC

***MESSAGE 6.1 : WARNING NDF. 2 MAY BE IGNORED

SGNC0 ELASTISCHE STREUMATRIX 0. ORDNUNG FUER 0 16

12.GRUPPE

0.84196E+00
0.15803E+00

SGNC1 ELASTISCHE STREUMATRIX 1. ORDNUNG FUER 0 16

12.GRUPPE

0.89880E-01
-0.48180E-01

SGNC2 ELASTISCHE STREUMATRIX 2. ORDNUNG FUER 0 16

12.GRUPPE

0.34100E-02
-0.26100E-02

SGNC3 ELASTISCHE STREUMATRIX 3. ORDNUNG FUER 0 16

12.GRUPPE

0.40000E-04
-0.40000E-04

SGNC4 ELASTISCHE STREUMATRIX 4. ORDNUNG FUER 0 16

12.GRUPPE

0.0
0.0

SGNC5 ELASTISCHE STREUMATRIX 5. ORDNUNG FUER 0 16

12.GRUPPE

-0.50000E-04
0.50000E-04

ERLAEUTERUNG
L-TE ORDNUNG, G-TE GRUPPE, I-TE ZEILE: MATRIXELEMENT L-TER ORDNUNG
FUER STREUUNG AUS DER G-TEN GRUPPE IN DIE (G+I-1)-TE GRUPPE, BEZOGEN
AUF DEN TOTALEN ELASTISCHEN QUERSCHNITT (TOTALES 0.MOMENT) DER
G-TEN GRUPPE

M A K R O W I C H T U N G F

ALLE MOMENTE WIE DAS 0. MOMENT MIT
F(E,1) (STANDARD F(E,1) = 1/E)

M I K R O W I C H T U N G FS (FEINSTRUKTUR)

ALLE MOMENTE MIT FS(E,1) = 1
(KEINE FEINSTRUKTURWICHTUNG)

G E S A M T W I C H T U N G F * FS

TOTALE ELASTISCHE GRUPPENSTREUQUERSCHNITTE SGN UND GRUPPENSTREUKOSINUS MUEL FUER 0 16

12.GRUPPE

3.70000E+00
4.17000E-02

ERLAEUTERUNG
G-TE GRUPPE, 1. ZEILE: TOTALER ELASTISCHER QUERSCHNITT DER G-TEN GRUPPE
G-TE GRUPPE, 2. ZEILE: MITTLERER STREUKOSINUS DER G-TEN GRUPPE

TOTALE GRUPPENQUERSCHNITTE SGT FUER 0 16

12.GRUPPE

3.70003E+00
3.70003E+00
3.70003E+00
3.70003E+00
3.70003E+00
3.70003E+00

ERLAEUTERUNG
G-TE GRUPPE, L-TE ZEILE: TOTALER QUERSCHNITT DER G-TEN GRUPPE,
GEWICHTET WIE DAS (L-1)-TE MOMENT DER STREUMATRIX

NORMIERUNGSINTEGRALE BIS ZUM 5. MOMENT

12.GRUPPE

7.65807E-01
7.658C7E-C1
7.65807E-C1
7.658C7E-C1
7.658C7E-C1
7.658C7E-C1

ERLAEUTERUNG
G-TE GRUPPE, L-TE ZEILE: (L-1)-TES MOMENT DES WICHTUNGSSPEKTRUMS
INTEGRIERT UEBER DIE G-TE GRUPPE

IN MODULE 6 1.07 SECONDS CPU-TIME ARE USED

DATE 22.11.76 TIME 18.47.07

PROGRAMM KENNZIFFER 9
PROGRAMM ZUR BERECHNUNG DER ELASTISCHEN STREUMATRIZEN FUER DIE REMC-KORREKTUR

FOR MATERIAL O 16 , TYPE SGNC THERE ARE 20 ANGULAR DISTRIBUTIONS WITH 21 ANGLE POINTS RETRIEVED FOR THIS TASK.
THE LOWEST CALCULATED ENERGY GROUP NUMBER WITH SGNC IS 3.

IN MODULE 9 128 K BYTES OF REGION.C NOT USED.

CALCULATION FOR GROUP 3
****

FOR THIS ENERGY GROUP CALCULATION WITH ANGULAR DISTRIBUTIONS.

NUMBER OF ENERGY POINTS RETRIEVED FOR MATERIAL O 16 IN THE ENERGY-RANGE 2.500000E+06 , 4.000000E+06 EV.

SGT	33
SGN	31
MUEL	33

TOTAL NUMBER OF DIFFERENT POINTS 34

GROUP= 3 NUMBER OF FINE INTERVALS= 70 MATERIAL 0 16

THE INTERVAL-BOUNDARIES ARE

2.5000000000D+06	2.5170707750D+06	2.5341415500D+06	2.5512123250D+06	2.5682831000D+06	2.5853538750D+06
2.6024246472D+06	2.6206107040D+06	2.6388146681D+06	2.6569682658D+06	2.6736218635D+06	2.6918781824D+06
2.7101345013D+06	2.7283908202D+06	2.7466471391D+06	2.7649034580D+06	2.7831830760D+06	2.8026626939D+06
2.8215423118D+06	2.8404219298D+06	2.8593015477D+06	2.8788257450D+06	2.8983499424D+06	2.9178741397D+06
2.9373983371D+06	2.9569225344D+06	2.9771133181D+06	2.9973041018D+06	3.0174948855D+06	3.0376856692D+06
3.0578764529D+06	3.0787565813D+06	3.0996367096D+06	3.1205168380D+06	3.1413969664D+06	3.1622770947D+06
3.1838710300D+06	3.2054631113D+06	3.2270561196D+06	3.2486491279D+06	3.2702421362D+06	3.2925728633D+06
3.3149025904D+06	3.3372328174D+06	3.3595630445D+06	3.3818932716D+06	3.4049858872D+06	3.4280785029D+06
3.4511711185D+06	3.4742637341D+06	3.4973563498D+06	3.5212373831D+06	3.5451184164D+06	3.5689994498D+06
3.5928804831D+06	3.6167615164D+06	3.6414578853D+06	3.6661542541D+06	3.6908506229D+06	3.7155469917D+06
3.7402433605D+06	3.7657829017D+06	3.7913224428D+06	3.8168619840D+06	3.8424015251D+06	3.8679410662D+06
3.8943525669D+06	3.9207640675D+06	3.9471755682D+06	3.9735870688D+06	3.9999985695D+06	

THE VALUES OF SGT

1.0834E+00	1.0891E+00	1.0970E+00	1.1005E+00	1.1038E+00	1.1085E+00	1.1121E+00	1.1146E+00	1.1177E+00	1.1215E+00
1.1259E+00	1.1301E+00	1.1328E+00	1.1357E+00	1.1393E+00	1.1433E+00	1.1483E+00	1.1511E+00	1.1524E+00	1.1542E+00
1.1563E+00	1.1588E+00	1.1616E+00	1.1651E+00	1.1694E+00	1.1731E+00	1.1773E+00	1.2102E+00	1.2683E+00	1.3391E+00
1.4284E+00	1.5361E+00	1.6403E+00	1.7403E+00	1.8771E+00	2.0272E+00	2.1975E+00	2.3608E+00	2.5067E+00	2.6964E+00
2.9286E+00	3.1488E+00	3.1416E+00	3.1065E+00	3.0625E+00	3.0117E+00	3.0163E+00	3.4876E+00	3.3902E+00	3.1098E+00
2.9511E+00	2.9673E+00	2.9900E+00	3.0184E+00	3.0377E+00	3.0171E+00	2.9866E+00	2.9630E+00	2.9482E+00	3.0611E+00
3.8995E+00	4.0912E+00	2.9131E+00	2.5995E+00	2.4398E+00	2.3468E+00	2.2748E+00	2.2145E+00	2.1558E+00	2.0816E+00

THE VALUES OF SGN

1.0834E+00	1.0891E+00	1.0970E+00	1.1005E+00	1.1038E+00	1.1085E+00	1.1121E+00	1.1146E+00	1.1177E+00	1.1215E+00
1.1259E+00	1.1301E+00	1.1328E+00	1.1357E+00	1.1393E+00	1.1433E+00	1.1483E+00	1.1511E+00	1.1524E+00	1.1542E+00
1.1563E+00	1.1588E+00	1.1616E+00	1.1651E+00	1.1694E+00	1.1731E+00	1.1773E+00	1.2102E+00	1.2683E+00	1.3391E+00
1.4284E+00	1.5361E+00	1.6403E+00	1.7403E+00	1.8771E+00	2.0272E+00	2.1975E+00	2.3608E+00	2.5067E+00	2.6964E+00
2.9286E+00	3.1488E+00	3.1416E+00	3.1065E+00	3.0625E+00	3.0117E+00	3.0163E+00	3.4876E+00	3.3902E+00	3.1098E+00
2.9511E+00	2.9673E+00	2.9900E+00	3.0184E+00	3.0377E+00	3.0162E+00	2.9844E+00	2.9599E+00	2.9441E+00	3.0562E+00
3.8939E+00	4.0849E+00	2.9059E+00	2.5910E+00	2.4288E+00	2.3323E+00	2.2566E+00	2.1942E+00	2.1161E+00	2.0104E+00

THE VALUES OF MUEL

2.5992E-01	2.5142E-01	2.3986E-01	2.3344E-01	2.3823E-01	2.4623E-01	2.5310E-01	2.5824E-01	2.6464E-01	2.7228E-01
2.8134E-01	2.8989E-01	2.9605E-01	3.0305E-01	3.1091E-01	3.0744E-01	2.9906E-01	2.9227E-01	2.8747E-01	2.8141E-01
2.7392E-01	2.6505E-01	2.5984E-01	2.5775E-01	2.5271E-01	2.2247E-01	1.7854E-01	1.5867E-01	1.7247E-01	1.8805E-01
2.0550E-01	2.2383E-01	2.3245E-01	2.3525E-01	2.3859E-01	2.3790E-01	2.2484E-01	2.0879E-01	1.9454E-01	1.7830E-01
1.6146E-01	1.5737E-01	1.6329E-01	1.7065E-01	1.8015E-01	1.9153E-01	2.0503E-01	2.2069E-01	2.3783E-01	2.6301E-01
2.8666E-01	2.9861E-01	3.1334E-01	3.3147E-01	3.4607E-01	3.5223E-01	3.5745E-01	3.6025E-01	3.6177E-01	3.5152E-01
3.0352E-01	2.6847E-01	2.5578E-01	3.3589E-01	3.7451E-01	3.6960E-01	3.6851E-01	3.7488E-01	3.9515E-01	4.2437E-01

THE VALUES OF FLUX

2.0269E-01	2.0133E-01	1.9998E-01	1.9864E-01	1.9732E-01	2.0269E-01	2.0132E-01	1.9995E-01	1.9863E-01	1.9731E-01
2.0270E-01	2.0132E-01	1.9997E-01	1.9864E-01	1.9732E-01	2.0270E-01	2.0132E-01	1.9998E-01	1.9863E-01	1.9733E-01
2.0270E-01	2.0133E-01	1.9998E-01	1.9864E-01	1.9732E-01	2.0270E-01	2.0133E-01	1.9996E-01	1.9864E-01	1.9733E-01
2.0269E-01	2.0132E-01	1.9997E-01	1.9864E-01	1.9733E-01	2.0269E-01	2.0132E-01	1.9997E-01	1.9864E-01	1.9732E-01
2.0269E-01	2.0132E-01	1.9997E-01	1.9864E-01	1.9732E-01	2.0269E-01	2.0133E-01	1.9998E-01	1.9864E-01	1.9733E-01
2.0268E-01	2.0131E-01	1.9996E-01	1.9863E-01	1.9731E-01	2.0270E-01	2.0134E-01	1.9998E-01	1.9864E-01	1.9733E-01
2.0270E-01	2.0134E-01	1.9998E-01	1.9865E-01	1.9733E-01	2.0270E-01	2.0134E-01	1.9998E-01	1.9865E-01	1.9733E-01

```
 ELASTIC SCATTERING MATRIX   SGNC0  FOR O  16      GROUP=    3
FROM GROUP    3 TO GROUP      3
  2.8632E-02   7.9558E-02   1.2307E-01   1.6376E-01   2.1609E-01   2.7194E-01   3.2652E-01   3.7685E-01   4.2176E-01   4.6435E-01
  5.0277E-01   5.3766E-01   5.6899E-01   5.9726E-01   6.2221E-01   6.3739E-01   6.5213E-01   6.6617E-01   6.8074E-01   6.9553E-01
  7.1061E-01   7.2600E-01   7.4295E-01   7.6184E-01   7.7901E-01   7.7885E-01   7.7749E-01   7.8457E-01   7.9851E-01   8.1060E-01
  8.2464E-01   8.5376E-01   8.8302E-01   9.0946E-01   9.3567E-01   9.5923E-01   9.7841E-01   9.9646E-01   1.0000E+00   1.0000E+00
  1.0000E+00   1.0000E+00   1.0000E+00   1.0000E+00   1.0000E+00   1.0000E+00   1.0000E+00   1.0000E+00   1.0000E+00   1.0000E+00
  1.0000E+00   1.0000E+00   1.0000E+00   1.0000E+00   1.0000E+00   1.0000E+00   1.0000E+00   1.0000E+00   1.0000E+00   1.0000E+00
  1.0000E+00   1.0000E+00   1.0000E+00   1.0000E+00   1.0000E+00   1.0000E+00   1.0000E+00   1.0000E+00   1.0000E+00   1.0000E+00
FROM GROUP    3 TO GROUP      4
  9.7137E-01   9.2044E-01   8.7693E-01   8.3624E-01   7.8391E-01   7.2806E-01   6.7348E-01   6.2315E-01   5.7824E-01   5.3565E-01
  4.9723E-01   4.6234E-01   4.3101E-01   4.0274E-01   3.7779E-01   3.6261E-01   3.4787E-01   3.3383E-01   3.1926E-01   3.0447E-01
  2.8939E-01   2.7400E-01   2.5705E-01   2.3816E-01   2.2099E-01   2.2115E-01   2.2251E-01   2.1543E-01   2.0149E-01   1.8940E-01
  1.7536E-01   1.4624E-01   1.1698E-01   9.0544E-02   6.4333E-02   4.0767E-02   2.1587E-02   3.5415E-03   0.0          0.0
  0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
  0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
  0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0

 ELASTIC SCATTERING MATRIX   SGNC1  FOR O  16      GROUP=    3
FROM GROUP    3 TO GROUP      3
  2.8124E-02   7.6294E-02   1.1488E-01   1.4867E-01   1.9101E-01   2.3413E-01   2.7420E-01   3.0943E-01   3.3936E-01   3.6692E-01
  3.9075E-01   4.1176E-01   4.2986E-01   4.4596E-01   4.5950E-01   4.6088E-01   4.5634E-01   4.5107E-01   4.4548E-01   4.3901E-01
  4.3150E-01   4.2311E-01   4.1452E-01   4.0639E-01   3.9624E-01   3.6830E-01   3.3272E-01   3.1388E-01   3.2610E-01   3.3912E-01
  3.4956E-01   3.4519E-01   3.3365E-01   3.1584E-01   2.9730E-01   2.7671E-01   2.4621E-01   2.1372E-01   1.9444E-01   1.7876E-01
  1.6288E-01   1.5749E-01   1.6546E-01   1.7403E-01   1.8276E-01   1.9168E-01   2.0487E-01   2.2092E-01   2.4290E-01   2.6612E-01
  2.8655E-01   3.0207E-01   3.1737E-01   3.3280E-01   3.4607E-01   3.5239E-01   3.5744E-01   3.6040E-01   3.6177E-01   3.5346E-01
  3.0952E-01   2.6565E-01   2.5623E-01   3.3873E-01   3.7393E-01   3.6932E-01   3.6848E-01   3.7486E-01   3.9532E-01   4.2424E-01
FROM GROUP    3 TO GROUP      4
  2.3207E-01   1.7351E-01   1.2499E-01   8.4612E-02   4.7913E-02   1.1998E-02  -2.0702E-02  -4.8798E-02  -7.2169E-02  -9.1873E-02
 -1.0833E-01  -1.2187E-01  -1.3277E-01  -1.4164E-01  -1.4958E-01  -1.5310E-01  -1.5699E-01  -1.5923E-01  -1.6035E-01  -1.6054E-01
 -1.6002E-01  -1.5827E-01  -1.5475E-01  -1.4904E-01  -1.4362E-01  -1.4882E-01  -1.5501E-01  -1.5629E-01  -1.5308E-01  -1.4981E-01
 -1.4365E-01  -1.2315E-01  -1.0122E-01  -8.0558E-02  -5.8867E-02  -3.8391E-02  -2.0908E-02  -3.5040E-03   0.0          0.0
  0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
  0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
  0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0

 ELASTIC SCATTERING MATRIX   SGNC2  FOR O  16      GROUP=    3
FROM GROUP    3 TO GROUP      3
  2.7131E-02   7.0042E-02   9.9624E-02   1.2133E-01   1.4679E-01   1.6935E-01   1.8704E-01   2.0005E-01   2.0910E-01   2.1664E-01
  2.2226E-01   2.2662E-01   2.3063E-01   2.3452E-01   2.3776E-01   2.2598E-01   2.0872E-01   1.9082E-01   1.7282E-01   1.5470E-01
  1.3639E-01   1.1801E-01   1.0039E-01   8.3672E-02   6.7266E-02   4.7688E-02   2.6604E-02   2.4064E-02   5.2627E-02   8.3693E-02
  1.1455E-01   1.2777E-01   1.3734E-01   1.4770E-01   1.6079E-01   1.7492E-01   1.8765E-01   2.0213E-01   2.0388E-01   2.0227E-01
  2.0095E-01   2.3333E-01   2.8736E-01   3.3097E-01   2.9572E-01   2.4296E-01   2.3676E-01   2.5273E-01   2.6849E-01   2.8433E-01
  2.8402E-01   2.5871E-01   2.2710E-01   1.8440E-01   1.4484E-01   1.7285E-01   2.1613E-01   2.2445E-01   2.3206E-01   2.4794E-01
  2.4797E-01   1.9314E-01   1.4255E-01   1.3931E-01   1.4052E-01   1.4159E-01   1.4164E-01   1.3322E-01   1.2272E-01   1.1216E-01
FROM GROUP    3 TO GROUP      4
  3.0845E-02  -2.2585E-02  -6.3029E-02  -9.2340E-02  -1.0515E-01  -1.1118E-01  -1.1206E-01  -1.0809E-01  -1.0089E-01  -9.1295E-02
 -7.9792E-02  -6.6708E-02  -5.3283E-02  -3.9871E-02  -2.6700E-02  -1.8354E-02  -1.1391E-02  -4.2416E-03   3.0887E-03   1.0504E-02
  1.8002E-02   2.5379E-02   3.2009E-02   3.7669E-02   4.3010E-02   5.1082E-02   6.0377E-02   7.0150E-02   7.9667E-02   8.7488E-02
  9.1992E-02   8.4364E-02   7.3982E-02   6.2793E-02   4.8863E-02   3.3915E-02   1.9594E-02   3.4299E-03   0.0          0.0
  0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
  0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
  0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
```

```
 ELASTIC SCATTERING MATRIX    SGNC3  FOR C  16      GROUP=    3
FROM GROUP     3 TO GROUP      3
  2.5690E-02  6.1332E-02  7.9325E-02  8.6706E-02  9.3568E-02  9.537CE-02  9.2515E-02  8.7387E-02  8.1321E-02  7.6172E-02
  7.2065E-02  6.9520E-02  6.9111E-02  7.0693E-02  7.3492E-02  6.5204E-02  5.3285E-02  4.2708E-02  3.3358E-02  2.5322E-02
  1.8492E-02  1.2826E-02  8.3665E-03  4.9604E-03  3.3713E-03  1.1791E-02  2.5271E-02  4.3613E-02  6.5881E-02  8.7423E-02
  1.0681E-01  1.1680E-01  1.2393E-01  1.2910E-01  1.3050E-01  1.2685E-01  1.1349E-01  9.5200E-02  8.7986E-02  8.4045E-02
  8.0105E-02  7.6257E-02  7.2474E-02  6.8053E-02  6.0264E-02  5.1702E-02  5.2221E-02  5.7026E-02  6.1575E-02  6.6476E-02
  7.2452E-02  7.9925E-02  8.4043E-02  8.2445E-02  8.1430E-02  9.7457E-02  1.2114E-01  1.4800E-01  1.6944E-01  1.6949E-01
  1.5988E-01  1.2594E-01  9.4662E-02  8.9508E-02  8.6907E-02  8.4169E-02  8.1324E-02  7.8267E-02  7.5335E-02  7.2314E-02
FROM GROUP     3 TO GROUP      4
 -2.1332E-02 -5.8518E-02 -7.8137E-02 -8.5895E-02 -8.5742E-02 -7.9055E-02 -6.7663E-02 -5.3958E-02 -3.9306E-02 -2.5523E-02
 -1.2791E-02 -1.4661E-03  7.8517E-03  1.5170E-02  2.0626E-02  2.5695E-02  3.0188E-02  3.3327E-02  3.5160E-02  3.5686E-02
  3.4873E-02  3.2800E-02  2.9479E-02  2.5089E-02  1.9990E-02  1.6245E-02  1.0775E-02  5.4773E-04 -1.3815E-02 -2.7080E-02
 -3.8377E-02 -4.1731E-02 -4.2353E-02 -4.1041E-02 -3.5975E-02 -2.7858E-02 -1.7732E-02 -3.3209E-03  0.0          0.0
  0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0

 ELASTIC SCATTERING MATRIX    SGNC4  FOR C  16      GROUP=    3
FROM GROUP     3 TO GROUP      3
  2.3858E-02  5.0880E-02  5.6603E-02  5.0799E-02  4.2643E-02  3.0504E-02  1.6995E-02  5.2857E-03 -3.5221E-03 -8.7091E-03
 -1.0548E-02 -9.1562E-03 -5.0435E-03  1.1569E-03  8.5279E-03  1.0982E-02  1.2291E-02  1.4348E-02  1.6877E-02  1.9585E-02
  2.2146E-02  2.4262E-02  2.5179E-02  2.4938E-02  2.3802E-02  2.7658E-02  3.1327E-02  3.0868E-02  2.6310E-02  2.0497E-02
  1.3208E-02  2.3568E-03 -9.0187E-03 -1.9135E-02 -2.6034E-02 -2.8737E-02 -2.5849E-02 -1.6022E-02 -1.5302E-02 -1.7761E-02
 -2.0138E-02 -1.1520E-02  4.1677E-03  1.7049E-02  6.3867E-03 -9.0488E-03 -5.2237E-03  7.5461E-03  2.0126E-02  3.2818E-02
  3.7446E-02  2.9567E-02  2.2637E-02  1.8102E-02  1.4312E-02  2.3076E-02  3.7011E-02  5.3558E-02  6.6910E-02  6.6900E-02
  6.1739E-02  4.4087E-02  2.7636E-02  2.4339E-02  2.2197E-02  2.0059E-02  1.8056E-02  1.7861E-02  1.8076E-02  1.8323E-02
FROM GROUP     3 TO GROUP      4
 -1.9493E-02 -4.7586E-02 -5.4382E-02 -4.9191E-02 -3.8882E-02 -2.4001E-02 -7.7871E-03  6.7453E-03  1.8241E-02  2.6290E-02
  3.0935E-02  3.2408E-02  3.1183E-02  2.7854E-02  2.3124E-02  1.8863E-02  1.4066E-02  8.4821E-03  2.4356E-03 -3.7926E-03
 -9.9173E-03 -1.5539E-02 -2.0186E-02 -2.3580E-02 -2.5868E-02 -2.9681E-02 -3.2378E-02 -2.9867E-02 -2.1303E-02 -1.1544E-02
 -1.0348E-03  6.8592E-03  1.3886E-02  1.9670E-02  2.2235E-02  2.0859E-02  1.5441E-02  3.1797E-03  0.0          0.0
  0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0

 ELASTIC SCATTERING MATRIX    SGNC5  FOR O  16      GROUP=    3
FROM GROUP     3 TO GROUP      3
  2.1707E-02  3.9518E-02  3.4199E-02  1.9244E-02  3.3969E-03 -1.2238E-02 -2.4399E-02 -3.1099E-02 -3.2596E-02 -3.0207E-02
 -2.4718E-02 -1.7514E-02 -9.8489E-03 -2.5163E-03  3.8657E-03  9.3055E-03  1.3877E-02  1.7046E-02  1.8614E-02  1.8580E-02
  1.6937E-02  1.3771E-02  9.3943E-03  4.1947E-03 -1.5395E-03 -9.7363E-03 -1.9124E-02 -2.5922E-02 -2.7158E-02 -2.5711E-02
 -2.1778E-02 -1.8080E-02 -1.3129E-02 -7.2250E-03 -2.3140E-03  9.9944E-05 -2.1980E-04 -9.2803E-03 -1.1454E-02 -1.0651E-02
 -9.8232E-03 -7.0454E-03 -3.0412E-03  6.0373E-04  1.1132E-03  9.5204E-04  1.1082E-03  1.4350E-03  1.7714E-03  2.1302E-03
  1.8119E-03  5.1073E-04 -1.2618E-03 -3.9408E-03 -6.2896E-03 -2.0798E-03  4.2457E-03  9.3155E-03  1.3121E-02  1.2566E-02
  1.0432E-02  4.7235E-03 -6.2974E-04 -2.1325E-03 -3.2640E-03 -4.4110E-03 -5.2205E-03 -2.7156E-03  5.9883E-04  3.8816E-03
FROM GROUP     3 TO GROUP      4
 -1.7513E-02 -3.6185E-02 -3.1722E-02 -1.7538E-02 -1.8866E-03  1.3635E-02  2.5643E-02  3.2202E-02  3.3566E-02  3.0946E-02
  2.5365E-02  1.8047E-02  1.0210E-02  2.7337E-03 -3.7901E-03 -9.2389E-03 -1.3759E-02 -1.6875E-02 -1.8431E-02 -1.8370E-02
 -1.6678E-02 -1.3470E-02 -9.0525E-03 -3.8096E-03  1.8395E-03  8.3379E-03  1.5565E-02  2.1232E-02  2.3019E-02  2.2143E-02
  1.8538E-02  1.3058E-02  5.7690E-03 -2.4635E-03 -9.6809E-03 -1.3783E-02 -1.2866E-02 -3.0095E-03  0.0          0.0
  0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0


IN MODULE  9   21.04 SECONDS CPU-TIME ARE USED

DATE 22.11.76    TIME 18.47.54
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PROGRAMM KENNZIFFER 9
PROGRAMM ZUR BERECHNUNG DER ELASTISCHEN STREUMATRIZEN FUER DIE REMO-KORREKTUR



FOR MATERIAL  O  16    , TYPE  SGNC       THERE ARE     0  ANGULAR DISTRIBUTIONS WITH      0  ANGLE POINTS RETRIEVED FOR THIS TASK.
THE LOWEST CALCULATED ENERGY GROUP NUMBER WITH SGNC IS 11.


IN MODULE  9        128  K BYTES OF REGION.G NOT USED.



CALCULATION FOR GROUP  12
*************************

FOR THIS ENERGY GROUP CALCULATION   WITHOUT  ANGULAR DISTRIBUTIONS.

NUMBER OF ENERGY POINTS RETRIEVED FOR MATERIAL  O  16      IN THE ENERGY-RANGE  4.649996E+03 ,  1.000000E+04 EV.

  SGT             2
  SGN             2
  MUEL            2

TOTAL NUMBER OF DIFFERENT POINTS          2

GROUP= 12 NUMBER OF FINE INTERVALS=   70 MATERIAL  O  16

THE INTERVAL-BOUNDARIES ARE

    4.6499960937D+03     4.7022783861D+03     4.7545606785D+03     4.8068429709D+03     4.8591252633D+03     4.9114075557D+03
    4.9666290313D+03     5.0218505069D+03     5.0770719825D+03     5.1322934581D+03     5.1875149337D+03     5.2458408263D+03
    5.3041667188D+03     5.3624926114D+03     5.4208185039D+03     5.4791443964D+03     5.5407492287D+03     5.6023540610D+03
    5.6639588932D+03     5.7255637255D+03     5.7871685577D+03     5.8522366637D+03     5.9173047697D+03     5.9823728757D+03
    6.0474409817D+03     6.1125090876D+03     6.1812351641D+03     6.2499612407D+03     6.3186873172D+03     6.3874133937D+03
    6.4561394702D+03     6.5287291595D+03     6.6013188487D+03     6.6739085380D+03     6.7464982272D+03     6.8190879165D+03
    6.8957584214D+03     6.9724289262D+03     7.0490994311D+03     7.1257699360D+03     7.2024404409D+03     7.2834211750D+03
    7.3644019090D+03     7.4453826431D+03     7.5263633771D+03     7.6073441112D+03     7.6928773850D+03     7.7784106588D+03
    7.8639439326D+03     7.9494772064D+03     8.0350104802D+03     8.1253522265D+03     8.2156939728D+03     8.3060357190D+03
    8.3963774653D+03     8.4867192116D+03     8.5821397509D+03     8.6775602903D+03     8.7729808296D+03     8.8684013690D+03
    8.9638219083D+03     9.0646067581D+03     9.1653916079D+03     9.2661764577D+03     9.3669613075D+03     9.4677461573D+03
    9.5741968861D+03     9.6806476148D+03     9.7870983436D+03     9.8935490723D+03     9.9999998011D+03

THE VALUES OF SGT
  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00
  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00
  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00
  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00
  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00
  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00
  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00
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THE VALUES OF SGN
  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00
  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00
  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00
  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00
  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00
  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00
  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00  3.7000E+00

THE VALUES OF MUEL
  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02
  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02
  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02
  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02
  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02
  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02
  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02

THE VALUES OF FLUX
  2.0432E-01  2.0206E-01  1.9985E-01  1.9771E-01  1.9558E-01  2.0433E-01  2.0206E-01  1.9986E-01  1.9770E-01  1.9557E-01
  2.0433E-01  2.0206E-01  1.9986E-01  1.9769E-01  1.9557E-01  2.0433E-01  2.0207E-01  1.9986E-01  1.9769E-01  1.9558E-01
  2.0432E-01  2.0207E-01  1.9985E-01  1.9769E-01  1.9559E-01  2.0433E-01  2.0207E-01  1.9985E-01  1.9770E-01  1.9558E-01
  2.0433E-01  2.0207E-01  1.9986E-01  1.9769E-01  1.9558E-01  2.0433E-01  2.0206E-01  1.9986E-01  1.9770E-01  1.9557E-01
  2.0432E-01  2.0206E-01  1.9985E-01  1.9770E-01  1.9558E-01  2.0432E-01  2.0207E-01  1.9985E-01  1.9770E-01  1.9557E-01
  2.0433E-01  2.0206E-01  1.9986E-01  1.9769E-01  1.9558E-01  2.0432E-01  2.0207E-01  1.9986E-01  1.9769E-01  1.9558E-01
  2.0433E-01  2.0207E-01  1.9986E-01  1.9769E-01  1.9558E-01  2.0432E-01  2.0206E-01  1.9986E-01  1.9769E-01  1.9558E-01
```

```
 ELASTIC SCATTERING MATRIX   SGNCO  FOR O  16      GROUP=  12
FROM GROUP   12 TO GROUP    12
  2.4930E-02  7.4146E-02  1.2229E-01  1.6940E-01  2.1551E-01  2.6189E-01  3.0851E-01  3.5411E-01  3.9873E-01  4.4241E-01
  4.8633E-01  5.3049E-01  5.7369E-01  6.1596E-01  6.5732E-01  6.9893E-01  7.4076E-01  7.8168E-01  8.2171E-01  8.6089E-01
  9.0030E-01  9.3992E-01  9.7867E-01  9.9994E-01  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00
  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00
  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00
  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00
  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00
FROM GROUP   12 TO GROUP    13
  9.7507E-01  9.2585E-01  8.7771E-01  8.3060E-01  7.8449E-01  7.3811E-01  6.9150E-01  6.4589E-01  6.0127E-01  5.5760E-01
  5.1367E-01  4.6951E-01  4.2631E-01  3.8404E-01  3.4268E-01  3.0107E-01  2.5924E-01  2.1832E-01  1.7829E-01  1.3911E-01
  9.9699E-02  6.0082E-02  2.1328E-02  6.4071E-05  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
```

```
 ELASTIC SCATTERING MATRIX   SGNC1  FOR O  16      GROUP=  12
FROM GROUP   12 TO GROUP    12
   2.4195E-02  6.9073E-02  1.0876E-01  1.4350E-01  1.7356E-01  1.9979E-01  2.2210E-01  2.3993E-01  2.5352E-01  2.6308E-01
   2.6891E-01  2.7093E-01  2.6913E-01  2.6371E-01  2.5486E-01  2.4237E-01  2.2618E-01  2.0676E-01  1.8429E-01  1.5995E-01
   1.3005E-01  9.7555E-02  6.2373E-02  4.1764E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02
   4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02
   4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02
   4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02
   4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02  4.1700E-02
FROM GROUP   12 TO GROUP    13
   1.7505E-02 -2.7374E-02 -6.7056E-02 -1.0180E-01 -1.3186E-01 -1.5809E-01 -1.8040E-01 -1.9323E-01 -2.1182E-01 -2.2138E-01
  -2.2721E-01 -2.2923E-01 -2.2743E-01 -2.2201E-01 -2.1316E-01 -2.0067E-01 -1.8448E-01 -1.6506E-01 -1.4259E-01 -1.1725E-01
  -8.8349E-02 -5.5855E-02 -2.0673E-02 -6.3965E-05  0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0

 ELASTIC SCATTERING MATRIX   SGNC2  FOR O  16      GROUP=  12
FROM GROUP   12 TO GROUP    12
   2.2773E-02  5.9644E-02  8.4723E-02  9.9697E-02  1.0612E-01  1.0526E-01  9.8065E-02  8.5812E-02  6.9790E-02  5.1172E-02
   3.0449E-02  8.5935E-03 -1.2811E-02 -3.2821E-02 -5.0589E-02 -6.5693E-02 -7.7126E-02 -8.3682E-02 -8.4711E-02 -7.9638E-02
  -6.7489E-02 -4.7244E-02 -1.8639E-02  7.3013E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04
   7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04
   7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04
   7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04
   7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04  7.9535E-04
FROM GROUP   12 TO GROUP    13
  -2.2003E-02 -5.8874E-02 -8.3954E-02 -9.8927E-02 -1.0535E-01 -1.0449E-01 -9.7295E-02 -8.5042E-02 -6.9020E-02 -5.0402E-02
  -2.9679E-02 -7.8243E-03  1.3581E-02  3.3591E-02  5.1359E-02  6.6463E-02  7.7896E-02  8.4452E-02  8.5481E-02  8.0408E-02
   6.8258E-02  4.8013E-02  1.9409E-02  6.3751E-05  0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0

 ELASTIC SCATTERING MATRIX   SGNC3  FOR O  16      GROUP=  12
FROM GROUP   12 TO GROUP    12
   2.0758E-02  4.7165E-02  5.5412E-02  5.0870E-02  3.7988E-02  1.9864E-02 -6.1161E-04 -2.0375E-02 -3.7482E-02 -5.0590E-02
  -5.9020E-02 -6.2021E-02 -5.9341E-02 -5.1481E-02 -3.9301E-02 -2.3496E-02 -5.4317E-03  1.2577E-02  2.8380E-02  3.9653E-02
   4.3890E-02  3.7668E-02  1.7619E-02  6.3371E-05  0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
FROM GROUP   12 TO GROUP    13
  -2.0759E-02 -4.7166E-02 -5.5413E-02 -5.0871E-02 -3.7989E-02 -1.9865E-02  6.1058E-04  2.0374E-02  3.7481E-02  5.0589E-02
   5.9019E-02  6.2020E-02  5.9340E-02  5.1480E-02  3.9300E-02  2.3495E-02  5.4306E-03 -1.2578E-02 -2.8381E-02 -3.9654E-02
  -4.3891E-02 -3.7669E-02 -1.7620E-02 -6.3432E-05  0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
```

```
 ELASTIC SCATTERING MATRIX   SGNC4  FOR O  16      GROUP=  12
FROM GROUP   12 TO GROUP     12
   1.8280E-02  3.3293E-02  2.6764E-02  9.9353E-03 -9.4079E-03 -2.6616E-02 -3.8343E-02 -4.2714E-02 -3.9891E-02 -3.1054E-02
  -1.7599E-02 -1.5954E-03  1.4121E-02  2.7240E-02  3.5906E-02  3.8857E-02  3.5161E-02  2.5138E-02  1.0466E-02 -5.9646E-03
  -2.0293E-02 -2.6227E-02 -1.5427E-02 -6.3262E-05 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07
  -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07
  -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07
  -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07
  -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07 -2.5103E-07
FROM GROUP   12 TO GROUP     13
  -1.8280E-02 -3.3294E-02 -2.6764E-02 -9.9355E-03  9.4076E-03  2.6616E-02  3.8342E-02  4.2714E-02  3.9891E-02  3.1053E-02
   1.7599E-02  1.5951E-03 -1.4122E-02 -2.7240E-02 -3.5906E-02 -3.8858E-02 -3.5161E-02 -2.5138E-02 -1.0466E-02  5.9643E-03
   2.0293E-02  2.6227E-02  1.5427E-02  6.3009E-05  0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0

 ELASTIC SCATTERING MATRIX   SGNC5  FOR O  16      GROUP=  12
FROM GROUP   12 TO GROUP     12
   1.5493E-02  1.9753E-02  3.8694E-03 -1.4678E-02 -2.7070E-02 -3.0199E-02 -2.4099E-02 -1.1559E-02  3.4979E-03  1.7329E-02
   2.7192E-02  3.0876E-02  2.7581E-02  1.8350E-02  5.3975E-03 -8.6760E-03 -2.0370E-02 -2.6060E-02 -2.3784E-02 -1.3665E-02
   1.7278E-03  1.5139E-02  1.2970E-02  6.2536E-05  0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
FROM GROUP   12 TO GROUP     13
  -1.5493E-02 -1.9753E-02 -3.8694E-03  1.4678E-02  2.7070E-02  3.0199E-02  2.4099E-02  1.1559E-02 -3.4980E-03 -1.7329E-02
  -2.7192E-02 -3.0876E-02 -2.7581E-02 -1.8350E-02 -5.3975E-03  8.6760E-03  2.0370E-02  2.6060E-02  2.3784E-02  1.3665E-02
  -1.7278E-03 -1.5139E-02 -1.2970E-02 -6.2536E-05  0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0

IN MODULE  9    3.40 SECONDS CPU-TIME ARE USED

DATE 22.11.76    TIME 18.48.07
```

Appendix B. Program Listing

On the following pages B 2 to B 144 the listing of the program MIGRØS-3 is given.

```
C      PROGRAMM ZUR STEUERUNG DES MIGROS-SYSTEMS                                10
C                                                                               20
       REAL*8 MAT1,N1,N2,MIGROS,DD                                              30
       DIMENSION XL(5000),NXL(5000)                                             40
       COMMON MAT1,K(2),NOUT,LIZ                                                50
       EQUIVALENCE (XL(1),NXL(1))                                               60
       DATA N1/'BLOC '/,N2/'ENDE '/,SGC/'SGC '/,MIGROS/'MIGR '/,                70
      1DD/'FT10F001'/                                                           80
       NINP=5                                                                   90
       NOUT=6                                                                  100
       KDE=1                                                                   110
       LIZ=3                                                                   120
       NF=8                                                                    130
       N6=10                                                                   140
       CALL FSPIE                                                              150
       READ (NINP,28) MAT1                                                     160
   28  FORMAT(A8)                                                              170
       IF(MAT1.EQ.MIGROS)  GO TO 27                                            180
       REWIND NINP                                                             190
       CALL BING(NOUT)                                                         200
   27  CALL NDFOPN (KDE,NXL,NUDAT,0)                                           210
       WRITE (NOUT,1) NUDAT                                                    220
    1  FORMAT(1H1/' STAND DER KERNDATENBIBLIOTHEK VOM ',I10)                   230
       WRITE (LIZ) LIZ                                                         240
       BACKSPACE LIZ                                                           250
       WRITE (NF) NF                                                           260
       BACKSPACE NF                                                            270
       ICON=0                                                                  280
       N=1                                                                     290
       CALL DDTEST (N,DD,ICON,NST)                                             300
       IF(NST.EQ.1)  GO TO 29                                                  310
       WRITE (N6) N6                                                           320
       BACKSPACE N6                                                            330
   29  CALL GAREA (XL,M,L)                                                     340
       IADR=M+L                                                                350
       M=M+1                                                                   360
       CALL FREE72 (NINP,NF,NOUT,XL(M),XL(M),XL(M))                            370
       IZI=0                                                                   380
    2  READ (NF)                                                               390
   16  READ (NF) MAT1,MAT2                                                     400
       IZI=IZI+2                                                               410
       IF(MAT1.EQ.N1.AND.MAT2.EQ.1) GO TO 3                                    420
       NE=26                                                                   430
       GO TO 4                                                                 440
    3  READ (NF) NE                                                            450
       READ (NF) MAT1,MAT2                                                     460
       IZI=IZI+2                                                               470
    4  IF(MAT1.EQ.N1.AND.MAT2.EQ.2) GO TO 5                                    480
       NFE=1                                                                   490
       LSPEC=1                                                                 500
       GO TO 6                                                                 510
    5  READ (NF) LSPEC,NFE                                                     520
       NFE=NFE+NE                                                              530
       READ (NF) MAT1,MAT2                                                     540
       IZI=IZI+2                                                               550
    6  IF(MAT1.EQ.N1.AND.MAT2.NE.3) GO TO 7                                    560
       READ (NF) NA                                                            570
       READ (NF) MAT1,MAT2                                                     580
       IZI=IZI+2                                                               590
       GO TO 9                                                                 600
    7  WRITE (NOUT,8)                                                          610
    8  FORMAT(1HO/' ***ERROR O. 1 : THE INPUT OF THE MODULE NUMBERS WAS N      620
      1OT FOUND')                                                              630
       STOP                                                                    640
    9  IF(MAT1.EQ.N1.AND.MAT2.EQ.4)  GO TO 10                                  650
       NT=3                                                                    660
       GO TO 11                                                                670
   10  READ (NF) NT                                                           680
       READ (NF) MAT1,MAT2                                                     690
       IZI=IZI+2                                                               700
   11  IF(MAT1.EQ.N1.AND.MAT2.EQ.5) GO TO 12                                   710
       MI=7                                                                    720
       GO TO 13                                                                730
   12  READ (NF) MI                                                           740
       READ (NF) MAT1,MAT2                                                     750
       IZI=IZI+2                                                               760
   13  IF(MAT1.EQ.N1.AND.MAT2.EQ.6) GO TO 14                                   770
       NTYP=8                                                                  780
                                                                               790
       GO TO 15                                                                800
   14  READ (NF) NTYP                                                          810
       BACKSPACE NF                                                            820
       N=M+NTYP-1                                                              830
       READ (NF) NTYP,(XL(I),XL(I+200),I=M,N)                                  840
   24  READ (NF) MAT1,MAT2                                                     850
       IZI=IZI+2                                                               860
       DO 26 I=M,N                                                             870
       IF(XL(I).EQ.SGC)  NTYP=NTYP+1                                           880
   26  CONTINUE                                                                890
   15  IF(MAT1.EQ.N1.AND.MAT2.LT.62)  GO TO 22                                 900
       IF(MAT1.EQ.N1.AND.MAT2.GT.62)  GO TO 23                                 910
       IF(MAT1.EQ.N2)  GO TO 23                                                920
       READ (NF) NMAT                                                          930
       IZI=IZI+1                                                               940
       GO TO 25                                                                950
   22  READ (NF)                                                               960
       READ(NF) MAT1,MAT2                                                      970
       IZI=IZI+2                                                               980
       GO TO 15                                                                990
   23  NMAT=1                                                                 1000
   25  DO 17 I=1,IZI                                                          1010
   17  BACKSPACE NF                                                           1020
       NM  =NTYP*2+M                                                          1030
       NZ=NM+NMAT*2                                                           1040
       NENG=NZ+NMAT                                                           1050
       NSPEC=NENG+NE                                                          1060
       NARB=NSPEC+NFE*(LSPEC+1)                                               1070
       NTEMP=NARB+NA*3                                                        1080
       NSI=NTEMP+NT                                                           1090
       NG=NSI+MI+1                                                            1100
       NN1=NG+NA                                                              1110
```

```
      NN2=NN1+NA*NE                                                     1110
      NFG=NN2+NA*NE                                                     1120
      NFI=NFG+NA*NE                                                     1130
      NGG=NFI+NA*NE                                                     1140
      NII=NGG+NE                                                        1150
      NFR=NII+NE                                                        1160
      I=NFR/2*2                                                         1170
      IF(I.EQ.NFR)  NFR=NFR+1                                           1180
      IF(NFR.LT.IADR)  GO TO 20                                         1190
      WRITE (NOUT,21)                                                   1200
   21 FORMAT(1HO/' ***ERROR 0. 2 : THE REGION - FIELD IS ALREADY TOO SHO 1210
     1RT FOR THE CONTROL MODULE')                                       1220
      STOP                                                              1230
   20 NX=NE+1                                                           1240
      CALL INPUT (XL(M),XL(NM),XL(NZ),                                  1250
     1                    XL(NENG),XL(NSPEC),XL(NARB),XL(NTEMP),XL(NSI),  1260
     1XI(NG),XL(NN1),XL(NN2),XL(NFG),XL(NFI),XL(NGG),XL(NII),           1270
     3 NMAT,MI+1,NE,LSPEC+1,NFE,NA,NT,NTYP,NFR,XL,NF,NX,IADR)           1280
      IZI=0                                                             1290
      READ (NF) MAT1                                                    1300
      IF(MAT1.NE.N2)  GO TO 16                                          1310
      I=0                                                               1320
      WRITE (LIZ) I,N2                                                  1330
      RETURN                                                            1340
      END                                                               1350
```

```
C     PROGRAMM ZUM LESEN UND PRUEFEN DER EINGABE FUER DAS MIGROS-SYSTEM    10
C                                                                          20
      SUBROUTINE INPUT (ITYP,NAME,TZ,ENG,EF,NR,TEMP,SIGO,NRE,NN1,NN2,      30
     1NFG,NFI,NG,NI,NMAT,MI,NE,NSPEC,NEE,NA,NT,NTYP,NFR,XL,NF,NX,IADR)     40
      REAL*8 MAT1,    MAT, ITYP,N2,NAME,SGC,SGA,SGF                        50
     1,DAT,TIME                                                           60
      DIMENSION ENG(NE),EF(NEE,NSPEC),NAME(NMAT),TZ(NMAT),MAZ(2),          70
     1                          NR(3,NA),TEMP(NT),SIGO(MI),ITYP(NTYP),     80
     1       IPM(2), NRE(NA),NN1(NA,NE),NN2(NA,NE),NFG(NA,NE),NFI(NA,NE)  90
     2,XL(1),NG(NE),NI(NE),ENBER(5),NWFUN(5),CONWFU(5),INTYP(3)           100
      COMMON MAT,ISTRUK,ISPA,NOUT,LIZ,NANF,NEND,KL                        110
      COMMON/CESDUR/ IDUR                                                 120
      EQUIVALENCE (MAT,IPM(1))                                            130
      DATA N2/'ENDE '/                                                    140
     1           ,SGC/'SGC     '/,SGA/'SGA     '/,SGF/'SGF     '/        150
      CALL ESPIE                                                          160
      MIBER=5                                                             170
      MABWF=0                                                             180
      MXINT=200                                                           190
      MABQ1=200                                                           200
      MABQ2=200                                                           210
      MABQ3=200                                                           220
      KMROM=20                                                            230
      LDIM=1500                                                           240
      IRF=300                                                             250
      ISTF=400                                                            260
      NTT=4000                                                            270
      NMAX=5                                                              280
      ICOS=21                                                             290
      ISM=400                                                             300
      ISD = 1000                                                          310
      NFCU = 2                                                            320
      NFF=200                                                             330
      ISCO=ISM*ICOS                                                       340
      ISEC=ISD                                                            350
      IREMO=0                                                             360
      MAXERR=5                                                            370
      NINA=0                                                              380
      READ (NF) MAT,ISTRUK                                                390
      WRITE(NOUT,3003)MAT                                                 400
 3003 FORMAT('1M I G R O S - 3  TASK FOR MATERIAL',A10,/' ',45('*'))      410
      READ (NF) MAT1,MAT2                                                 420
      ISPA=0                                                              430
C     ISPA IS ONLY EXISTENT BECAUSE OF HISTORICAL REASONS                 440
      IF(MAT2-1)1,7,8                                                     450
    7 READ (NF) NE,(ENG(I),I=1,NE)                                        460
      READ (NF) MAT1,MAT2                                                 470
      DO 9 I=2,NE                                                         480
      IF(ENG(I).LT.ENG(I-1)) GO TO 10                                     490
    9 CONTINUE                                                            500
      GO TO 14                                                            510
   10 WRITE (NOUT,12) (ENG(I),I=1,NE)                                     520
   12 FORMAT(1HO/' ***ERROR 0. 3 : THE ENERGY GROUP BOUNDARIES'/(8E16.8)  530
     1)                                                                   540
      WRITE (NOUT,13)                                                     550
   13 FORMAT(' ARE NOT GIVEN IN AN INCREASING ORDER')                     560
      GO TO 5000                                                          570
    8 NE=26                                                               580
      ENG(1)=0.215                                                        590
      ENG(2)=0.465                                                        600
      ENG(3)=1.                                                           610
      DO 15 K=1,5                                                         620
      DO 15 J=1,3                                                         630
      MO=3*(K-1)+J                                                        640
   15 ENG(MO+3)=ENG(MO)*10.                                               650
      ENG(19)=3.2E6                                                       660
      ENG(20)=0.456                                                       670
      ENG(21)=0.856                                                       680
      ENG(22)=1.456                                                       690
      ENG(23)=2.5E6                                                       700
      ENG(24)=4.0E6                                                       710
      ENG(25)=6.5E6                                                       720
      ENG(26)=1.05E7                                                      730
   14 IF(MAT2-2)1,16,17                                                   740
   16 READ (NF) LSP,NFE,((EF(I,J),I=1,NFE),J=1,NSPEC)                    750
      READ (NF) MAT1,MAT2                                                 760
      DO 18 I=2,NFE                                                       770
      IF(EF(I,1).LE.EF(I-1,1)) GO TO 19                                   780
   18 CONTINUE                                                            790
      GO TO 20                                                            800
   19 WRITE (NOUT,21)                                                     810
```

```
 21 FORMAT(1HO/' ***ERROR O. 4 : THE ENERGY POINTS OF THE MACROSCOPIC
   1WEIGHTING FUNCTION ARE NOT GIVEN IN AN INCREASING ORDER')
    GO TO 5000
 17 NFE=1
    LSP=0
 20 DO 3001 NT=2,NSPEC
    NSPEC1=NT-1
    IF(NSPEC .GT.2)WRITE(NOUT,3002)NSPEC1
3002 FORMAT(/' PRINTOUT FOR SPECTRUM NR.',I5)
3001 CALL PRPHI(NFE,EF(1,1),EF(1,NT))
    IF(MAT2-3)1,22,23
 22 READ (NF) NA,(NR(1,I),NR(2,I),NR(3,I),I=1,NA)
    DO 11 I=1,NA
    IF(NR(2,I).GE.NR(3,I).AND.NR(2,I).LE.(NE-1))  GO TO 11
    IF(NR(1,I).EQ.10.AND.NR(3,I).LE.NE)  GO TO 11
    WRITE (NOUT,54) NR(1,I)
 54 FORMAT(1HO/' ***ERROR O. 5 : THE CHOICE OF ENERGY GROUP BOUNDARIES
   1 FOR PROGRAM',I6,' IS NOT VALID')
    GO TO 5000
 11 CONTINUE
    IF(NFE.EQ.1)  GO TO 114
    MIN=1
    MAX=NE-1
    DO 112 I=1,NA
    IF(NR(2,I).GT.MIN)  MIN=NR(2,I)
    IF(NR(3,I).LT.MAX)  MAX=NR(3,I)
112 CONTINUE
    AN=ENG(NE-MIN)
    END=ENG(NE-MAX+1)
    KL=NE-MIN
    M=NE-MAX+1
    J=1
    DO 200 I=KL,M
202 IF(ENG(I).EQ.EF(J,1))  GO TO 200
    IF(ENG(I).LT.EF(J,1))  GO TO 201
    J=J+1
    GO TO 202
201 DO 203 NT=1,NSPEC
    DO 203 N=J,NFE
    K=NFE-N+J
203 EF(K+1,NT)=EF(K,NT)
    NFE=NFE+1
    IF(ENG(I).GT.(EF(J-1,1)+EF(J+1,1))*0.5)  GO TO 206
    DO 204 NT=2,NSPEC
204 EF(K,NT)=EF(K+1,NT)-(EF(K+1,NT)-EF(K-1,NT))/(EF(K+1,1)-
   1EF(K-1,1))*(EF(K+1,1)-ENG(I))
    GO TO 205
206 DO 207 NT=2,NSPEC
207 EF(K,NT)=EF(K-1,NT)+(EF(K+1,NT)-EF(K-1,NT))/(EF(K+1,1)-EF(K-1,1))*
   1(ENG(I)-EF(K-1,1))
205 EF(K,1)=ENG(I)
200 CONTINUE
    IF(EF(1,1).GT.AN)  GO TO 113
    IF(EF(NFE,1).GE.END)  GO TO 114
113 WRITE (NOUT,115)
115 FORMAT(1HO/' ***ERROR O. 6 : THE MACROSCOPIC WEIGHTING FUNCTION DO
   1ES NOT INCLUDE ALL ENERGY GROUPS DESIRED')
    GO TO 5000
114 CONTINUE
    READ (NF) MAT1,MAT2
    GO TO 24
 23 WRITE (NOUT,25)
 25 FORMAT(1HO/' ***ERROR O. 7 : THE IDENTIFICATION NUMBERS OF MODULES
   1 TO BE CALLED CAN NOT BE FOUND')
    GO TO 5000
 24 IF(MAT2-4)1,26,27
 26 READ (NF) NT,(TEMP(I),I=1,NT)
    READ (NF) MAT1,MAT2
    DO 28 I=1,NA
    IF(NR(1,I).EQ.1.OR.NR(1,I).EQ.2) GO TO 29
 28 CONTINUE
    WRITE (NOUT,30)
 30 FORMAT(1HO/' ***WARNING O. 2 : THE DECLARATION OF THE TEMPERATURE
   1IS NOT NECESSARY AND IS IGNORED')
    GO TO 29
 27 DO 31 I=1,NA
    IF(NR(1,I).EQ.1.OR.NR(1,I).EQ.2) GO TO 32
 31 CONTINUE
    NT=0
    GO TO 29
 32 IF(ISTRUK.EQ.0) GO TO 34
    NT=3
    TEMP(1)=300.
    TEMP(2)=900.
    TEMP(3)=2100.
    GO TO 29
 34 NT=1
    TEMP(1)=0.
 29 IF(MAT2-5)1,33,35
 33 READ (NF) MI,(SIGO(I),I=1,MI)
    MS=MI
    IF(SIGO(MI).GE.10.**6)  GO TO 2002
    MS=MI+1
2002 READ (NF) MAT1,MAT2
    DO 36 I=1,NA
    IF(NR(1,I).EQ.1.OR.NR(1,I).EQ.2.OR.NR(1,I).EQ.3) GO TO 37
 36 CONTINUE
    WRITE (NOUT,38)
 38 FORMAT(1HO/' ***WARNING O. 3 : THE DECLARATION OF THE BACKGROUND C
   1ROSS SECTIONS IS NOT NECESSARY AND IS IGNORED')
    GO TO 37
 35 DO 39 I=1,NA
    IF(NR(1,I).EQ.1.OR.NR(1,I).EQ.2.OR.NR(1,I).EQ.3) GO TO 40
 39 CONTINUE
    MI=0
    GO TO 37
 40 MI=7
    MS=MI
    SIGO(1)=0.
    DO 41 I=1,6
```

```
 41 SIGO(I+1)=10.**I                                                    1920
 37 IF(MAT2-6)1,42,43                                                   1930
 42 READ (NF) NTYP,(ITYP(I),I=1,NTYP)                                  1940
    READ (NF)MAT1,MAT2                                                  1950
    DO 149 I=1,NTYP                                                     1960
    IF(ITYP(I).EQ.SGC)  GO TO 150                                       1970
149 CONTINUE                                                            1980
    GO TO 151                                                           1990
150 DO 152 J=1,NTYP                                                     2000
    IF(ITYP(J).EQ.SGA)  GO TO 153                                       2010
152 CONTINUE                                                            2020
    ITYP(I)=SGA                                                         2030
153 DO 154 J=1,NTYP                                                     2040
    IF(ITYP(J).EQ.SGF)  GO TO 155                                       2050
154 CONTINUE                                                            2060
    IF(ITYP(I).EQ.SGA)  GO TO 156                                       2070
    ITYP(I)=SGF                                                         2080
    GO TO 151                                                           2090
156 NTYP=NTYP+1                                                         2100
    ITYP(NTYP)=SGF                                                      2110
    GO TO 151                                                           2120
155 IF(ITYP(I).EQ.SGA)  GO TO 151                                       2130
    NTYP=NTYP-1                                                         2140
    DO 157 J=I,NTYP                                                     2150
157 ITYP(J)=ITYP(J+1)                                                   2160
151 DO 44 I=1,NA                                                        2170
    IF(NR(1,I).EQ.4) GO TO 45                                           2180
 44 CONTINUE                                                            2190
    WRITE (NOUT,46)                                                     2200
 46 FORMAT(1HO/' ***WARNING 0. 4 : THE DECLARATION OF THE CROSS SECTIO 2210
   1N TYPES IS NOT NECESSARY AND IS IGNORED')                           2220
    GO TO 45                                                            2230
 43 DO 47 I=1,NA                                                        2240
    IF(NR(1,I).EQ.4.OR.NR(1,I).EQ.10)  GO TO 48                         2250
 47 CONTINUE                                                            2260
    NTYP=0                                                              2270
    GO TO 45                                                            2280
 48 NTYP=8                                                              2290
    CALL DOPW (8HMUEL     ,ITYP(1))                                     2300
    CALL DOPW (8HNUE      ,ITYP(2))                                     2310
    CALL DOPW (8HSGA      ,ITYP(3))                                     2320
    CALL DOPW (8HSGF      ,ITYP(4))                                     2330
    CALL DOPW (8HSGT      ,ITYP(5))                                     2340
    CALL DOPW (8HSGN      ,ITYP(6))                                     2350
    CALL DOPW (8HSG2N     ,ITYP(7))                                     2360
    CALL DOPW (8HSGT      ,ITYP(8))                                     2370
 45 IF(MAT2-11)1,49,50                                                  2380
 49 READ (NF) NRES                                                      2390
    READ (NF) MAT1,MAT2                                                 2400
    DO 51 I=1,NA                                                        2410
    IF(NR(1,I).EQ.1) GO TO 52                                           2420
 51 CONTINUE                                                            2430
    WRITE (NOUT,53)                                                     2440
 53 FORMAT(1HO/' ***WARNING 0. 5 : THE DECLARATION OF THE NUMBER OF RE 2450
   1SONANCES IS NOT NECESSARY AND IS IGNORED')                          2460
    GO TO 52                                                            2470
 50 NRES=-1                                                             2480
 52 IF(MAT2-12)1,56,57                                                  2490
 56 READ (NF) ERROR                                                     2500
    READ (NF) MAT1,MAT2                                                 2510
    DO 58 I=1,NA                                                        2520
    IF(NR(1,I).EQ.1) GO TO 59                                           2530
 58 CONTINUE                                                            2540
    WRITE (NOUT,60)                                                     2550
 60 FORMAT(1HO/' ***WARNING 0. 6 : THE DECLARATION OF THE ALLOWED INTE 2560
   1GRATION ERROR IS NOT NECESSARY AND IS IGNORED')                     2570
    GO TO 59                                                            2580
 57 ERROR=0.01                                                          2590
 59 DO 3004 I=1,NA                                                      2600
    IF(NR(1,I).EQ.3)  GO TO 3005                                        2610
3004 CONTINUE                                                           2620
    IP=0                                                                2630
    GO TO 3006                                                          2640
3005 IP=1                                                               2650
3006 IF(MAT2-31)1,300,301                                               2660
 300 IF(IP.EQ.1)  GO TO 3008                                            2670
    WRITE (NOUT,3007)                                                   2680
3007 FORMAT(/' ***WARNING 0.16 : THE INPUT FOR MODULE 3 IS NOT NECESSAR 2690
   1Y')                                                                 2700
3008 READ(NF) EPSROM,DRINWA                                             2710
    READ(NF) MAT1,MAT2                                                  2720 1
    GOTO 302                                                            2730 8
 301 EPSROM=5.0E-5                                                      2740 5
    DRINWA=5.0                                                          2750 1
 302 IF(MAT2-32) 1,303,304                                              2760
 303 IF(IP.EQ.1)  GO TO 3009                                            2770
    WRITE (NOUT,3007)                                                   2780
3009 READ(NF) ITEST,IZPUMS,ITUMS                                        2790
    READ(NF) MAT1,MAT2                                                  2800
    GOTO 305                                                            2810
 304 ITEST=0                                                            2820
    IZPUMS=-1                                                           2830
    ITUMS=ITEST                                                         2840
 305 IF(MAT2-33) 1,306,307                                              2850
 306 IF(IP.EQ.1)  GO TO 3010                                            2860
    WRITE (NOUT,3007)                                                   2870
3010 READ(NF) NENBER,(ENBER(I),NWFUN(I),CONWFU(I),I=1,NENBER)           2880
    READ(NF) MAT1,MAT2                                                  2890
    IF(NENBER.GE.1.AND.NENBER.LE.MAXEBR) GOTO 308                       2900
    WRITE(NOUT,3016) NENBER,MAXEBR                                      2910
3016 FORMAT(1HO/' ***ERROR 0.16 : NUMBER OF INTEGRATION REGIONS NENBER  2920
   *IS EQUAL',I5,'./17X,'BUT IT MUST BE GREATER THAN ZERO AND LESS OR 2930
   * EQUAL THAN ',I2,'.')                                              2940
    GO TO 5000                                                          2950
 307 NENBER=1                                                           2960
    ENBER(1)=-1.0                                                       2970
    IF(NFE.LE.1) NWFUN(1)=0                                             2980
    IF(NFE.GT.1) NWFUN(1)=-1                                            2990
    CONWFU(1)=1.0                                                       3000
 308 DO 3011 I=1,NA                                                     3010
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```
      IF(NR(1,I).EQ.5)  GO TO 3012                                      3020
 3011 CONTINUE                                                          3030
      IP=0                                                              3040
      GO TO 3013                                                        3050
 3012 IP=1                                                              3060
 3013 IF(MAT2.EQ.51)  GO TO 400                                         3070
      KINEM=1                                                           3080
      GO TO 401                                                         3090
  400 IF(IP.EQ.1)  GO TO 3014                                           3100
      WRITE (NOUT,3015)                                                 3110
 3015 FORMAT(/' ***WARNING 0. 7 : THE INPUT FOR MODULE 5 IS NOT NECESSAR 3120
     1Y')                                                               3130
 3014 READ(NF) KINEM                                                    3140
      READ(NF) MAT1,MAT2                                                3150
  401 IF(MAT2-52)1,63,64                                                3160
   63 IF(IP.EQ.1)  GO TO 3018                                           3170
      WRITE (NOUT,3015)                                                 3180
 3018 READ (NF) XNUE                                                    3190
      READ (NF) MAT1,MAT2                                               3200
      GO TO 66                                                          3210
   64 XNUE=0.16                                                         3220
   66 IF(MAT2.EQ.53)  GO TO 402                                         3230
      NIN=2                                                             3240
      INTYP(1)=1                                                        3250
      INTYP(2)=2                                                        3260
      GO TO 403                                                         3270
  402 IF(IP.EQ.1)  GO TO 3017                                           3280
      WRITE (NOUT,3015)                                                 3290
 3017 READ(NF) NIN,(INTYP(IS),IS=1,NIN)                                 3300
      READ(NF) MAT1,MAT2                                                3310
  403 DO 77 I=1,NA                                                      3320
      IF(NR(1,I ).EQ.6) GO TO 78                                        3330
   77 CONTINUE                                                          3340
      IP=0                                                              3350
      GO TO 79                                                          3360
   78 IP=1                                                              3370
      LSPEC=NEE*LSP                                                     3380
   79 IF(MAT2-61)1,80,81                                                3390
   80 IF(IP.EQ.1) GO TO 82                                              3400
      WRITE (NOUT,83)                                                   3410
   83 FORMAT(1HO/' ***WARNING 0. 8 : THE INPUT FOR MODULE 6 IS NOT NECES 3420
     1SARY')                                                            3430
   82 READ (NF) ISEL,NLE                                                3440
      READ (NF) MAT1,MAT2                                               3450
      NLA=0                                                             3460
      IF(NLE.LT.1)  NLE=1                                               3470
      IF(NLE.GT.5)  NLE=5                                               3480
      GO TO 84                                                          3490
   81 NLA=0                                                             3500
      NLE=5                                                             3510
      ISEL=2                                                            3520
   84 IF(IP.EQ.0)  GO TO 141                                            3530
      IF(NEE.GT.0.AND.EE(1,1).EQ.0) EE(1,1)=1.E-3                       3540
  141 IF(MAT2-62)1,133,134                                              3550
  133 IF(IP.EQ.1)  GO TO 135                                            3560
      WRITE (NOUT,83)                                                   3570
  135 READ (NF) NMAT,(NAME(I),TZ(I),I=1,NMAT)                           3580
      READ (NF) MAT1,MAT2                                               3590
      NTK=1                                                             3600
      GO TO 136                                                         3610
  134 NTK=0                                                             3620
  136 IF(MAT2-63)1,137,140                                              3630
  137 IF(IP.EQ.1)  GO TO 139                                            3640
      WRITE(NOUT,83)                                                    3650
  139 READ (NF) MW                                                      3660
      IF (MW.EQ.1)  GO TO 1000                                          3670
      IF(NTK.EQ.1)  GO TO 2000                                          3680
      WRITE (NOUT,2001)                                                 3690
 2001 FORMAT(1HO/' ***ERROR 0.15 : MODULE 6 CANNOT BE STARTED, BECAUSE 8 3700
     1LOC 12 MUST BE GIVEN IF MW=2 IN BLOC 13')                         3710
      GO TO 5000                                                        3720
 2000 MAZ(1)=0                                                          3730
      MAZ(2)=1                                                          3740
      GO TO 1001                                                        3750
 1000 MAZ(1)=1                                                          3760
      MAZ(2)=0                                                          3770
 1001 READ (NF) MAT1,MAT2                                               3780
      IF(MAZ(1).EQ.0)  GO TO 138                                        3790
      IF(LSP.EQ.0)  GO TO 138                                           3800
      IF(LSP-(NLE+1))142,138,138                                        3810
  142 LP=NLE+1                                                          3820
      WRITE (NOUT,143) LP                                               3830
  143 FORMAT(1HO/' ***ERROR 0. 8 : THE NUMBER OF WEIGHTING FUNCTIONS IS  3840
     'LESS THAN THE NUMBER OF LEGENDRE MOMENTS.'/I5,' NUMBER OF WEIGHTIN 3850
     2G FUNCTIONS ARE NEEDED')                                          3860
      GO TO 5000                                                        3870
  140 MAZ(1)=0                                                          3880
      MAZ(2)=0                                                          3890
  138 IF(MAT2-64)1,145,146                                              3900
  145 IF(IP.EQ.1)  GO TO 147                                            3910
      WRITE(NOUT,83)                                                    3920
  147 READ(NF)   NK,NRR                                                 3930
      NS=NE                                                             3940
      READ(NF)MAT1,MAT2                                                 3950
      GO TO 148                                                         3960
  146 NS=NE                                                             3970
      NK=70                                                             3980
      NRR=16                                                            3990
  148 IF(MAT2-81)1,85,86                                                4000
   85 READ (NF) EPS                                                     4010
      READ(NF) MAT1,MAT2                                                4020
      GO TO 87                                                          4030
   86 EPS=0.01                                                          4040
   87 DO 68 I=1,NA                                                      4050
      IF(NR(1,I).EQ.9)  GO TO 69                                        4060
   68 CONTINUE                                                          4070
      IP=0                                                              4080
      GO TO 70                                                          4090
   69 IP=1                                                              4100
   70 IF(MAT2-91)1,71,72                                                4110
```

```
 71 IF(IP.EQ.1)  GO TO 73                                                4120
    WRITE (NOUT,74)                                                      4130
 74 FORMAT(1HO/' ***WARNING O. 9 : THE INPUT FOR MODULE 9 IS NOT NECES 414C
   1SARY')                                                               4150
 73 READ (NF) ERR,NJM,NUJM                                               4160
    READ (NF) MAT1,MAT2                                                  4170
    GO TO 75                                                             4180
 72 IF(IP.EQ.0)  GO TO 75                                                4190
    ERR=0.01                                                             4200
    NJM=10                                                               4210
    NUJM=10                                                              4220
 75 IF(MAT2-92)1, 76, 103                                                4230
 76 IF(IP.EQ.1)  GO TO 104                                               424C
    WRITE (NOUT,74)                                                      4250
104 READ (NF) ISELR,NLRA,NLRE,NCALL                                      4260
    IF(NCALL.NE.0)  GO TO 158                                            4270
    READ(NF)MAT1,MAT2                                                    428C
    GO TO 105                                                            4290
158 IS=0                                                                 4300
    DO 109 I=1,NA                                                        4310
    IF(NR(1,I).EQ.9)  IS=IS+1                                            4320
109 CONTINUE                                                             4330
    IF(IS.EQ.NCALL)  GO TO 110                                           4340
    WRITE (NOUT,111) IS,NCALL                                            4350
111 FORMAT(1HO/' ***ERROR O. 9 : MODULE 9 IS CALLED ',I3,' TIMES, IN T 4360
   1HE INPUT BLOC 92 NCALL IS SET TO',I3)                                4370
    GO TO 5000                                                           438C
110 DO 106 I=1,NCALL                                                     4390
    READ (NF)NGRE,(NN1(I,J),NN2(I,J),NFG(I,J),NFI(I,J),J=1,NGRE)         44CC
    NRE(I)=NGRE                                                          4410
    DO 106 J=1,NGRE                                                      4420
    IF(NN1(I,J).GE.NN2(I,J))  GO TO 106                                  443C
    WRITE (NOUT,107) I                                                   4440
107 FORMAT(1HO/' ***ERROR O.10 : IN BLOC 92 THE INPUT OF THE ENERGY GR 4450
   1OUPS IS NOT VALID FOR THE ',I3,'. PROGRAM CALL')                     4460
    GO TO 5000                                                           4470
106 CONTINUE                                                             448C
    READ(NF)MAT1,MAT2                                                    4490
    GO TO 108                                                            4500
103 NLRA=0                                                               4510
    NLRE=5                                                               4520
    ISELR=1                                                              453C
    NCALL=0                                                              4540
105 NFG(1,1)=14                                                          4550
    NFI(1,1)=5                                                           4560
    NRE(1)=1                                                             4570
108 IF(MAT1.EQ.92)  GO TO 88                                             458C
  1 WRITE (NOUT,89)                                                      4590
 89 FORMAT(1HO/' ***ERROR O.11 : THE INPUT IS NOT ORDERED IN INCREASIN 4600
   1G ARGUMENTS')                                                        4610
    GO TO 5000                                                           4620
 88 NGR=0                                                                463C
    KL=1                                                                 4640
    ISPATF=ISPA                                                          4650
1CC NANF=NR(2,KL)                                                        4660
    NEND=NR(3,KL)                                                        467C
    CALL DATUM (DAT,TIME)                                                468C
    WRITE (NOUT,3000) DAT,TIME                                           4690
3000 FORMAT(/' DATE ',A8,'    TIME ',A8)                                 47CC
    IF(NR(1,KL).EC.1) GC TO 90                                           4710
    IF(NR(1,KL).EC.2) GC TO 91                                           472C
    IF(NR(1,KL).EQ.3) GC TO 92                                           473C
    IF(NR(1,KL).EQ.4) GO TO 93                                           4740
    IF(NR(1,KL).EC.5) GC TC 94                                           475C
    IF(NR(1,KL).EQ.6) GO TO 95                                           4760
    IF(NR(1,KL).EC.7) GO TO 96                                           477C
    IF(NR(1,KL).EQ.8) GC TO 97                                           4780
    IF(NR(1,KL).EQ.9)  GO TO 119                                         4790
    IF(NR(1,KL).EC.10)  GC TO 120                                        48CC
    WRITE (NOUT,98) NR(1,KL)                                             4810
  98 FORMAT(1HO/' ***ERROR O.12 : THE DESIRED MODULE',I6,' IS NOT CONTA 4820
   1INED IN MIGROS')                                                     4830
    GC TO 5000                                                           4840
 126 IRE=IRE+IREP                                                        4850
    ISTE=ISTE+ISTEP                                                      4860
    B=ZEIT(A)                                                            487C
    WRITE (NOUT,1004) NR(1,KL),B                                         4880
  90 NGR=0                                                               4890
    C=C.                                                                 49CC
    A=ZEIT(C)                                                            4910
    IJ=NFR+7*MI+3*NE+7*IRE+6*ISTE                                        492C
    JI=IABS(IADR-IJ)                                                     4930
    IF(IADR.LT.IJ)  GO TO 121                                            4940
    WRITE (NOUT,1003) NR(1,KL),JI                                        495C
1003 FORMAT(1HO/1HO/' IN MODULE',I3,I8,' WORDS ARE NOT USED IN THE REGI 4960
   1CN FIELD')                                                           4970
    CALL FGFM(MI,SIGO,NE,ENG,NFE,EF(1,1),EF(1,2),NT,TEMP,ERRCR,NRES,     4980
   1NGR,XL(NFR),XL(NFR+7*MI),IRE,IREP,XL(NFR+7*MI+3*NE),XL(NFR+7*MI+     4990
   23*NE+IRE),XL(NFR+7*MI+3*NE+IRE*2),XL(NFR+7*MI+3*NE+3*IRE),           5000
   3XL(NFR+7*MI+3*NE+4*IRE),XL(NFR+7*MI+3*NE+5*IRE),                     5010
   4XL(NFR+7*MI+3*NE+6*IRE),ISTE,ISTEP,XL(NFR+7*MI+3*NE+7*IRE),          5020
   5XL(NFR+7*MI+3*NE+7*IRE+5*ISTE))                                      5030
    IF(IREP.GT.0.OR.ISTEP.GT.0)  GO TO 126                               5040
    B=ZEIT(A)                                                            5050
    WRITE (NOUT,1004) NR(1,KL-1),B                                       5060
1004 FORMAT(1HO/' IN MODULE',I3,F8.2,' SECONDS CPU-TIME ARE USED')       507C
    IF(NGR.EQ.0)  GO TO 101                                              5080
    KL=KL-1                                                              5090
    NR(1,KL)=2                                                           5100
    NANF=MINO(NE-NGR,NR(2,KL))                                           5110
    GC TC 91                                                             512C
 101 IF(KL.LE.NA)  GO TO 100                                             5130
    GC TC 102                                                            5140
  91 IJ=NFR+35*MI                                                        5150
    C=0.                                                                 5160
    A=ZEIT(C)                                                            517C
    JI=IABS(IADR-IJ)                                                     5180
    IF(IADR.LT.IJ)  GO TO 121                                            5190
    WRITE (NOUT,1CC3) NR(1,KL),JI                                        5200
    CALL FSTAT(MI,SIGO,NE,ENG,NFE,EF(1,1),EF(1,2),NT,TEMP,XL(NFR),       5210
```

```
     1XL(NFR+15*MS),XL(NFR+30*MS))                                              5220
      B=ZEIT(A)                                                                 5230
      WRITE (NOUT,1004) NR(1,KL-1),B                                            5240
      NGR=0                                                                     5250
      IF(KL.LE.NA)  GO TO 100                                                   5260
      GO TO 102                                                                 5270
  125 MIBER=MIBER+MIBERP                                                        5280
      MABWF=MABWF+MABWFP                                                        5290
      MXINT=MXINT+MXINTP                                                        5300
      MABQ1=MABQ1+MABQ1P                                                        5310
      MABQ2=MABQ2+MABQ2P                                                        5320
      MABQ3=MABQ3+MABQ3P                                                        5330
      KMROM=KMROM+KMROMP                                                        5340
      B=ZEIT(A)                                                                 5350
      WRITE (NOUT,1004) NR(1,KL),B                                              5360
   92 ISIG=0                                                                    5370
      C=0.                                                                      5380
      A=ZEIT(C)                                                                 5390
      IF(SIGO(MI).GE.1.E6)  GO TO 144                                           5400
      ISIG=1                                                                    5410
      MI=MI+1                                                                   5420
      SIGO(MI)=1.E6                                                             5430
  144 IF(NFE.GT.1.AND.MABWF.LT.50) MABWF=50                                     5440
      MRF=1                                                                     5450
      IF(ISPATE.EQ.0) MRF=7                                                     5460
      IF(ISPATE.EQ.1) MRF=8                                                     5470
      IJ=NFR+3*MIBER+6*MI+MXINT+4*(MABWF+MABQ1+MABQ2+MABQ3)+2*KMROM+            5480
     *4*MRF*MI                                                                  5490
      IF(IADR.LT.(IJ+10000)) GOTO 244                                           5500
      JI=(IADR-IJ)/18                                                           5510
      MXINT=MXINT+JI                                                            5520
      MABQ1=MABQ1+JI                                                            5530
      MABQ3=MABQ3+JI                                                            5540
  244 L1=NFR                                                                    5550
      L2=L1+MIBER                                                               5560
      L3=L2+MIBER                                                               5570
      L4=L3+MIBER                                                               5580
      L5=L4+6*MI                                                                5590
      L6=L5+4*MABWF                                                             5600
      L7=L6+MXINT                                                               5610
      L8=L7+4*MABQ1                                                             5620
      L9=L8+4*MABQ2                                                             5630
      L10=L9+4*MABQ3                                                            5640
      L10=L10+((L10+1)-((L10+1)/2)*2)                                           5650
      L11=L10+2*KMROM                                                           5660
      L12=L11+2*MRF*MI                                                          5670
      IJ=L12+2*MRF*MI                                                           5680
      JI=IABS(IADR-IJ)                                                          5690
      IF(IADR.LT.IJ)  GO TO 121                                                 5700
      WRITE (NOUT,1003) NR(1,KL),JI                                             5710
      CALL FSTRUK(MI,SIGO,NE,ENG,NFE,EF(1,1),EF(1,2),                           5720
     *NFNBER,FNBER,NWFUN,CONWFU,EPSRCM,DRINWA,ITEST,I7PUMS,ITUMS,ISPATE,        5730
     *MIBER,XL(L1),MIBERP,XL(L2),XL(L3),XL(L4),MABWF,XL(L5),MABWFP,             5740
     *MXINT,XL(L6),MXINTP,MABQ1,XL(L7),MABQ1P,MABQ2,XL(L8),MABQ2P,              5750
     *MABQ3,XL(L9),MABQ3P,KMROM,XL(L10),KMROMP,XL(L11),MRF,XL(L12),MRFP)        5760
      IF(ISIG.EQ.1)  MI=MI-1                                                    5770
      IF(MIBERP.GT.0.OR.MABWFP.GT.0.OR.MXINTP.GT.0.OR.MABQ1P.GT.0.OR.           5780
     *MABQ2P.GT.0.OR.MABQ3P.GT.0.OR.KMROMP.GT.0.OR.MRFP.GT.0) GOTO 125          5790
      B=ZEIT(A)                                                                 5800
      WRITE (NOUT,1004) NR(1,KL-1),B                                            5810
      IF(KL.LE.NA)  GO TO 100                                                   5820
      GO TO 102                                                                 5830
  124 LDIM=LDIM+LDIMP                                                           5840
      B=ZEIT(A)                                                                 5850
      WRITE (NOUT,1004) NR(1,KL),B                                              5860
   93 IJ=NFR+6*NE+2*LDIM                                                        5870
      C=C.                                                                      5880
      A=ZEIT(C)                                                                 5890
      JI=IABS(IADR-IJ)                                                          5900
      IF(IADR.LT.IJ)  GO TO 121                                                 5910
      WRITE (NOUT,1003) NR(1,KL),JI                                             5920
      CALL SUND (NE,ENG,NFE,EF(1,1),EF(1,2),NTYP,ITYP,XL(NFR),                  5930
     1XL(NFR+NE),XL(NFR+2*NE),XL(NFR+3*NE),XL(NFR+4*NE),XL(NFR+5*NE),           5940
     2LDIM,LDIMP,XL(NFR+6*NE),XL(NFR+6*NE+LDIM))                                5950
      IF(LDIMP.GT.0)  GO TO 124                                                 5960
      B=ZEIT(A)                                                                 5970
      WRITE (NOUT,1004) NR(1,KL-1),B                                            5980
      IF(KL.LE.NA)  GO TO 100                                                   5990
      GO TO 102                                                                 6000
   94 C=C.                                                                      6010
      A=ZEIT(C)                                                                 6020
      IF(KINEM.NE.0.AND.KINEM.NE.1.AND.KINEM.NE.2) GO TO 3                      6030
      NIN=NIN-NINA                                                              6040
      DO 208 IS=1,NIN                                                           6050
      INTYP(IS)=INTYP(NINA+IS)                                                  6060
      IF(INTYP(IS).NE.1.AND.INTYP(IS).NE.2.AND.INTYP(IS).NE.3) GO TO 3          6070
  208 CONTINUE                                                                  6080
      GO TO 6                                                                   6090
    3 WRITE (NOUT,1010)                                                         6100
 1010 FORMAT(1HO/' PROGRAM 5 CANNOT BE STARTED, BECAUSE KINEM WAS NOT SE        6110
     1T EQUAL TO 0, 1 OR 2'/'  OR FIELD INTYP WAS NOT SET EQUAL TO 1, 2         6120
     2OR 3 IN THE INPUT')                                                       6130
      KL=KL+1                                                                   6140
      GO TO 5                                                                   6150
    6 NINA=0                                                                    6160
      CALL SCAT(NE,ENG,XNUE,NFE,EF(1,1),EF(1,2),NX,KINEM,NIN,NINA,INTYP,        6170
     1XL(NFR),XL(NFR),IADR-NFR+1,IJ)                                            6180
      IJ=NFR+IJ                                                                 6190
      JI=IABS(IADR-IJ)                                                          6200
      IF(IADR.LT.IJ) GO TO 121                                                  6210
    5 WRITE(NOUT,1003) NR(1,KL-1),JI                                            6220
      B=ZEIT(A)                                                                 6230
      WRITE (NOUT,1004) NR(1,KL-1),B                                            6240
      IF(KL.LE.NA)  GO TO 100                                                   6250
      GO TO 102                                                                 6260
  123 NECU=NECU+NECUP                                                           6270
      ISM=ISM+ISMP                                                              6280
      ISD=ISD+ISDP                                                              6290
      ICOS=ICOS+ICOSP                                                           6300
      ISCO=MAX0(ISM*ICOS,ISCC+ISCOP)                                            6310
```

```
      ISCO=MAXO(ISCC,NECU*ISC)                                          6320
      ISEC=MAXO(ISM*NECU,ISEC+ISECP)                                    6330
      ISEC=MAXO(ISEC,ISD)                                               6340
      NTT=NTT+NTTP                                                      6350
      NANF=NANF-KIM                                                     6360
      B=ZEIT(A)                                                         6370
      WRITE (NOUT,1004) NR(1,KL),B                                      6380
   95 L=NFR+5*ISM                                                       6390
      C=C.                                                              6400
      A=ZEIT(C)                                                         6410
      M=L+7*ISD                                                         6420
      N=M+2*ICOS                                                        6430
      NN=N+4*NX                                                         6440
      MM=NN+7*NE                                                        6450
      IJ=MM+ISCO+ISEC+6*NECU*NE+8*NE+2*NTT+2*ISD                        6460
      JI=IABS(IADR-IJ)                                                  6470
      IF(IADR.LT.IJ)  GO TO 121                                         6480
      WRITE (NOUT,1003) NR(1,KL),JI                                     6490
      CALL FLUMMI(XL(NFR),XL(NFR+ISM),XL(NFR+2*ISM),XL(NFR+3*ISM),      6500
     1XL(NFR+4*ISM),XL(NFR+5*ISM),XL(L+ISD),XL(L+2*ISD),                6510
     2XL(L+3*ISD),XL(L+4*ISD),XL(L+5*ISD),XL(L+6*ISD),XL(L+7*ISD),      6520
     3XL(M+ICOS),XL(M+2*ICOS),XL(N+NX),XL(N+2*NX),XL(N+3*NX),ENG,       6530
     4XL(N+4*NX),XL(NN+NE),              EF(1,1),EF(1,2),XL(NN+7*NE),   6540
     5XL(MM+ISCO),XL(MM+ISCO+ISEC),XL(MM+ISCO+ISEC+6*NECU*NE),          6550
     6XL(MM+ISCO+ISEC+6*NECU*NE+2*NF),                                  6560
     8XL(MM+ISCO+ISEC+6*NECU*NE+2*NF+NTT),NAME,TZ,                      6570
     6NIA,NLE,ISEL,NMAX,NF,NX,NFE,LSPEC,MAZ,NTK,NMAT,NTT,NTTP,          6580
     6                          ICOS,ICOSP,NECU,NECUP,ISM,ISMP,ISD,     6590
     7ISCP,ISCO,ISCOP,ISEC,ISECP,KIM,NS,NK,NRR,XL(MM+ISCO+ISEC+6*NECU*  6600
     8NE+2*NE+2*NTT),XL(MM+ISCO+ISEC+6*NECU*NE+2*NE+2*NTT+ISD),XL(MM+   6610
     9ISCO+ISEC+6*NECU*NE+2*NE+2*NTT+2*ISD))                            6620
       IF(NECUP.GT.0.OR.ISMP.GT.0.OR.ISCP.GT.0.OR.ISCOP.GT.0.OR.        6630
     1ICOSP.GT.0.OR.ISECP.GT.0.OR.NTTP.GT.0)  GO TO 123                 6640
       B=ZEIT(A)                                                        6650
       WRITE (NOUT,1004) NR(1,KL-1),B                                   6660
       IF(KL.LE.NA)  GO TO 100                                          6670
       GO TO 102                                                        6680
   96  IJ=NFR+NE                                                        6690
       C=0.                                                             6700
       A=ZEIT(C)                                                        6710
       JI=IABS(IADR-IJ)                                                 6720
       IF(IADR.LT.IJ)  GO TO 121                                        6730
       WRITE (NOUT,1003) NR(1,KL),JI                                    6740
       CALL SPALT (NE,ENG,XL(NFR))                                      6750
       B=ZEIT(A)                                                        6760
       WRITE (NOUT,1004) NR(1,KL-1),B                                   6770
       IF(KL.LE.NA)  GO TO 100                                          6780
       GO TO 102                                                        6790
   97  C=0.                                                             6800
       A=ZEIT(C)                                                        6810
       IJ=NFR+NE+2*NEF                                                  6820
       JI=IABS(IADR-IJ)                                                 6830
       IF(IADR.LT.IJ)  GO TO 121                                        6840
       WRITE (NOUT,1003) NR(1,KL),JI                                    6850
       CALL EDV (NE,ENG,NFE,EF(1,1),EF(1,2),EPS,XL(NFR),NEF,XL(NFR+NE),  6860
     1XL(NFR+NE+NEF),IW)                                                6870
       B=ZEIT(A)                                                        6880
       WRITE (NOUT,1004) NR(1,KL-1),B                                   6890
       IF(IW.EQ.1)  GO TO 97                                            6900
       IF(KL.LE.NA)  GO TO 100                                          6910
       GO TO 102                                                        6920
  119  IREMO=IREMO+1                                                    6930
       C=0.                                                             6940
       A=ZEIT(C)                                                        6950
       IF(NCALL.EQ.C)  IREMO=1                                          6960
       L=NANF-NEND+1                                                    6970
       M=NRE(IREMO)                                                     6980
       NN=NEND                                                          6990
       IF(NCALL.EQ.0)  NN1(1,1)=NANF                                    7000
       IF(NCALL.EQ.0)  NN2(1,1)=NEND                                    7010
       DO 128 N=1,M                                                     7020
  129  NG(NN)=NFG(IREMO,N)                                              7030
       NI(NN)=NFI(IREMO,N)                                              7040
       NN=NN+1                                                          7050
       IF(NN.LE.NEND+NN1(IREMO,N)-NN2(IREMO,N)+1)  GO TO 129            7060
  128  CONTINUE                                                         7070
       IF(NN-1.EQ.NEND+L)  GO TO 130                                    7080
       WRITE(NOUT,131)                                                  7090
  131  FORMAT(1HO/' ***ERROR 0.13 : FOR MODULE 9 THE INPUT BLOCS 4 AND 16 7100
     1 DO NOT CORRESPOND')                                              7110
       KL=KL+1                                                          7120
       GO TO 132                                                        7130
  130  CALL REMO(NE,ENG,NFE,EF(1,2),EF(1,1),ERR,NLRA,NLRE,L,NG,NI,NJM,  7140
     1NUJM,ISELR,XL(NFR),XL(NFR),IADR-NFR+1)                            7150
       B=ZEIT(A)                                                        7160
       WRITE (NOUT,1004) NR(1,KL-1),B                                   7170
  132  IF(KL.LE.NA)  GO TO 100                                          7180
       GO TO 102                                                        7190
  120  IJ=IADR-NFR                                                      7200
       WRITE (NOUT,1003) NR(1,KL),IJ                                    7210
       C=0.                                                             7220
       A=ZEIT(C)                                                        7230
       CALL THERM (NE,NTYP,ITYP)                                        7240
       B=ZEIT(A)                                                        7250
       WRITE (NOUT,1004) NR(1,KL-1),B                                   7260
       IF(KL.LE.NA)  GO TO 100                                          7270
       GO TO 102                                                        7280
  121  WRITE (NOUT,122) NR(1,KL),JI                                     7290
  122  FORMAT(1HO/' ***ERROR 0.14 : THE REGION PARAMETER IN THE JOB- CARD 7300
     1 IS NOT GREAT ENOUGH TO START MODULE',I3,                         7310
     2' ;',I8,' WORDS ARE MISSED AT LEAST')                             7320
       IDUR=0                                                           7330
       B=ZEIT(A)                                                        7340
       WRITE (NOUT,1004) NR(1,KL),B                                     7350
       IF(NR(1,KL).EQ.5.AND.NINA.GT.0.AND.NINA.LT.NIN) GO TO 94         7360
       KL=KL+1                                                          7370
       IF(KL.LE.NA)  GO TO 100                                          7380
  102  CALL DATUM (DAT,TIME)                                            7390
       WRITE (NOUT,3000) DAT,TIME                                       7400
       RETURN                                                           7410
 5000  I=0                                                              7420
       WRITE (LTZ) I,N2                                                 7430
       STOP                                                             7440
       END                                                              7450
```

```
      SUBROUTINE PRPHI(NSP,E,F)                                          10
      DIMENSION E(NSP),F(NSP)                                            20
      COMMON A(4),NOUT                                                   30
      WRITE(NOUT,100)                                                    40
      IF(NSP.GT.1)GOTO 1                                                 50
      WRITE(NOUT,101)                                                    60
      GOTO 2                                                             70
    1 CALL TRAP(NSP,E,F,FINT)                                            80
      WRITE(NOUT,102)NSP,FINT                                            90
    2 CONTINUE                                                          100
      RETURN                                                            110
  100 FORMAT('///' FOR THE WEIGHTING SPECTRUM')                         120
  101 FORMAT('+',27X,'THE FUNCTION PHI(E) OR DPHI(E) WILL BE USED.')    130
  102 FORMAT('+',27X,'POINTWISE INPUT-DATA WILL BE USED. NUMBER OF POINT 140
     *S',I5,'. INTEGRAL',1PE16.7,'.')                                   150
      END                                                               160
```

```
      SUBROUTINE TRAP(N,X,Y,FINT)                                        10
C                                                                        20
C  SIMPLE TRAPEZOIDAL INTEGRATION                                        30
C                                                                        40
      DIMENSION X(N),Y(N)                                                50
      COMMON A(4),ICUT                                                   60
      FINT=0.                                                            70
      N1=N-1                                                             80
      IF(N1.LE.0)GOTO 2                                                  90
      DO 1 I=1,N1                                                       100
      DX=X(I+1)-X(I)                                                    110
      IF(DX.LT.0.)WRITE(IOUT,100)I,X(I),X(I+1)                          120
    1 FINT=FINT+DX*(Y(I+1)+Y(I))                                        130
      FINT=FINT*0.5                                                     140
    2 RETURN                                                            150
  100 FORMAT(' ***WARNING 0.15: ARGUMENTS NOT IN INCREASING ORDER DURING 160
     1 TRAPEZOIDAL INTEGRATION.',/                                      170
     *' ***              POINT I=',I5,' X(I)=',1PE12.4,' X(I+1)=',E12.4) 180
      END                                                               190
```

```
GAREA    START   0                                                       10
         BC      15,12(0,15)                                             20
         DC      XL1'07'                                                 30
         DC      CL7'GAREA  '                                            40
         STM     14,12,12(13)                                            50
         BALR    10,0                                                    60
         USING   *,10                                                    70
         ST      13,AREA+4                                               80
         LA      4,AREA                                                  90
         ST      4,8(0,13)                                              100
         LR      13,4                                                   110
BEGIN    SR      2,2                                                    120
         ST      2,LF+4                                                 130
         L       2,0(0,1)        ADRESSE DES 1. ARGUMENTS               140
         L       3,4(0,1)        ADRESSE DES 2. ARGUMENTS               150
         L       4,8(0,1)        ADRESSE DES 3. ARGUMENTS               160
         L       5,16(0,0)       CVT-ADRESSE                            170
         L       5,0(0,5)                                               180
         L       5,0(0,5)        TCB-ADRESSE                            190
         L       5,152(0,5)      D-PQE-ADRESSE                          200
         L       5,8(0,5)        PQE-ADRESSE                            210
         L       6,0(0,5)        ADRESSE DES 1. FBQE                    220
         L       7,4(0,5)        ADRESSE DES LETZTEN FBQE               230
STM3     LR      8,7                                                    240
         CLC     LF+5(3),9(6)                                           250
         BH      STM1                                                   260
         MVC     LF+5(3),9(6)    LAENGE DES FBQE WEGSPEICHERN           270
STM1     SR      8,6                                                    280
         BE      STM2                                                   290
         L       6,0(0,6)                                               300
         B       STM3                                                   310
STM2     L       5,LF+4                                                 320
         S       5,=X'00002800'                                         330
         ST      5,LF+4                                                 340
         GETMAIN VC,LA=LF,A=ADDR                                        350
         LTR     15,15                                                  360
         BE      STM4                                                   370
         SR      15,15           FEHLERAUSGANG                          380
         ST      15,0(0,3)                                              390
         ST      15,0(0,4)                                              400
         B       ENDE                                                   410
STM4     L       5,ADDR                                                 420
         SR      5,2                                                    430
         SRA     5,2(0)                                                 440
         ST      5,0(0,3)        SPEICHERN DES INKREMENTS (WORTE)       450
         L       5,ADDR+4                                               460
         SRA     5,2(0)                                                 470
         ST      5,0(0,4)        SPEICHERN DER LAENGE (WORTE)           480
ENDE     L       13,AREA+4                                              490
         LM      14,12,12(13)                                           500
         MVI     12(13),X'FF'                                           510
         BCR     15,14                                                  520
         DS      0F                                                     530
LF       DC      X'00000008'                                            540
         DS      1F                                                     550
ADDR     DS      2F                                                     560
AREA     DS      18F                                                    570
         END     GAREA                                                  580
```

```
      SUBROUTINE EING (NOUT)                                                    10
      WRITE (NOUT,1)                                                            20
    1 FORMAT(1HI/1HO/1HO/                                                       30
     1' INPUT DESCRIPTION FOR THE PROGRAM SYSTEM MIGROS-3'                //    40
     1' ************************************************'                ////  50
     2' INTRODUCTION'                                                     //    60
     3' THE PROGRAM SYSTEM MIGROS CALCULATES MICROSCOPIC GROUP'           /     70
     4' CONSTANTS FROM NUCLEAR CROSS SECTION DATA STORED IN THE'          /     80
     5' NUCLEAR DATA LIBRARY KEDAK. THE SYSTEM CONSISTS OF THE'           /     90
     6' FOLLOWING MODULES:'                                               //    100
     7' MODULE NO.   PURPOSE'                                             //    110
     8'      1       CALCULATION OF GROUP CROSS SECTIONS FOR INFINITE'    /     120
     9'              DILUTION AND OF RESONANCE SELF SHIELDING FACTORS'    /     130
     A'              FROM RESOLVED RESONANCE PARAMETERS.'                 //    140
     B'      2       CALCULATION OF GROUP CROSS SECTIONS FOR INFINITE'    /     150
     C'              DILUTION AND OF RESONANCE SELF SHIELDING FACTORS'    /     160
     D'              FROM STATISTICAL RESONANCE PARAMETERS.'              //    170
     E'      3       CALCULATION OF GROUP CROSS SECTIONS FOR INFINITE'    /     180
     F'              DILUTION AND OF RESONANCE SELF SHIELDING FACTORS'    /     190
     G'              FROM POINT CROSS SECTION DATA.'/)                          200
      WRITE (NOUT,2)                                                            210
    2 FORMAT(                                                                   220
     1'      4       CALCULATION OF WEIGHTED GROUP AVERAGES FOR'          /     230
     2'              INFINITE DILUTION.'                                  //    240
     3'      5       CALCULATION OF NORMALIZED TRANSFER MATRICES FOR'     /     250
     4'              INELASTIC SCATTERING, (N,2N) AND (N,3N) PROCESSES.'/       260
     4/                                                                         270
     5'      6       CALCULATION OF NORMALIZED ELASTIC SCATTERING'        /     280
     6'              MATRICES UP TO 5-TH ORDER (LEGENDRE REPRESENTA-'     /     290
     7'              TION), OF ELASTIC GROUP CROSS SECTIONS, OF THE'      /     300
     8'              AVERAGE ELASTIC SCATTERING COSINE AND OF TOTAL'      /     310
     9'              GROUP CROSS SECTIONS WITH ORDER-DEPENDENT'           /     320
     A'              WEIGHTING.'                                          //    330
     B'      7       CALCULATION OF FISSION SPECTRA.'                     //    340
     C'      8       CALCULATION OF WEIGHTED 1/V GROUP AVERAGES.'         //    350
     D'      9       CALCULATION OF NORMALIZED ELASTIC SCATTERING'        /     360
     E'              MATRICES UP TO 5-TH ORDER (LEGENDRE REPRESENTA-'     /     370
     F'              TION), OF WEIGHTED TOTAL AND ELASTIC SCATTERING'     /     380
     G'              GROUP CROSS SECTIONS AND OF GROUP-AVERAGED '         /     390
     H'              SCATTERING COSINES FOR THE REMO CORRECTION.'/)              400
      WRITE (NOUT,3)                                                            410
    3 FORMAT(                                                                   420
     1'     10       CALCULATION OF THERMAL CROSS SECTIONS.')                   430
      WRITE(NOUT,5)                                                             440
    5 FORMAT(1HI/1HO/1HO/                                                       450
     1' THE FOLLOWING INPUT MUST BE PROVIDED. IF GROUP CONSTANTS ARE'     /     460
     2' TO BE CALCULATED FOR SEVERAL MATERIALS THE COMPLETE INPUT MUST'/        470
     3' BE REPEATED FOR EACH ONE. THE INPUT IS FORMAT-FREE FOLLOWING'     /     480
     4' THE FREEFO CONVENTIONS: EACH DATA RECORD STARTS IN COLUMN 1 OF'/        490
     5' A DATA CARD. IF IT IS NOT POSSIBLE TO PLACE ALL THE DATA OF'      /     500
     6' ONE DATA RECORD ON ONE CARD, A SECOND, THIRD, ETC. CARD MAY'      /     510
     7' BE USED, WHICH MUST HAVE A BLANK IN COLUMN 1. OR: A NON BLANK'    /     520
     8' COLUMN 1 IN THE INPUT CARD IS AN INDICATION FOR A NEW INPUT'      /     530
     9' RECORD. ONE HAS TO DISTINGUISH BETWEEN AN ALPHAMERIC WORD OF'     /     540
     A' THE LENGTH REAL*4 AND OF THE LENGTH REAL*8. A REAL*4 WORD MUST'/        550
     B' BE ENCLOSED IN APOSTROPHIES AND IS STORED LEFT-ADJUSTED IN'       /     560
     C' THE COMPUTER AND FILLED UP WITH BLANKS IF NOT ALL 4 BYTES ARE'    /     570
     D' OCCUPIED. EXAMPLE: ''ARG'' OR ''ABCD''. A REAL*8 WORD MAY BE')          580
      WRITE(NOUT,4)                                                             590
    4 FORMAT(                                                                   600
     1' ENCLOSED IN APOSTROPHIES COMPRISING AT LEAST 5 CHARACTERS AND'    /     610
     2' AT MOST 8 CHARACTERS, WHICH ARE STORED LEFT-ADJUSTED IN THE '     /     620
     3' COMPUTER IF NOT ALL 8 BYTES ARE OCCUPIED. A SPECIAL CASE ARE'     /     630
     4' REAL*8 WORDS WITH A NUMBER OF OCCUPIED BYTES LESS THAN OR'        /     640
     5' EQUAL TO 5. THESE WORDS MAY BE ALSO ENCLOSED IN @-SIGNS. THEY'    /     650
     6' ARE ALSO STORED LEFT-ADJUSTED IN THE COMPUTER AND FILLED UP'      /     660
     7' WITH BLANKS. EXAMPLES: ''PU239''=''PU239    ''=@PU239@;'          /     670
     8' ''RES   ''=@RES@. FIXED POINT AND FLOATING POINT NUMBERS ARE'     /     680
     9' WRITTEN IN THE USUAL MANNER, E. G: FIXED POINT NUMBERS: 1  10'    /     690
     A' 875 AND FLOATING POINT NUMBERS: 10.  5.E3  0.7E-3  0.01 .'        /     700
     B' THE INPUT DATA ITEMS ARE SEPARATED BY ONE OR MORE BLANKS.')             710
      WRITE (NOUT,6)                                                            720
    6 FORMAT(1HI/1HO/1HO/                                                       730
     1' CARD 1'                                                           /     740
     2'   MAT            MATERIAL NAME IN KEDAK NOMENCLATURE'             /     750
     3'                  (8-BYTE ALPHAMERIC REPRESENTATION).'              /     760
     4'   ISTRUK  =0 : DOPPLER BROADENING IS NEGLIGIBLE AS IS TYPICAL'     /     770
     5'                  FOR S-WAVE RESONANCES OF STRUCTURAL MATERIALS,'   /     780
     6'           =1 : DOPPLER BROADENING MUST BE ACCOUNTED FOR AS IS'     /     790
     7'                  TYPICAL FOR HEAVY NUCLIDES.'                      //    800
     8'                  MORE SPECIFICALLY: IF MODULES 1 AND 2 ARE'        /     810
     9'                  UTILIZED, INFINITE DILUTION GROUP CROSS SEC-'     /     820
     A'                  TIONS AND RESONANCE SELF SHIELDING FACTORS ARE'   /     830
     B'                  CALCULATED FROM RESONANCE PARAMETERS FOR THE'     /     840
     C'                  FOLLOWING STANDARD TEMPERATURES :'                /     850
     D'                  T=0 K                  IF ISTRUK=0,'              /     860
     E'                  T=300, 900, 2100 K     IF ISTRUK=1.')                 870
      WRITE (NOUT,7)                                                            880
    7 FORMAT(                                                                   890
     1'                  IF MODULE 3 IS UTILIZED THE SAME QUANTITIES ARE'/      900
     2'                  CALCULATED FROM POINT DATA FOR THAT TEMPERATURE'/      910
     3'                  FOR WHICH THE POINT DATA ARE STORED (T=0 K IN'    /    920
     4'                  THE PRESENT VERSION, KEDAK-3), REGARDLESS OF'     /    930
     5'                  THE ISTRUK VALUE.'                                /    940
     6'                  IF TEMPERATURES DIFFERING FROM THE STANDARD'      /    950
     7'                  TEMPERATURES ARE TO BE USED, THIS MUST BE SPE-'   /    960
     8'                  CIFIED ON CARD 9 BELOW.'                          ///  970
     9' IF GROUP BOUNDARIES DIFFERING FROM THOSE OF THE 26-GROUP ABBN'     /    980
     A' SET ARE TO BE USED (VIZ. 0.215EV, 0.465EV, 1EV, 2.15EV, 4.65EV'/        990
     B' 10EV, 21.5EV, 46.5EV, 100EV, 215EV, 465EV, 1KEV, 2.15KEV,'       /    1000
     C' 4.65KEV, 10KEV, 21.5KEV, 46.5KEV, 100KEV, 200KEV, 400KEV,'       /    1010
     D' 800KEV, 1.4MEV, 2.5MEV, 4MEV, 6.5MEV, 10.5MEV) TWO MORE CARDS'   /    1020
     E' FOLLOW:'/)                                                              1030
      WRITE (NOUT,8)                                                            1040
    8 FORMAT(                                                                   1050
     1' CARD 2'                                                           /    1060
     2'   @BLOC@    1         INVARIANT'                                   /    1070
     3' CARD 3'                                                           /    1080
     4'   NE                 NUMBER OF ENERGY GROUP BOUNDARIES'           /    1090
     5'                      (ARBITRARY),'                                /    1100
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     6'   (ENG(I),I=1,NE)    ENERGY GROUP BOUNDARIES IN UNITS OF EV'     / 1110
     7'                      IN ASCENDING ORDER.'                       // 1120
     8' NOTE THAT THE NUMBER OF ENERGY GROUPS THAT MIGROS CAN TREAT'    / 1130
     9' IS NOT RESTRICTED TO 26.'                                      /// 1140
     A' THE STANDARD WEIGHTING FUNCTION IS THE COLLISION DENSITY'       / 1150
     B' F(I,1)=PHI(E(I))=1./E(I). ALTERNATIVELY ONE CAN EMPLOY OTHER'   / 1160
     C' WEIGHTING FUNCTIONS AFTER LINKAGE OF AN APPROPRIATE FUNCTION'   / 1170
     D' PHI(E) WITH MIGROS. IF IN THIS CASE MODULE 3 IS USED ONE MUST'  / 1180
     E' LINK AN ADDITIONAL FUNCTION DPHI(E) YIELDING BASICALLY THE'     / 1190
     F' SAME RESULT AS PHI BUT WITH DOUBLE PRECISION. A THIRD ALTERNA-'/ 1200
     G' TIVE IS UTILIZATION OF A POINTWISE GIVEN COLLISION DENSITY FOR'/ 1210
     H' WHICH ONE NEEDS THE FOLLOWING CARDS:')                          1220
      WRITE (NOUT,9)                                                    1230
   9 FORMAT(1H1/1HC/1H0/                                                1240
     1' CARD 4'                                                       / 1250
     2'   @BLOC@   2          INVARIANT'                              / 1260
     3' CARD 5'                                                       / 1270
     4'   NSPEC               NUMBER OF SPECTRA,'                     / 1280
     5'   NFE                 NUMBER OF ENERGY GRID POINTS,'          / 1290
     6'   (EE(I),I=1,NFE),((F(I,J),I=1,NFE),J=1,NSPEC)   WITH'       / 1300
     7'                       EE: ENERGY GRID POINTS IN UNITS OF EV'  / 1310
     8'                           IN ASCENDING ORDER,'                / 1320
     9'                        F: COLLISION DENSITY VALUES.'         // 1330
     A' IF THE NUMBER OF SPECTRA (COLLISION DENSITY FUNCTIONS) IS'     / 1340
     B' GREATER THAN 1 THE SPECTRA 2, 3,... ARE INTERPRETED ONLY IN'   / 1350
     C' MODULE 6 WHERE THEY ARE TAKEN AS THE WEIGHTING FUNCTIONS FOR'  / 1360
     D' THE 1ST, 2ND,... MOMENT OF THE ELASTIC SCATTERING MATRIX'      / 1370
     E' (MW=1 ON CARD 35). MAKE SURE THAT THE NUMBER OF SPECTRA IS'    / 1380
     F' CONSISTENT WITH THE NUMBER OF MOMENTS CALCULATED. IF ONLY ONE' / 1390
     G' SPECTRUM IS SPECIFIED IT WILL BE EMPLOYED FOR ALL REQUIRED')    1400
      WRITE (NOUT,10)                                                   1410
  10 FORMAT(                                                            1420
     1' MOMENTS OF THE ELASTIC SCATTERING MATRIX. A SPECIAL MODIFICA-'  / 1430
     1' TION, HOWEVER, ALLOWS AN IMPROVED TREATMENT OF FINE-STRUCTURE'  / 1440
     1' WEIGHTING (SEE CARDS 32-35). THE NUMBER OF GRID'                / 1450
     2' POINTS IS ARBITRARY BUT CARE SHOULD BE TAKEN THAT THE SPECTRA'  / 1460
     3' COVER THE WHOLE ENERGY RANGE OF INTEREST.'                     /// 1470
     4' CARD 6'                                                       / 1480
     5'   @BLOC@   3          INVARIANT'                              / 1490
     6' CARD 7'                                                       / 1500
     7'   NA                  NUMBER OF MODULES UTILIZED,'            / 1510
     8'   ((NR(I,J),I=1,3),J=1,NA)   WITH'                           / 1520
     9'                       NR(I,J)  NUMBER OF MODULE,'             / 1530
     A'                       NR(2,J)  NUMBER OF ENERGY GROUP WHERE CAL-'/ 1540
     B'                                CULATION WITH MODULE NR(1,J) IS'  / 1550
     C'                                TO BEGIN,'                     / 1560
     D'                       NR(3,J)  NUMBER OF ENERGY GROUP UP TO'  / 1570
     E'                                WHICH CALCULATION WITH MODULE'  / 1580
     F'                                NR(1,J) IS TO BE EXTENDED.')      1590
      WRITE (NOUT,11)                                                   1600
  11 FORMAT(                                                            1610
     1'                                THE LIMITS NR(2,J), NR(3,J) ARE'  / 1620
     2'                                TO BE GIVEN IN THE USUAL SENSE OF'/ 1630
     3'                                ASCENDING ENERGY. NOTE THAT THEN' / 1640
     4'                                NR(3,J)<=NR(2,J), SINCE GROUPS'   / 1650
     5'                                ARE CONVENTIONALLY LABELED IN THE'/ 1660
     6'                                REVERSE SENSE, I. E. GROUP NUMBER'/ 1670
     7'                                1 IS ASSIGNED TO THE GROUP BE-'   / 1680
     8'                                TWEEN THE HIGHEST TWO ENERGY'     / 1690
     9'                                VALUES ON CARD 3.'               // 1700
     A' COMMENT:'                                                       / 1710
     B' MODULES CAN BE CALLED MORE THAN ONCE. THIS IS NECESSARY IF'     / 1720
     C' SEVERAL UNCONNECTED RANGES OF ENERGY GROUPS MUST BE TREATED.'   / 1730
     D' FOR EACH RANGE ONE CALL MUST BE MADE.'                          / 1740
     E' NR(2,J) AND NR(3,J) ARE INTERPRETED AS REFERRING TO OUT-SCAT-'  / 1750
     F' TERING GROUPS IN THE CASE OF ELASTIC AND INELASTIC SCATTERING')  1760
      WRITE (NOUT,12)                                                   1770
  12 FORMAT(1H1/1HC/1HC/                                                1780
     1' MATRICES. THE CALCULATION IS PERFORMED FOR ALL IN-SCATTERING'   / 1790
     2' GROUPS, I. E. ALL GROUPS LISTED IN @BLOC@ 1 INTO WHICH A'       / 1800
     3' NEUTRON CAN GET IN THE COURSE OF SCATTERING PROCESSES. THE'     / 1810
     4' THERMAL GROUP IS INCLUDED AS IN-SCATTERING GROUP.'            /// 1820
     5'                    *****'                                     /// 1830
     6' IF MODULE 1 AND 2 FOR CALCULATION OF SELF-SHIELDING FACTORS'    / 1840
     7' FROM RESOLVED AND STATISTICAL RESONANCE PARAMETERS ARE CALLED,'/ 1850
     8' AND TEMPERATURES OTHER THAN THE STANDARD TEMPERATURES (0KELVIN'/ 1860
     9' FOR STRUCTURAL MATERIALS, ISTRUK=0, 300, 900 AND 2100 KELVIN'   / 1870
     A' FOR HEAVY NUCLEI, ISTRUK=1) ARE NEEDED, TWO MORE CARDS MUST'    / 1880
     B' FOLLOW:'                                                       // 1890
     C' CARD 8'                                                       / 1900
     D'   @BLOC@   4          INVARIANT'                              / 1910
     E' CARD 9'                                                       / 1920
     F'   NT                  NUMBER OF TEMPERATURES (ARBITRARY),'    / 1930
     G'   (TEMP(I),I=1,NT)    TEMPERATURES IN KELVIN.'//)              1940
      WRITE(NOUT,13)                                                    1950
  13 FORMAT(                                                            1960
     1' IF SELF-SHIELDING FACTORS ARE TO BE CALCULATED (WITH MODULE 1,'/ 1970
     2' 2 OR 3) FOR DILUTION CROSS SECTIONS SIGMA0 (SIGO(I)) DIFFERING'/ 1980
     3' FROM THOSE OF THE ABBN GROUP CONSTANT SET (VIZ. 0, 10, 100,'    / 1990
     4' 1000, 10000, 100000 AND 1000000 BARN) THE FOLLOWING CARDS ARE'  / 2000
     5' NEEDED:'                                                       // 2010
     6' CARD 10'                                                      / 2020
     7'   @BLOC@   5          INVARIANT'                              / 2030
     8' CARD 11'                                                      / 2040
     9'   MI                  NUMBER OF DILUTION CROSS SECTIONS'      / 2050
     A'                       (ARBITRARY),'                           / 2060
     B'   (SIGO(I),I=1,MI)    DILUTION CROSS SECTION VALUES (SIGMA0-'  / 2070
     C'                       VALUES) IN BARN.'                     /// 2080
     D'                         *****'                              /// 2090
     E' IF WEIGHTED GROUP AVERAGES FOR INFINITE DILUTION ARE TO BE'     / 2100
     F' CALCULATED (WITH MODULES 4 AND 10) FOR DATA TYPES OTHER THAN'   / 2110
     G' THE 8 STANDARD TYPES MUEL, NUE, SGA, SGF, SGI, SGN, SG2N, AND' ) 2120
      WRITE (NOUT,14)                                                   2130
  14 FORMAT(                                                            2140
     1' SGT THE FOLLOWING CARDS ARE NEEDED:'                           // 2150
     2' CARD 12'                                                      / 2160
     3'   @BLOC@   6            INVARIANT'                            / 2170
     4' CARD 13'                                                      / 2180
     5'   NTYP                  NUMBER OF DATA TYPES (ARBITRARY),'    / 2190
     6'   (ITYP(I),I=1,NTYP)    DATA TYPES (KEDAK NOMENCLATURE).')     2200
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      WRITE (NOUT,15)                                                   2210
   15 FORMAT(1H1/1HO/1HO/                                               2220
     1' COMMENT:'                                                     / 2230
     2' WEIGHTED GROUP AVERAGES CAN BE CALCULATED FOR ALL DATA TYPES' / 2240
     3' WHICH CAN BE REPRESENTED AS ONE-VALUED FUNCTIONS OF A SINGLE' / 2250
     4' ARGUMENT (INCIDENT NEUTRON ENERGY). THE POSSIBLE TYPES ARE'   / 2260
     5' LISTED IN KFK 1725 OR KFK 2234. SPECIAL DEFINITIONS OF GROUP' / 2270
     6' AVERAGES ARE USED FOR COMPOSITE QUANTITIES SUCH AS ALPHA, ETA,'/ 2280
     7' MUEL OR NUE (CF. KFK 1784). IF THE CROSS SECTION TYPES SGF AND'/ 2290
     8' SGA (SEE KFK 2234) ARE TREATED THE CROSS SECTION TYPE'        / 2300
     9' SGC=SGA-SGF IS AUTOMATICALLY TREATED, TOO.'                  /// 2310
     A'                          *****'                              /// 2320
     B' IF RESONANCE SELF-SHIELDING FACTORS ARE TO BE CALCULATED FROM' / 2330
     C' INDIVIDUAL RESONANCE PARAMETERS (MODULE 1), BUT ONLY WITH A'  / 2340
     D' LIMITED NUMBER OF RESONANCES ON EITHER SIDE OF EACH ENERGY'   / 2350
     E' GRID POINT, TWO MORE CARDS FOLLOW:'/)                           2360
      WRITE (NOUT,16)                                                   2370
   16 FORMAT(                                                           2380
     1' CARD 14'                                                      / 2390
     2'   @BLOCA    11       INVARIANT'                              / 2400
     3' CARD 15'                                                      / 2410
     4'   NRES               NUMBER OF RESONANCES TO BE CONSIDERED ON'/ 2420
     5'                      EITHER SIDE OF A GIVEN ENERGY.'         /// 2430
     6' IF MODULE 1 IS TO BE EMPLOYED, BUT NOT WITH THE STANDARD VALUE'/ 2440
     7' 0.01 OF THE MAXIMUM ADMISSIBLE RELATIVE ERROR FOR THE INTEGRA-'/ 2450
     8' TION, ONE NEEDS THE FOLLOWING TWO CARDS:'                    // 2460
     9' CARD 16'                                                      / 2470
     A'   @BLOCA    12       INVARIANT'                              / 2480
     B' CARD 17'                                                      / 2490
     C'   ERROR              MAXIMUM ADMISSIBLE RELATIVE INTEGRATION'/ 2500
     D'                      ERROR.'                                 /// 2510
     E'                         *****'                               /// 2520
     F' IF GROUP CROSS SECTIONS AND SELF-SHIELDING FACTORS ARE TO BE' / 2530
     G' CALCULATED FROM POINT DATA (MODULE 3) BUT NOT WITH THE STAN-')  2540
      WRITE (NOUT,17)                                                   2550
   17 FORMAT(                                                           2560
     1' DARD VALUES EPSROM=5.0E-05, ORINWA=5.0, (EXPLAINED BELOW)'    / 2570
     2' ONE NEEDS THE FOLLOWING TWO CARDS:'                          // 2580
     3' CARD 18'                                                      / 2590
     4'   @BLOCA    31       INVARIANT'                              / 2600
     5' CARD 19'                                                      / 2610
     6'   EPSROM             RELATIVE ACCURACY FOR THE ROMBERG INTEGRA-' / 2620
     7'                      TION. THE ITERATION STOPS IF THE RELATIVE'  / 2630
     8'                      DIFFERENCE BETWEEN TWO SUCCESSIVE APPROXI-' / 2640
     9'                      MATIONS IS NOT GREATER THAN EPSROM,')       2650
       WRITE (NOUT,18)                                                  2660
   18 FORMAT(1H1/1HO/1HO/                                               2670
     1'   ORINWA             CONTROL OF ERROR PRINTING IN THE ROMBERG'  / 2680
     2'                      ITERATION SUBROUTINE. IF THE ITERATION IS' / 2690
     3'                      STOPPED (E. G. BY ROUND-OFF ERRORS) BEFORE' / 2700
     4'                      THE EPSROM CRITERION IS FULFILLED, AN ERROR'/ 2710
     5'                      MESSAGE IS PRINTED ONLY IF THE CRITERION IS'/ 2720
     6'                      NOT EVEN FULFILLED WITH ORINWA TIMES EPSROM.' 2730
     7//)                                                               2740
      WRITE(NOUT,19)                                                    2750

   19 FORMAT(                                                           2760
     1' IF MODULE 3 IS TO BE EMPLOYED BUT NOT WITH THE DEFAULT VALUES' / 2770
     2' ITEST=0, IZPUMS=-1 AND ITUMS=0 (CF. CARD 21), THE FOLLOWING'  / 2780
     3' TWO CARDS ARE NEEDED:'                                       // 2790
     4' CARD 20'                                                      / 2800
     5'   @BLOCA    32       INVARIANT'                              / 2810
     6' CARD 21'                                                      / 2820
     7'   ITEST              CONTROL OF ERROR MESSAGES AND WARNINGS' / 2830
     8'                      =0: NORMAL PRINT-OUT FOR PRODUCTION RUNS,' / 2840
     9'                      =1: EXTENDED PRINT-OUT FOR PROGRAM'     / 2850
     A'                          DEBUGGING,'                         / 2860
     B'                      =2: AS ITEST=1 WITH ADDITIONAL PRINT-OUT,' / 2870
     C'                      =3: AS ITEST=2 WITH FURTHER EXTENDED PRINT-'/ 2880
     D'                          OUT,'                               / 2890
     E'                      =4, 5, ..9: AS ITEST=3,'                / 2900
     F'                      =10, 11, 12, 13: AS ITEST=0, 1, 2, 3 WITH' / 2910
     G'                          ADDITIONAL ERROR MESSAGES FOR EACH' / 2920
     H'                          SIGO VALUE,')                       2930
      WRITE (NOUT,20)                                                   2940
   20 FORMAT(                                                           2950
     1'                      >13: AS ITEST=13.'                      / 2960
     2'   IZPUMS             CONTROL OF ITEST FOR DIFFERENT GROUPS'  / 2970
     3'                      <=-1: ITEST IS UNCHANGED,'              / 2980
     4'                      =IGR: BEGINNING WITH THE IGR-TH GROUP UP TO'/ 2990
     5'                            THE NR(3,J)-TH GROUP (CF. CARD 7)' / 3000
     6'                            ITEST HAS THE NEW VALUE ITUMS (SEE' / 3010
     7'                            BELOW). IGR MUST BE LESS THAN OR'  / 3020
     8'                            EQUAL TO NR(2,J) (CF. CARD 7). THIS' / 3030
     9'                            IS VALID FOR ALL J WITH NR(1,J)=3,  '/ 3040
     A'                            I. E. WHENEVER MODULE 3 IS CALLED.' / 3050
     B'   ITUMS              NEW VALUE OF ITEST.'                    /// 3060
     C' IF MODULE 3 IS TO BE UTILIZED BUT NOT WITH THE DEFAULT VALUES' / 3070
     D' NENBER=1, ENBER(1)=-1.0, CONWFU(1)=1.0, OR NOT WITH NWFUN(1)=0'/ 3080
     E' IN CASE OF A CALCULATED COLLISION DENSITY, OR NOT WITH'       / 3090
     F' NWFUN(1)=-1 IN CASE OF A POINTWISE GIVEN COLLISION DENSITY'   / 3100
     6' (CF. CARD 23) ONE NEEDS THE NEXT TWO CARDS:'/)                  3110
      WRITE (NOUT,21)                                                   3120
   21 FORMAT(                                                           3130
     1' CARD 22'                                                      / 3140
     2'   @BLOCA    33       INVARIANT'                              / 3150
     3' CARD 23'                                                      / 3160
     4'   NENBER             NUMBER OF ENERGY INTERVALS WITH  DIFFERENT' / 3170
     5'                      WEIGHTING FUNCTIONS AND/OR DIFFERENT INTE-' / 3180
     6'                      GRATION METHODS,')                         3190
      WRITE(NOUT,22)                                                    3200
   22 FORMAT(1H1/1HO/1HO/                                               3210
     1'   (ENBER(I),NWFUN(I),CONWFU(I),I=1,NENBER)  WITH'             / 3220
     2'                      ENBER(I): UPPER LIMIT OF I-TH ENERGY INTER-'/ 3230
     3'                      VAL, EQUAL TO LOWER LIMIT OF (I+1)-TH'  / 3240
     4'                      ENERGY INTERVAL, SO THAT'               / 3250
     5'                      ENBER(I) < ENBER(I+1).'                 / 3260
     6'                      THE LOWER LIMIT FOR THE FIRST ENERGY INTER-'/ 3270
     7'                      VAL IS TAKEN AS EQUAL TO THE BEGINNING OF' / 3280
     8'                      THE CURRENT ENERGY GROUP RANGE (SMALLEST' / 3290
     9'                      ENERGY VALUE) AS SPECIFIED ON CARD 3 (OR IN'/ 3300
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  A'                    THE PROGRAM AND IN CARD 7 IN CASE OF SEVE-' / 3310
  B'                    RAL DISCONNECTED ENERGY GROUP RANGES).'     / 3320
  C'                    ENBER(NENBER) MUST BE AT LEAST AS GREAT AS' / 3330
  D'                    THE LARGEST ENERGY OF THE CURRENT ENERGY'   / 3340
  E'                    GROUP RANGE.'                               / 3350
  F'                    SPECIAL CASE FOR NENBER=1:'                 / 3360
  G'                    ENBER(1)=-1.0. THIS MEANS THE WHOLE SPECI-') 3370
   WRITE (NOUT,23)                                                  3380
23 FORMAT(                                                          3390
  1'                    FIED ENERGY GROUP RANGE.'                   / 3400
  2'                    NWFUN(I): TYPE OF WEIGHTING FUNCTION AND'   / 3410
  3'                    METHOD OF INTEGRATION USED IN INTERVAL I.'  / 3420
  4'                    METHOD OF INTEGRATION:'                     / 3430
  5'                    NWFUN(I)<=0:  NUMERICAL INTEGRATION WITH '  / 3440
  6'                                  THE ROMBERG METHOD,'          / 3450
  7'                    NWFUN(I)>0 :  ANALYTICAL INTEGRATION.'      / 3460
  8'                    TYPE OF WEIGHTING FUNCTION:'                / 3470
  9'                    |NWFUN(I)|=C: ARBITRARY FUNCTION WITH THE' / 3480
  A'                                  NAME OPHI.(OPHI=1./E BY DE-'  / 3490
  B'                                  FAULT IF NOT GIVEN BY THE'    / 3500
  C'                                  USER AS A FUNCTION SUBROUTINE'/ 3510
  D'                                  TO THE PROGRAM),'             / 3520
  E'                    |NWFUN(I)|=1: POINTWISE WEIGHTING FUNCTION,'/ 3530
  F'                    |NWFUN(I)|=2: OPHI=CONWFU(I)/E (FOR CONWFU' ) 3540
   WRITE (NOUT,24)                                                  3550
24 FORMAT(                                                          3560
  1'                                  SEE NEXT INPUT VARIABLE).'    / 3570
  2'                                  CAUTION: BECAUSE IN SOME'     / 3580
  3'                                  CASES ROUNDING ERRORS APPEAR' / 3590
  4'                                  WHEN THE ANALYTICAL INTEGRA-' / 3600
  5'                                  TION IS CHOSEN, WE RECOMMEND' / 3610
  6'                                  TO USE ONLY NWFUN(I)<=0.'     / 3620
  7'                                  THERE IS NO DIFFERENCE IN THE'/ 3630
  8'                                  CPU TIMES BETWEEN ROMBERG AND'/ 3640
  9'                                  ANALYTICAL INTEGRATION.'      / 3650
  A'                    CONWFU(I):    FACTOR IN THE WEIGHTING FUNC-'/ 3660
  B'                                  TION OPHI=CONWFU(I)/E. ONLY'  / 3670
  C'                                  USED IF |NWFUN(I)|=2.'      /// 3680
  D'                      *****'                                  //) 3690
   WRITE (NOUT,25)                                                  3700
25 FORMAT(                                                          3710
  1' THREE DIFFERENT OPTIONS ARE AVAILABLE FOR THE TRANSFER PROBA-' / 3720
  2' BILITIES NEEDED FOR THE CALCULATION (WITH MODULE 5) OF NORMA-' / 3730
  3' LIZED TRANSFER MATRICES FOR INELASTIC SCATTERING WITH EXCITA-' / 3740
  4' TION OF DISCRETE LEVELS AT EXCITATION ENERGIES EJ:'            / 3750
  5' (1)  F(EP-->E)=DELTA(EP-E-EJ)       IF KINEM=0,'               / 3760
  6'      WHERE DELTA DENOTES DIRAC''S DELTA FUNCTION. THIS FORM'   / 3770
  7'      WAS USED IN THE ORIGINAL VERSION OF MIGROS-2 (KFK 1784).') 3780
   WRITE (NOUT,26)                                                  3790
26 FORMAT(1H1/1H0/1H0/                                              3800
  1' (2)  F(EP-->E)=DELTA(EP-E-EJ*(A+1.)/A)        IF KINEM=1'      / 3810
  2'      THIS FORM WAS USED IN THE REVISED VERSION OF MIGROS-2'    / 3820
  3'      (TRANSFORMATION OF EJ FROM CMS TO LAB COORDINATES)."      / 3830
  4' (3)  F(EP-->E)=DELTA(E-EP*(A**2+1.)/(A+1.)**2'                 / 3840
  5'                     +EJ*A/(A+1.))             IF KINEM=2'      / 3850
  6'      THIS APPROXIMATION WAS RECOMMENDED BY SEGEV (SEGEV,'      / 3860
  7'      NSE 45 (1971)269 AND VERTES, NSE 52 (1973)485) AND IS'    / 3870
  8'      ALSO PROPOSED FOR THE PROCESSING OF ENDF/B DATA (DRAKE,'  / 3880
  9'      BNL 50274 (T-6C1) ENDF 102, VOL.1).'                      / 3890
  A' FORM (2), I. E. KINEM=1, IS THE DEFAULT OPTION IN MODULE 5. IF'/ 3900
  B' EITHER FORM (1) OR (3) IS TO BE USED ONE NEEDS THE FOLLOWING'  / 3910
  C' ADDITIONAL INPUT:'                                            // 3920
  D' CARD 24'                                                       / 3930
  E'   @BLOC@   51       INVARIANT'                                 / 3940
  F' CARD 25')                                                      3950
   WRITE (NOUT,27)                                                  3960
27 FORMAT(                                                          3970
  1'   KINEM             TAG FOR TREATMENT OF DISCRETE LEVELS'     / 3980
  2'                      (SEE ABOVE).'                           /// 3990
  3' IF FOR THE MATERIAL OF INTEREST THE NUCLEAR DATA LIBRARY DOES' / 4000
  4' NOT CONTAIN ANY INFORMATION ON THE ENERGY DISTRIBUTION OF'     / 4010
  5' SECONDARY NEUTRONS (SED1C, SED2N, SED3N) IN THE ENERGY REGION' / 4020
  6' OF CONTINUOUS LEVEL EXCITATION OF THE RESIDUAL NUCLEUS AN'     / 4030
  7' EVAPORATION MODEL IS EMPLOYED IN MODULE 5. THE PARAMETER XNUE' / 4040
  8' FOR THE CALCULATION OF THE NUCLEAR TEMPERATURE,'               / 4050
  9' THETA(EP)=SQRT(EP/(XNUE*A)), IS SET EQUAL TO XNUE=0.16/MEV BY' / 4060
  A' DEFAULT. (A= ATOMIC WEIGHT OF THE TARGET NUCLEUS.) IF OTHER'   / 4070
  A' XNUE VALUES ARE TO BE USED ONE NEEDS THE FOLLOWING ADDITIONAL' / 4080
  B' INPUT:'                                                       // 4090
  C' CARD 26'                                                       / 4100
  D'   @BLOC@   52       INVARIANT'                                 / 4110
  E' CARD 27'                                                       / 4120
  F'   XNUE               EVAPORATION MODEL PARAMETER'             / 4130
  G'                      (IN UNITS OF 1/MEV).'                   //) 4140
   WRITE (NOUT,28)                                                  4150
28 FORMAT(                                                          4160
  1' IF MODULE 5 IS CALLED THE TRANSFER MATRICES FOR INELASTIC'     / 4170
  2' SCATTERING AND FOR (N,2N) ARE CALCULATED BY DEFAULT. IF OTHER' / 4180
  3' REACTION TYPES ARE WANTED ONE NEEDS THE FOLLOWING ADDITIONAL'  / 4190
  4' INPUT:'                                                       // 4200
  5' CARD 28'                                                       / 4210
  6'   @BLOC@   53          INVARIANT'                             / 4220
  7' CARD 29'                                                       / 4230
  8'   NIN                  NUMBER OF REACTION TYPES,'             / 4240
  9'   (INTYP(I),I=1,NIN)   REACTION TYPE INDICATORS:'             / 4250
  A'                        INTYP=1  FOR INELASTIC SCATTERING,'    / 4260
  B'                        INTYP=2  FOR (N,2N) PROCESSES,'        / 4270
  C'                        INTYP=3  FOR (N,3N) PROCESSES.'       /// 4280
  D'                       *****')                                 4290
   WRITE (NOUT,29)                                                  4300
29 FORMAT(1H1/1H0/1H0/                                              4310
  E' IF MODULE 6 IS TO BE USED BUT NOT WITH THE STANDARD VALUES'    / 4320
  F' ISEL=2, NLE=5 ONE NEEDS THE FOLLOWING CARDS:'                 // 4330
  G' CARD 30'                                                       / 4340
  H'   @BLOC@   61       INVARIANT'                                 / 4350
  1' CARD 31'                                                       / 4360
  2'   ISEL               TAG FOR POSSIBLE CROSS SECTION MODIFICATION'/ 4370
  3'                      AND ADDITIONAL PRINT-OUT (DEFAULT VALUE: 2)'/ 4380
  4'                      |ISEL|=2: NO CROSS SECTION MODIFICATION;'  / 4390
  5'                      |ISEL|=1: BELOW 1CKEV, IN THE RESOLVED'    / 4400
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 6'                              RESONANCE RANGE, THE ELASTIC'      / 4410
 7'                              SCATTERING AND TOTAL CROSS SEC-'   / 4420
 8'                              TIONS ARE SET EQUAL TO 1 BARN'     / 4430
 9'                              (MAINLY TO SIMPLIFY THE CALCULA-'  / 4440
 A'                              TION OF APPROXIMATE SCATTERING'    / 4450
 B'                              PROBABILITIES AND AVERAGE ELASTIC'/ 4460
 C'                              SCATTERING COSINES FOR HEAVY ELE-'/ 4470
 D'                              MENTS, AND TO SAVE CORE MEMORY'    / 4480
 E'                              SPACE).')                          4490
  WRITE (NOUT,30)                                                   4500
30 FORMAT(                                                          4510
 1'                      ISEL<0:   ADDITIONAL PRINT-OUT OF INTERME-' / 4520
 2'                                DIATE INFORMATION.'               / 4530
 3'   NLE                HIGHEST ORDER IN LEGENDRE EXPANSION (MAX 5)'/ 4540
 4'                      THE ACTUAL VALUE USED IS MAX(1,NLE) BECAUSE'/ 4550
 5'                      OF THE NORMALIZATION OF THE AVERAGE SCATTE-'/ 4560
 6'                      RING COSINES TO THE KEDAK MOEL VALUES. THE' / 4570
 6'                      MODULE ALWAYS CALCULATES SCATTERING '       / 4580
 6'                      MATRICES FROM MOMENT ZERO TO MOMENT NLE.' /// 4590
 7' IF MODULE 6 IS CALLED AND FINE-STRUCTURE WEIGHTING WITH'         / 4600
 8' 1./SGT**(L+1) IS TO BE EMPLOYED FOR THE L-TH MOMENT ADD THE '    / 4610
 8' CARDS 32 UP TO 35:'                                            // 4620
 9' ADD THE FOLLOWING CARDS:'                                      // 4630
 A' CARD 32'                                                        / 4640
 B'   @BLOC@   62       INVARIANT'                                  / 4650
 C' CARD 33'                                                        / 4660
 D'   NMAT              NUMBER OF MATERIALS IN THE MIXTURE WHOSE'   / 4670
 E'                     MACROSCOPIC TOTAL CROSS SECTION IS TO BE'   / 4680
 F'                     USED FOR FINE-STRUCTURE WEIGHTING;')        4690
  WRITE (NOUT,31)                                                   4700
31 FORMAT(                                                          4710
 1'   (NAME(I),TZ(I),I=1,NMAT)   WITH'                             / 4720
 2'                     NAME: MATERIAL NAME (8-BYTE ALPHAMERIC'     / 4730
 3'                           REPRESENTATION),'                     / 4740
 4'                     TZ  : NUCLEAR DENSITY (NUCLEI PER CM**3)'   / 4750
 5'                           TIMES 1.E-24.'                     /// 4760
 6' IF MODULE 6 IS CALLED AND NOT ALL MOMENTS ARE TO BE WEIGHTED'    / 4770
 7' BY THE COLLISION DENSITY F(I,1) (CF. CARD 5) OF THE 0-TH MO-'    / 4780
 8' MENT, THE FOLLOWING CARDS ARE NEEDED:'                         // 4790
 9' CARD 34'                                                        / 4800
 A'   @BLOC@   63       INVARIANT'                                  / 4810
 B' CARD 35'                                                        / 4820
 C'   MW               TAG FOR WEIGHTING,'                         / 4830
 D'                     MW=1: WEIGHT F(I,L+1) FOR L-TH MOMENT,'     / 4840
 E'                           NSPEC=NLE+1 MUST OCCUR ON CARD 5 WITH'/ 4850
 F'                           NLE GIVEN ON CARD 31 OR BY DEFAULT;')  4860
  WRITE (NOUT,32)                                                   4870
32 FORMAT(1H1/1HO/1HO/                                              4880
 1'                     MW=2: WEIGHT F(I,1)/SGT**(L+1) FOR L-TH'    / 4890
 2'                           MOMENT (CARD 33 MUST PRECEDE).'    /// 4900
 3' IF MODULE 6 IS USED BUT NOT WITH THE STANDARD GRID POINT'       / 4910
 4' NUMBERS PER GROUP (NK=70, NR=16, SEE BELOW) ONE NEEDS THE'      / 4920
 5' FOLLOWING CARDS:'                                              // 4930
 6' CARD 36'                                                        / 4940
 7'   @BLOC@   64       INVARIANT'                                  / 4950
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 8' CARD 37'                                                        / 4960
 9'   NK                NK*MIN(1,ALOG(ENG(I)/ENG(I-1))/          ' / 4970
 A'                     ALOG(1/ALFA)) IS THE NUMBER OF BASIC GRID' / 4980
 B'                     POINTS IN THAT ENERGY REGION WITHIN GROUP I'/ 4990
 C'                     FROM WHICH ELASTIC SCATTERING INTO ADJACENT'/ 5000
 D'                     GROUPS IS POSSIBLE, ALFA=((A-1)/(A+1))**2,' / 5010
 E'                     A= ATOMIC WEIGHT IN NEUTRON MASS UNITS;')    5020
  WRITE (NOUT,33)                                                   5030
33 FORMAT(                                                          5040
 1'   NR                NR IS THE NUMBER OF BASIC GRID POINTS IN'   / 5050
 2'                     THAT ENERGY REGION OF EACH GROUP FROM WHICH'/ 5060
 3'                     ELASTIC SCATTERING INTO ADJACENT GROUPS IS' / 5070
 4'                     IMPOSSIBLE. (THIS REGION POSSIBLY MAY NOT'  / 5080
 5'                     EXIST, THEN NR HAS NO MEANING.)'          /// 5090
 4'                       *****'                                  /// 5100
 5' IF 1/V AVERAGES ARE TO BE CALCULATED (WITH MODULE 8), BUT NOT'  / 5110
 6' WITH THE MAXIMUM ADMISSIBLE RELATIVE INTEGRATION ERROR'         / 5120
 7' EPS=0.01, ONE NEEDS THE FOLLOWING CARDS:'                      // 5130
 8' CARD 38'                                                        / 5140
 9'   @BLOC@   81       INVARIANT'                                  / 5150
 A' CARD 39'                                                        / 5160
 B'   EPS               MAXIMUM ADMISSIBLE RELATIVE INTEGRATION'    / 5170
 C'                     ERROR.'                                   /// 5180
 D'                       *****'                                  /// 5190
 E' IF REMO DATA ARE TO BE CALCULATED (WITH MODULE 9) BUT NOT WITH') 5200
  WRITE (NOUT,34)                                                   5210
34 FORMAT(                                                          5220
 1' THE STANDARD VALUES (SEE BELOW) ERR=0.01, NJM=10, NUJM=10,'     / 5230
 2' ONE NEEDS THE FOLLOWING TWO CARDS:'                            // 5240
 3' CARD 40'                                                        / 5250
 4'   @BLOC@   91       INVARIANT'                                  / 5260
 5' CARD 41'                                                        / 5270
 6'   ERR               MAXIMUM ADMISSIBLE RELATIVE INTEGRATION'    / 5280
 7'                     ERROR;'                                     / 5290
 8'   NJM               2**NJM+1 IS THE MAXIMUM NUMBER OF GRID'     / 5300
 9'                     POINTS FOR THE ANGULAR INTEGRATION;'        / 5310
 A'   NUJM              2**NUJM+1 IS THE MAXIMUM NUMBER OF GRID'    / 5320
 B'                     POINTS FOR THE ENERGY INTEGRATION.')        5330
  WRITE (NOUT,35)                                                   5340
35 FORMAT(1H1/1HO/1HO/                                              5350
 1' IF MODULE 9 IS TO BE USED BUT NOT WITH THE DEFAULT VALUES'      / 5360
 2' (EXPLAINED BELOW) ISELR=1 FOR ISTRUK=0, ISELR=0 FOR ISTRUK=1,'  / 5370
 3' NLRA=0, NLRE=5, NCALL=0, NFG=14, NFI=5, ONE NEEDS THE'          / 5380
 4' FOLLOWING CARDS:'                                              // 5390
 5' CARD 42'                                                        / 5400
 6'   @BLOC@   92       INVARIANT'                                  / 5410
 7' CARD 43'                                                        / 5420
 8'   ISELR             =1: SCATTERING PROBABILITIES ARE CALCULATED'/ 5430
 9'                         ACCORDING TO EQ. 8.3 OF KFK 1784 WITH'  / 5440
 A'                         THE KEDAK VALUES FOR THE SCATTERING'    / 5450
 B'                         CROSS SECTION SGN(E),'                  / 5460
 C'                     =0: IN EQ. 8.3 OF KFK 1784 THE SCATTERING'  / 5470
 D'                         CROSS SECTION SGN(E) IS TAKEN AS 1 BARN;' 5480
 D/                                                                 5490
 E'   NLRA              LOWEST LEGENDRE ORDER;'                     / 5500
 F'   NLRE              HIGHEST LEGENDRE ORDER;')                   5510
  WRITE (NOUT,36)                                                   5520
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36 FORMAT(                                                              5530
  1'   NCALL              =0: EACH TIME MODULE 9 IS CALLED ALL ENERGY'/ 5540
  2'                          GROUPS ARE SUBDIVIDED INTO 14 SUBGROUPS'/ 5550
  3'                          WITH 5 ENERGY INTERVALS EACH,'           / 5560
  4'                      >0  NUMBER OF CALLS FOR MODULE 9 (MUST BE'   / 5570
  5'                          CONSISTENT WITH CARD 7).'              /// 5580
  6' IN CASE NCALL>0 THE FOLLOWING CARD IS NEEDED NCALL TIMES:'       // 5590
  7' CARD 44'                                                          / 5600
  8'   NGRP               NUMBER OF ENERGY GROUP RANGES WITH DIFFE-'  / 5610
  9'                      RENT ENERGY GRIDS;'                         / 5620
  A'   (N1(I),N2(I),NFG(I),NFI(I),I=1,NGRE)    WITH'                 / 5630
  B'                      N1 : NUMBER OF FIRST GROUP IN RANGE,'       / 5640
  C'                      N2 : NUMBER OF LAST GROUP IN RANGE,'        / 5650
  D'                      NFG: NUMBER OF SUBGROUPS PER GROUP,'        / 5660
  E'                      NFI: NUMBER OF ENERGY INTERVALS PER '       / 5670
  F'                          SUBGROUP.'                             /// 5680
  G'                     *****'                                       // 5690
   WRITE (NOUT,37)                                                    5700
37 FORMAT(                                                            5710
  1' THE LAST CARD FOR A GIVEN MATERIAL IS AS FOLLOWS:'               // 5720
  2' CARD 45'                                                          / 5730
  3'   @ENDE@   111      INVARIANT'                                   /// 5740
  4'                     *****'                                       /// 5750
  5' CARDS 1 TO 45 HAVE TO BE REPEATED FOR EACH MATERIAL WANTED'       / 5760
  6' AND/OR EACH WEIGHTING SPECTRUM TO BE USED. THE LAST CARD FOR'     / 5770
  7' THE ENTIRE JOB IS:'                                              // 5780
  7' CARD 46'                                                          / 5790
  8'   @ENDE@   112      INVARIANT'                                   /// 5800
  9'                     *****')                                      5810
   WRITE (NOUT,49)                                                    5820
49 FORMAT(1HI/1HO/1HO/                                                5830
  1' PRINTING OF THE PRESENT INPUT DESCRIPTION CAN BE SUPPRESSED BY'/ 5840
  2' PLACING THE FOLLOWING CARD (WITH THE M PUNCHED IN COLUMN 1) IN'/ 5850
  3' FRONT OF THE FIRST INPUT CARD:'                                  // 5860
  4' CARD )'                                                           / 5870
  5'   MIGR               INVARIANT'                                   // 5980
  6' THIS CARD DOES NOT APPEAR IN THE FREEFO DISPLAY OF INPUT DATA.'/ 5890
  7//'                        *****'                                  /// 59CC
  8' THE PROGRAM SYSTEM MIGROS REQUIRES DD-CARDS FOR THE FOLLOWING' / 5910
  9' EXTERNAL STORAGE DEVICES:'                                       // 5920
  A' 8      UNIT ON WHICH THE DECODED INPUT IS WRITTEN BY FREEFO,'    / 5930
  B' 1      UNIT FROM WHICH THE NUCLEAR DATA LIBRARY IS AVAILABLE,'   / 5940
  C' 3      UNIT ON WHICH ALL MODULES WRITE RESULTS,'                 / 5950
  D' 10     TEMPORARY INTERMEDIATE LIBRARY NEEDED ONLY BY MODULE 6.'// 5960
  E/                                                                  5970
  E'                         *****'                                  //) 5980
   WRITE (NOUT,38)                                                    5990
38 FORMAT(                                                            6000
  1' THE REQUIRED ARRAY LENGTHS DEPEND ON THE INPUT AND ON THE'       / 6010
  2' CALLED MODULES. THE NOTATION OF THE INPUT DESCRIPTION IS USED'   / 6020
  3' IN WHAT FOLLOWS. ALL ARRAY LENGTHS ARE GIVEN IN TERMS OF'        / 6030
  4' 4-BYTE WORDS UNLESS STATED OTHERWISE.'                           // 6040
  5' THE CONTROL PHASE NEEDS'                                         / 6050
  6' 2*NTYP+3*NMAT+NFE*(NSPEC+1)+NT+MI+1+3*NE+4*NA*(1+NE)  WORDS,'    / 6060
  7' WHERE THE DEFAULT VALUES ARE USED FOR QUANTITIES NOT SPECIFIED'/ 6070
  8' IN THE INPUT, VIZ. NTYP=7, NFE=1, NSPEC=1, NT=3, MI=7, NMAT=1,'/ 6080
  9' AND NE=26.'                                                      / 6090
  A' TO THIS ONE MUST ADD THE MEMORY SPACE OCCUPIED BY THE UTILIZED'/ 6100
  B' MODULE WITH THE LARGEST STORAGE REQUIREMENT. THE STORAGE'       / 6110
  C' REQUIREMENTS OF THE VARIOUS MODULES ARE AS FOLLOWS:'           // 6120
  D' MODULE NO.    STORAGE REQUIREMENT (4-BYTE WORDS)'              // 6130
  E'      1        7*MI+3*NE+7*MAX(300,NUMBER OF RESONANCES ON'      / 6140
  F'               KEDAK)+6*MAX(400,MAXIMUM NUMBER OF GRID ENERGIES'/ 6150
  G'               FOR INTEGRATION OVER ONE ENERGY GROUP)   WORDS')   6160
   WRITE (NOUT,39)                                                    6170
39 FORMAT(                                                            6180
  1'               COMMENT: THE USER CANNOT DETERMINE THE NUMBER OF' / 6190
  2'               GRID ENERGIES IN ADVANCE. IF 400 WORDS ARE NOT'   / 6200
  3'               SUFFICIENT THE SPACE FOR DATA STORAGE IS ENLARGED'/ 6210
  4'               PROVIDED THE AVAILABLE REGION ADMITS THIS. IF THE'/ 6220
  5'               REGION IS NOT LARGE ENOUGH THE MODULE IS BY-'     / 6230
  6'               PASSED. IT IS RECOMMENDED IN THIS CASE TO ENLARGE'/ 6240
  7'               THE REGION BY AT LEAST 2K BYTES.'                 / 6250
  8'      2        35*MI    WORDS.'                                  / 626C
  9'      3        3*MIBER+6*MI+MXINT+4*(MABWF+MABC1+MABQ2+MABQ3)'   / 6270
  A'               +2*KMROM+4*MRF*MI    WORDS.')                     6280
   WRITE (NOUT,40)                                                    6290
40 FORMAT(1HI/1HO/1HO/                                                6300
  1'               MIBER: MAXIMUM NUMBER OF RANGES WITH DIFFERENT'   / 6310
  2'                      WEIGHTING FUNCTIONS OR DIFFERENT INTEGRA-' / 6320
  3'                      TION METHODS. MIBER IS SET EQUAL TO 5 IN'  / 6330
  4'                      THE SUBROUTINE INPUT.'                     / 6340
  5'               MABWF: MAXIMUM NUMBER OF ENERGY POINTS IN ONE'    / 6350
  6'                      GROUP OF THE POINTWISE GIVEN WEIGHTING'    / 6360
  7'                      FUNCTION. MABWF HAS THE VALUE 0 IF NO'     / 6370
  8'                      POINTWISE GIVEN WEIGHTING FUNCTION IS'     / 6380
  9'                      PROVIDED IN THE INPUT. OTHERWISE IT HAS'   / 6390
  A'                      THE MINIMUM VALUE 50.'                     / 6400
  B'               MXINT: MAXIMUM NUMBER OF ENERGY POINTS IN ONE'    / 6410
  C'                      GROUP SUMMED OVER ALL PARTICIPATING CROSS' / 6420
  D'                      SECTIONS (AND EVENTUALLY THE POINTWISE'    / 643C
  E'                      GIVEN WEIGHTING FUNCTION), MINIMUM VALUE=' / 6440
  F'                      200.')                                     6450
   WRITE (NOUT,41)                                                    6460
41 FORMAT(                                                            6470
  1'               MABQ1: MAXIMUM NUMBER OF ENERGY POINTS IN ONE'    / 648C
  2'                      GROUP FOR THE CROSS SECTION TYPES SGT,'    / 6490
  3'                      SGA, SGN AND, IF EXISTENT, SGF, MINIMUM'   / 6500
  4'                      VALUE = 200.'                              / 6510
  5'               MABQ2: MAXIMUM NUMBER OF ENERGY POINTS IN ONE'    / 6520
  6'                      GROUP FOR THE CROSS SECTION TYPE NUEL,'    / 6530
  7'                      MINIMUM VALUE = 200.'                      / 6540
  8'               MABQ3: MAXIMUM NUMBER OF ENERGY POINTS IN ONE'    / 655C
  9'                      GROUP FOR THE CROSS SECTION TYPE SGT,'     / 6560
  A'                      MINIMUM VALUE = 200.'                      / 6570
  B'               KMROM: KMROM-1 = MAXIMUM NUMBER OF BISECTIONS IN' / 6580
  C'                      THE ROMBERG INTEGRATION ROUTINE FSROMB,'   / 6590
  D'                      MINIMUM VALUE = 20.'                       / 66CC
  E'               MRF  : 7 FOR NON-FISSIONABLE MATERIAL,'           / 6610
  F'                      8 FOR FISSIONABLE MATERIAL.')              6620
   WRITE (NOUT,42)                                                    6630
42 FORMAT(                                                            6640
  1'               WITH THE MINIMUM VALUES A MINIMUM MEMORY DEMAND'  / 6650
  2'               OF 3121 4-BYTE WORDS (POINTWISE WEIGHTING SPEC-'  / 6660
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     3'                TRUM GIVEN, FISSIONABLE MATERIAL) IS NECESSARY TO'/ 6670
     4'                RUN MODULE 3 (FSTRUK). BUT WE RECOMMEND TO USE'   / 6680
     5'                ABOUT 10000 4-BYTE WORDS, BECAUSE SOME OR ALL OF' / 6690
     6'                THE MINIMUM VALUES MUST BE INCREASED DURING THE'  / 6700
     7'                CALCULATIONS.'                                    / 6710
     8'       4        6*NE+2*MAX(1500,NUMBER OF SGN VALUES, NUMBER OF'  / 6720
     9'                SGF VALUES ON KEDAK IN THE ENERGY INTERVAL'       / 6730
     A'                CONSIDERED)    WORDS'                             / 6740
     B'       5        MAX(7*NE*NE+7*NE+2*NE27+4*NAE+3*ISG+2*NISGD,'     / 6750
     C'                    4+2*NE*NE+3*NE+NE27+2*NISGC+NISGI+NEP+4*NEP*' / 6760
     D'                    NF)    WORDS'                                 / 6770
     E'                NE27: NUMBER OF ENERGY GROUP BOUNDARIES OF'       / 6780
     F'                      IN-SCATTERING GROUPS. STANDARD ESTIMATE: 27') 6790
      WRITE (NOUT,43)                                                    6800
   43 FORMAT(                                                            6810
     1'                      (THE STANDARD ESTIMATES ARE USED AS STAR-'  / 6820
     2'                      TING VALUES IN THE PROGRAM BUT MAY BE MODI-'/ 6830
     3'                      FIED AUTOMATICALLY DEPENDING ON THE ACTUAL' / 6840
     4'                      JOB CHARACTERISTICS).'                      / 6850
     5'                NAE:  MAXIMUM NUMBER OF EXCITED LEVELS THAT CON-' / 6860
     6'                      TRIBUTE IN A GIVEN OUT-SCATTERING GROUP.'   / 6870
     7'                      STANDARD ESTIMATE: 30.')                    6880
      WRITE (NOUT,44)                                                    6890
   44 FORMAT(1H1/1H0/1H0/                                                6900
     1'                ISG : MAXIMUM NUMBER OF ENERGY GRID POINTS IN ONE'/ 6910
     2'                      OF THE CONSIDERED OUT-SCATTERING GROUPS.'   / 6920
     3'                      THIS NUMBER IS DETERMINED BY THE COMBINA-'  / 6930
     4'                      TION OF THE ENERGY GRID POINTS OF ALL'      / 6940
     5'                      EXCITED LEVELS WHICH MUST BE USED IN THE'   / 6950
     6'                      OUT-SCATTERING GROUP AND OF THOSE GRID'     / 6960
     7'                      POINTS OF THE SPECTRUM THAT LIE IN THE'     / 6970
     8'                      OUT-SCATTERING GROUP. STANDARD ESTIMATE:200'/ 6980
     9'                NISGD:ISG+MAXIMUM NUMBER OF ENERGY GRID POINTS OF'/ 6990
     A'                      ANY EXCITED LEVEL (SGIZ) WHICH CONTRIBUTE'  / 7000
     B'                      IN THE OUT-SCATTERING GROUP. STANDARD ESTI-'/ 7010
     C'                      MATE: 400.'                                 / 7020
     D'                NISGC:MAXIMUM NUMBER OF ENERGY GRID POINTS OF'    / 7030
     E'                      SGI (SG2N, SG3N) ON KEDAK IN ONE OF THE'    / 7040
     F'                      OUT-SCATTERING GROUPS. STANDARD ESTIMATE:'  / 7050
     G'                      200.')                                      7060
      WRITE(NOUT,45)                                                     7070
   45 FORMAT(                                                            7080
     1'                NISGI:MAXIMUM NUMBER OF ENERGY POINTS AS OBTAINED'/ 7090
     2'                      BY COMBINING THE KEDAK POINTS OF SGI (SG2N,'/ 7100
     3'                      SG3N) AND THE MESH POINTS OF THE SPECTRUM'  / 7110
     4'                      IN ANY OUT-SCATTERING GROUP. STANDARD'      / 7120
     5'                      ESTIMATE: 300.'                             / 7130
     6'                NEP : NUMBER OF INCIDENT-NEUTRON ENERGIES, FOR'   / 7140
     7'                      WHICH THE DISTRIBUTIONS SECIC (SEC2N,'      / 7150
     8'                      SEC3N) ARE GIVEN ON KEDAK. STANDARD ESTI-'  / 7160
     9'                      MATE: 30.'                                  / 7170
     A'                NF  : NUMBER OF DIFFERENT ANALYTICAL DISTRIBU-'   / 7180
     B'                      TIONS GIVEN ON KEDAK FOR SECIC (SEC2N,'     / 7190
     C'                      SEC3N) FROM WHICH THE TOTAL DISTRIBUTION'   / 7200
     D'                      MUST BE COMPOSED. STANDARD ESTIMATE: 5'     / 7210
     E'       6        APPROXIMATELY 30000 (STANDARD) TO 200000 (MANY'   / 7220
     F'                GROUPS, LARGE ENERGY DEGRADATION) WORDS. THE'     / 7230
     G'                EXACT STORAGE REQUIREMENT DEPENDS ON THE MOSTLY') 7240
      WRITE (NOUT,46)                                                    7250
   46 FORMAT(                                                            7260
     1'                UNKNOWN DISTRIBUTION OF THE KEDAK DATA OVER THE'  / 7270
     2'                ENERGY GROUPS. IT IS RECOMMENDED TO BEGIN WITH'   / 7280
     3'                THE STANDARD VALUE AND TO INCREASE THE STORAGE'   / 7290
     4'                SPACE ONLY IF THIS DOES NOT WORK. THE PROGRAM'    / 7300
     5'                TRIES IN ANY CASE TO ORGANIZE THE CALCULATIONS IN'/ 7310
     6'                ACCORDANCE WITH THE AVAILABLE MEMORY SPACE.'      / 7320
     7'       7        NE WORDS.'                                        / 7330
     8'       8        NE+2*NFE  WORDS.'                                 / 7340
     9'       9        45+NM1*IMAX*(3+NUJM)+ICOS*(4+NIV)+IMAX+2*NJM+NE'  / 7350
     A'                +15*NMAX+NZM*(2+IZV)+BUF  WORDS.'                 / 7360
     B'                NM1 : NLRE+1.'                                    / 7370
     C'                IMAX: MAXIMUM ENERGY DEGRADATION IN TERMS OF'     / 7380
     D'                      ENERGY GROUPS (=2 FOR SIMPLE SCATTERING'    / 7390
     E'                      INTO THE ADJACENT GROUP).'                  / 7400
     F'                ICOS: NUMBER OF ANGULAR GRID POINTS OF THE SGNC'  / 7410
     G'                      DATA ON KEDAK.')                            7420
      WRITE (NOUT,47)                                                    7430
   47 FORMAT(                                                            7440
     1'                NIV : NUMBER OF ENERGY GRID POINTS OF THE SGNC'   / 7450
     2'                      DATA ON KEDAK.'                             / 7460
     3'                NMAX: MAXIMUM NUMBER OF ENERGY GRID POINTS WITHIN'/ 7470
     4'                      ONE ENERGY GROUP FOR THE DATA TYPES SGT,'   / 7480
     5'                      SGN OR MUEL ON KEDAK.')                     7490
      WRITE (NOUT,48)                                                    7500
   48 FORMAT(1H1/1H0/1H0/                                                7510
     1'                NZM : MAXIMUM NUMBER OF ENERGY INTERVALS IN ONE'  / 7520
     2'                      SUBGROUP TIMES MAXIMUM NUMBER OF SUBGROUPS' / 7530
     3'                      PER GROUP.'                                 / 7540
     3'                IZV : MAX(4,IMAX*NM1).'                           / 7550
     4'                BUF : MAX(2+IMAX*NZM,NTOT), WHERE NTOT IS THE'    / 7560
     5'                      MAXIMUM NUMBER OF DATA POINTS WITHIN ONE'   / 7570
     6'                      GROUP FOR THE TYPES SGT, SGN AND MUEL (ALL' / 7580
     7'                      THREE CONSIDERED AS A JOINT POINT SET) ON'  / 7590
     8'                      KEDAK.'                                     / 7600
     9'      10        NO SPACE FOR DATA ARRAYS REQUIRED.'             /// 7610
     A' THE REGION PARAMETER ON THE JOB CARD IS THE SUM OF'              / 7620
     B'     -MAXIMUM LENGTH OF DATA ARRAYS,'                             / 7630
     C'     -170K BYTES FOR THE MIGROS PROGRAM,'                         / 7640
     D'     -BUFFER LENGTH.')                                            7650
      RETURN                                                             7660
      END                                                                7670
C                                                                        10
C     ROUTINE FOR PRODUCING AN UNFORMATTED INPUT-FILE                    20
C                                                                        30
C                                                                        40
      SUBROUTINE FREEFO (INP,NFI,NFO,LF,F,NF)                            50
      DIMENSION LF(1),F(1),NF(1),JZ(2),IREAL(2)                          60
      REAL*8 N8,NV8/5HNUFIN/,VC,REAL                                     70
      LOGICAL*1 JF(8),JX(2),LVS,LVCRI,LNACHI                             80
```

```
      INTEGER*2 NFE(80),LV(19),JY(4),LL,JKFE,STERN/2H* /                    90
      EQUIVALENCE (JZ(1),IFE(1),JY(1),NE),(LL,JX(1))                        100
      EQUIVALENCE (REAL,IREAL(1),LVS)                                       110
      EQUIVALENCE (LVOR,LVOR1),(LNACH,LNACH1)                               120
      DATA LV(1)/1H /,LV(2)/1HC/,LV(3)/1H1/,LV(4)/1H2/,LV(5)/1H3/,          130
     1LV(6)/1H4/,LV(7)/1H5/,LV(8)/1H6/,LV(9)/1H7/,LV(10)/1H8/,              140
     2LV(11)/1H9/,LV(12)/1H*/,LV(13)/1H+/,LV(14)/1H-/,LV(15)/1H./,          150
     3LV(16)/1HE/,LV(17)/1H0/,LV(18)/1H'/,LE/4HFEXA/,LFO/4HFORM/            160
     4,LSPE/4HSPEC/,LNO/4HNORM/,LV(19)/1HD/                                 170
C                                                                           180
C                                                                           190
C                                                                           200
      IY=80                                                                 210
      GOTO 9111                                                             220
C                                                                           230
C                                                                           240
      ENTRY FREE72 (INP,NFI,NFO,LF,F,NF)                                    250
      IY=72                                                                 260
C                                                                           270
C                                                                           280
 9111 V=1.                                                                  290
      MV=1                                                                  300
      LFP=0                                                                 310
      NF(1)=0                                                               320
      LPFP=0                                                                330
      LVCR=0                                                                340
      LNACH=0                                                               350
      LZ=0                                                                  360
      LW=0                                                                  370
      REAL=0.0+0                                                            380
      LSL=0                                                                 390
      LS=0                                                                  400
      LP=0                                                                  410
      NS=0                                                                  420
      LO=0                                                                  430
      N=0                                                                   440
      LL=LV(1)/256                                                          450
      KSPNO=0                                                               460
      KOUT=0                                                                470
C                                                                           480
C                                                                           490
C                                                                           500
   33 IF(NF(1).EQ.LE) GOTO 2                                                510
      IF(NF(1).EQ.LFO) GOTO 2                                               520
      GOTO 201                                                              530
  200 KOUT=1                                                                540
      GOTO 12                                                               550
  201 JZ(1)=NF(1)                                                           560
      JZ(2)=NF(2)                                                           570
      IF(N8.EQ.NV8) GOTO 200                                                580
      READ (INP,1,END=200,ERR=3) (NFE(I),I=1,80)                            590
    1 FORMAT(80A1)                                                          600
      GO TO 4                                                               610
    2 IF(NFI)203,203,202                                                    620
  202 REWIND NFI                                                            630
  203 RETURN                                                                640
    3 WRITE (NFO,5)                                                         650
    5 FORMAT(1HO/48H ERROR-CONDITION IN DATA TRANSFER OR INPUT-ERROR)       660
      STOP                                                                  670
    4 IF (IY.EQ.80) GOTO 6667                                               680
      JKFE=NFE(73)                                                          690
      NFE(73)=STERN                                                         700
 6667 WRITE (NFO,6) (NFE(I),I=1,80)                                         710
    6 FORMAT(1X,80A1)                                                       720
      IF (IY.EQ.80) GOTO 6668                                               730
      NFE(73)=JKFE                                                          740
C                                                                           750
C                                                                           760
C                                                                           770
 6668 IF(NF(1).EQ.LNO) GOTO 500                                             780
      IF(NF(1).EQ.LSPE) GOTO 501                                            790
      GOTO 502                                                              800
  500 KSPNO=0                                                               810
      GOTO 11                                                               820
  501 KSPNO=1                                                               830
      GOTO 11                                                               840
  502 IF(NFE(1).EQ.LV(1)) GOTO 10                                           850
      IF(N)11,11,12                                                         860
   12 IF(NFI)13,13,144                                                      870
  144 IF(KSPNO)145,145,14                                                   880
   14 WRITE (NFI) N,(NF(I),I=1,N)                                           890
  111 IF(KOUT)11,11,2                                                       900
  145 WRITE (NFI) (NF(I),I=1,N)                                             910
      GOTO 111                                                              920
   13 NS=NS+1                                                               930
      LF(NS)=N                                                              940
      N1=NS+1                                                               950
      N2=NS+N                                                               960
      N=0                                                                   970
      DO 15  I=N1,N2                                                        980
      N=N+1                                                                 990
   15 LF(I)=NF(N)                                                           1000
      NS=N2                                                                 1010
      GOTO 111                                                              1020
   11 N=0                                                                   1030
      J=0                                                                   1040
      GO TO 16                                                              1050
   10 J=1                                                                   1060
   16 J=J+1                                                                 1070
C                                                                           1080
C                                                                           1090
C                                                                           1100
   97 DO 20  K=1,19                                                         1110
      IF(NFE(J).EQ.LV(K)) GO TO 21                                          1120
   20 CONTINUE                                                              1130
      GO TO 3                                                               1140
C                                                                           1150
   21 IF (LW.GT.0) GOTO 221                                                 1160
      IF (K.LT.2.OR.K.GT.11) GOTO 221                                       1170
      JJ=J                                                                  1180
```

```
 8003 JJ=JJ+1                                                          1190
      IF (JJ.LE.IY) GOTO 8000                                          1200
 8002 LW=1                                                             1210
      GOTO 97                                                          1220
 8000 IF (NFE(JJ).EQ.LV(1)) GOTO 8002                                 1230
      IF (NFE(JJ).NE.LV(15)) GOTO 8003                                 1240
      LPPP=1                                                           1250
      GOTO 8002                                                        1260
C                                                                      1270
  221 IF(K-1)30,30,22                                                  1280
   30 IF(LS)31,31,32                                                   1290
   31 IF(J-IY)16,33,33                                                 1300
C                                                                      1310
C                                                                      1320
C                                                                      1330
   32 IF(LPP)40,40,41                                                  1340
   40 N=N+1                                                            1350
      NF(N)=LSU*MV                                                     1360
   47 LSU=0                                                            1370
      LS=0                                                             1380
      LO=0                                                             1390
      LW=0                                                             1400
      MV=1                                                             1410
      V=1.                                                             1420
      GOTO 31                                                          1430
C                                                                      1440
C                                                                      1450
C                                                                      1460
   41 M=LP-LS                                                          1470
      IF(M)44,45,46                                                    1480
   44 IF(78+M)3,3,45                                                   1490
   46 IF(75-M)3,3,45                                                   1500
   45 N=N+1                                                            1510
      VC=V                                                             1520
      REAL=REAL*VC*1.D+1**M                                            1530
      IF (LPPP.EQ.1) GOTO 8010                                         1540
      NF(N)=IREAL(1)                                                   1550
      N=N+1                                                            1560
      NF(N)=IREAL(2)                                                   1570
      GOTO 8011                                                        1580
 8010 IF (IREAL(2).GE.0) GOTO 8012                                     1590
      LVCR1=LVS                                                        1600
      IREAL(1)=IREAL(1)+1                                              1610
      LNACH1=LVS                                                       1620
      IF (LVOR.EQ.LNACH) GOTO 8012                                     1630
      IREAL(1)=LNACH+1048576                                           1640
 8012 NF(N)=IREAL(1)                                                   1650
 8011 LP=0                                                             1660
      LZ=0                                                             1670
      LPP=0                                                            1680
      LPPP=0                                                           1690
      REAL=0.D+0                                                       1700
      GO TO 47                                                         1710
C                                                                      1720
C                                                                      1730
C                                                                      1740
   22 IF(K-11)50,50,23                                                 1750
   50 LS=LS+1                                                          1760
      IF (LPPP.GT.0) GOTO 8004                                         1770
      IF (LS.LE.9) GOTO 8005                                           1780
      IF (LSU.GT.214748364) GOTO 3                                     1790
      IF ((K-2).GT.7) GOTO 3                                           1800
 8005 LSU=10*LSU+K-2                                                   1810
   51 IF (J-IY) 16,32,32                                               1820
 8004 IF (LZ.GT.0) GOTO 8006                                           1830
      IF ((K-2).EQ.0) GOTO 8006                                        1840
      LZ=LZ+1                                                          1850
      JJ=J                                                             1860
      LZZ=0                                                            1870
 9001 JJ=JJ+1                                                          1880
      DO 8007 KK=2,11                                                  1890
      IF (NFE(JJ).EQ.LV(KK)) GOTO 8008                                 1900
 8007 CONTINUE                                                         1910
      GOTO 8009                                                        1920
 8008 LZ=LZ+1                                                          1930
      IF ((KK-2).NE.0) GOTO 9000                                       1940
      LZZ=LZZ+1                                                        1950
      GOTO 9001                                                        1960
 9000 LZZ=0                                                            1970
      GOTO 9001                                                        1980
 8009 LZ=LZ-LZZ                                                        1990
      IF (LZ.GT.16) GOTO 3                                             2000
 8006 REAL=REAL*1.D+1+K-2                                              2010
      IF (LPP) 51,51,883                                               2020
  883 LC=-1                                                            2030
      J=J+1                                                            2040
      IF (J-IY) 884,884,32                                             2050
C                                                                      2060
C                                                                      2070
C                                                                      2080
   23 IF(K-14)60,60,24                                                 2090
   60 IF(LC)61,61,3                                                    2100
   61 LO=1                                                             2110
      IF(K-14)62,63,63                                                 2120
   63 V=-1.                                                            2130
      MV=-1                                                            2140
   62 IF(J-IY)64,3,3                                                   2150
   64 J=J+1                                                            2160
      DO 65  K=2,11                                                    2170
      IF(NFE(J).EQ.LV(K)) GO TO 21                                     2180
   65 CONTINUE                                                         2190
      IF(NFE(J).EQ.LV(15)) GO TO 70                                    2200
      GO TO 3                                                          2210
C                                                                      2220
C                                                                      2230
C                                                                      2240
   24 IF(K-15)70,70,25                                                 2250
   70 IF(LP)71,71,3                                                    2260
   71 LP=LS                                                            2270
      LPP=1                                                            2280
```

```
      LPPP=1
      IF(J-IY)72,73,73
   73 IF(LS)3,3,41
   72 J=J+1
      DO 74  K=2,11
      IF(NFE(J).EQ.LV(K)) GO TO 50
   74 CONTINUE
      IF(NFE(J).EQ.LV(1)) GO TO 73
      IF(NFE(J).EQ.LV(16)) GO TO 81
      IF (NFE(J).EQ.LV(19)) GOTO 8013
      LC=0
  884 LA=0
      LV1=1
      LP1=0
      IF(J-IY)882,882,3
C
C
C
   25 IF(K-16)80,80,226
  226 IF (K-19) 26,8013,8013
 8013 LPPP=2
   80 IF(LPP)3,3,81
   81 LA=0
      LC=1
      LV1=1
      LP1=0
      IF(J-IY)82,3,3
   82 J=J+1
      IF(NFE(J).EQ.LV(1)) GO TO 83
  882 IF(NFE(J).EQ.LV(12)) GO TO 83
      IF(NFE(J).EQ.LV(13)) GO TO 83
      IF(NFE(J).EQ.LV(14)) GO TO 84
      IF(LC)97,3,85
   84 LV1=-1
   83 IF(J-IY)86,3,3
   86 J=J+1
   85 DO 87 K=2,11
      IF(NFE(J).EQ.LV(K)) GO TO 88
   87 CONTINUE
      IF(NFE(J).EQ.LV(1)) GO TO 89
      GO TO 3
   89 IF(LA)3,3,90
   88 LA=1
      LP1=10*LP1+K-2
      IF(J-IY)36,90,90
   90 LP=LP+LP1*LV1
      GO TO 41
C
C
C
   26 IF(K-17)300,300,301
  300 M=5
      K7=17
      GO TO 117
  301 M=4
      K7=18
  117 LC=0
  116 LA=0
      DO 100  L=1,4
  100 JY(L)=LV(L)
  110 J=J+1
      IF(J-IY)101,102,102
  102 IF(NFE(J).EQ.LV(K7)) GOTO 120
      LC=0
      GOTO 121
  120 J=J-1
  121 IF(LC)33,3,112
  101 IF(NFE(J).EQ.LV(K7)) GO TO 106
      GO TO 107
  106 IF(LC)105,3,102
  107 LA=LA+1
      LC=1
      LL=NFE(J)
      JF(LA)=JX(1)
      IF(LA-M)110,112,112
  112 N=N+1
      NF (N)=JZ(1)
      IF(K-17)433,433,434
  433 N=N+1
      NF (N)=JZ(2)
  434 LC=-1
      IF(NFE(J+1).EQ.LV(K7)) GOTO 110
      GOTO 116
  105 IF(NFE(J+1).EQ.LV(1)) GOTO 16
      GO TO 3
      END
```

```
C     SUBROUTINEN ZUM LESEN DER KERNDATENBIBLIOTHEK
C
C     SUBROUTINEN NDFOPN , LDFOPN ZUM ERÖFFNEN DER KERNDATENBIBLIOTHEK
C
      SUBROUTINE NDF
      DIMENSION IDAT(2),IAD(1003),ISATZ(880),DAT1(60),I(4),IR(3),IW(3),
     1NNAM(4),INAM(20),KDAT1(60),MNAM(20),NUNA(2),IWNA(880),XNAM(20),
     2XJDAT(880),JDAT(880),NN(4),IREST(2),DAT2(60),Z(60),XWNA(880)
      EQUIVALENCE (I(1),IR(1)),(Z(1),KDAT1(1)),(IWNA(1),XWNA(1)),
     1(JDAT(1),XJDAT(1))
      DATA I/'KEDA','BIBL','IOTH','    '/,NSZ/100/,NCLTP/6/
C
      ENTRY NDFOPN (LBN,ICAT,IFD,ISPR)
      JJ=1
      ICAT(1)=I(4)
      ICAT(2)=I(4)
      GOTO 50
C
      ENTRY LDFOPN (LBN,IFD,*)
      JJ=2
```

```
   50 NSZ=880                                                                  210
      DEFINE FILE 1 (6000,880,U,K8)                                           220
      MNAM(1)=0                                                               230
      NUNA(1)=0                                                               240
      IS=1                                                                    250
      READ (LBN'IS) (ISATZ(II),II=1,NSZ)                                      260
      IS=IS+1                                                                 270
      DO 1 J=1,3                                                              280
      IF(ISATZ(J)-I(J))2,1,2                                                  290
    2 WRITE (NOUTP,4)                                                         300
    4 FORMAT(1HO/' ***ERROR NDF. 1 : THE DD-CARD FOR UNIT 1 DOES NOT CHA      310
     1RACTERIZE A VALID KEDAK LIBRARY')                                       320
      STOP                                                                    330
    1 CONTINUE                                                                340
      IFD=ISATZ(4)                                                            350
      IAD(1)=ISATZ(5)                                                         360
      IAD(2)=ISATZ(8)                                                         370
      IAD(3)=ISATZ(11)                                                        380
      K=4                                                                     390
      IR(1)=ISATZ(6)                                                          400
      IR(2)=ISATZ(9)                                                          410
      IR(3)=ISATZ(12)                                                         420
      IW(1)=ISATZ(7)                                                          430
      IW(2)=ISATZ(10)                                                         440
      IW(3)=ISATZ(13)                                                         450
      DO 3 J=1,3                                                              460
      N=IR(J)                                                                 470
      IWJ=IW(J)                                                               480
      IF(IS-N-1)5,6,5                                                         490
    5 READ (LBN'N) (ISATZ(II),II=1,NSZ)                                       500
      IS=N+1                                                                  510
    6 IF(J-3)10,11,11                                                         520
   10 L=3                                                                     530
      GO TO 326                                                               540
   11 L=4                                                                     550
  326 IMP=IAD(J)*L+IWJ-1                                                      560
    8 IF(IMP-NSZ)13,14,15                                                     570
   14 N=1                                                                     580
      GO TO 16                                                                590
   15 N=2                                                                     600
   16 DO 12 L=IWJ,NSZ                                                         610
      IAD(K)=ISATZ(L)                                                         620
   12 K=K+1                                                                   630
      GO TO (3,17),N                                                          640
   17 IMP=IMP-NSZ                                                             650
      IWJ=1                                                                   660
      READ (LBN'IS) (ISATZ(II),II=1,NSZ)                                      670
      IS=IS+1                                                                 680
      GO TO 8                                                                 690
   13 DO318 L=IWJ,IMP                                                         700
      IAD(K)=ISATZ(L)                                                         710
  318 K=K+1                                                                   720
    3 CONTINUE                                                                730
      RETURN                                                                  740
C                                                                             750
C                                                                             760
C     SUBROUTINEN NDFLOC , LDFLOC , IDFLCC                                    770
C                                                                             780
      ENTRY NDFLOC (KONTR,NNAM,DAT1,ID,KC)                                    790
      IF(NSZ.NE.880)  GO TO 1004                                              800
      ID=0                                                                    810
      KC=0                                                                    820
      DO 403 LS=1,2                                                           830
      IF (DAT1(LS).NE.MNAM(LS))  GO TO 104                                    840
  403 CONTINUE                                                                850
      MGL=2                                                                   860
      GOTO 107                                                                870
  104 MGL=1                                                                   880
  107 J=NNAM(1)*2                                                             890
      DO 51 N=1,J                                                             900
   51 Z(N)=DAT1(N)                                                            910
      L=1                                                                     920
      LS=1                                                                    930
      DO 18 N=1,J                                                             940
      IF(N-4)19,218,20                                                        950
   19 IF(N-3)20,218,218                                                       960
   20 MNAM(L)=KDAT1(N)                                                        970
      L=L+1                                                                   980
      GOTO 18                                                                 990
  218 IBEST(LS)=KDAT1(N)                                                      1000
      LS=LS+1                                                                 1010
   18 CONTINUE                                                                1020
      KK=1                                                                    1030
      GOTO427                                                                 1040
C                                                                             1050
      ENTRY LDFLOC (KONTR,NNAM,INAM,DAT2)                                     1060
      IF(NSZ.NE.880)  GO TO 1004                                              1070
      DO 127 LS=1,2                                                           1080
      IF (INAM(LS).NE.MNAM(LS))  GO TO 128                                    1090
  127 CONTINUE                                                                1100
      MGL=2                                                                   1110
      GOTO 129                                                                1120
  128 MGL=1                                                                   1130
  129 J=NNAM(1)*2                                                             1140
      DO 21 N=1,J                                                             1150
   21 MNAM(N)=INAM(N)                                                         1160
      KK=2                                                                    1170
  427 K=4                                                                     1180
      IWJ=0                                                                   1190
      DO 22 LS=1,3,2                                                          1200
      IWJ=IWJ+1                                                               1210
      N=IAD(IWJ)*3                                                            1220
      DO 23 M=1,N                                                             1230
      IF (MNAM(LS).NE.IAD(K))  GO TO 23                                       1240
      IF (MNAM(LS+1).EQ.IAD(K+1))  GO TO 26                                   1250
   23 K=K+3                                                                   1260
      WRITE (NOUTP,2000) (MNAM(M),M=1,4)                                      1270
 2000 FORMAT(1HO/' ***WARNING NDF. 1 : THE DATA FOR **',2A4,'**',1X,'**',     1280
     12A4,'* ARE NOT INCLUDED'/' IN THE CONVERSIONTABLE OF THE KEDAK LIB      1290
     2RARY')                                                                  1300
```

```
      MNAM(1)=1                                                         1310
      KONTR=0                                                           1320
      IF(JJ-1)98,98,96                                                  1330
   26 NUNA(IWJ)=IAD(K+2)                                                1340
   22 K=K+4                                                             1350
      GO TO (227,228),MGL                                               1360
C                                                                       1370
      ENTRY IDFLOC (KONTR,NNAM,INAM,DAT2)                               1380
      IF(NSZ.NE.880)  GO TO 1004                                        1390
      KK=3                                                              1400
      IF(INAM(1)-NUNA(1))130,131,130                                    1410
  131 MGL=2                                                             1420
      GOTO 132                                                          1430
  130 MGL=1                                                             1440
  132 NUNA(1)=INAM(1)                                                   1450
      NUNA(2)=INAM(2)                                                   1460
      IF(NNAM(1)-2)27,27,52                                             1470
   52 J=NNAM(1)                                                         1480
      DO 53 LS=3,J                                                      1490
   53 MNAM(2*LS-1)=INAM(LS)                                             1500
   27 GO TO (227,228),MGL                                               1510
  227 N=IAD(3)*4                                                        1520
      IWJ=(IAD(1)+IAD(2))*3+4                                           1530
      DO 28 LS=1,N,4                                                    1540
      IF(NUNA(1)-IAD(IWJ))28,29,28                                      1550
   28 IWJ=IWJ+4                                                         1560
      KONTR=0                                                           1570
      GO TO 24                                                          1580
   29 NT=IAD(IWJ+1)                                                     1590
      JR=IAD(IWJ+2)                                                     1600
      JW=IAD(IWJ+3)                                                     1610
  228 KR=JR                                                             1620
      KW=JW                                                             1630
      IVY=0                                                             1640
      IF(IS-KR-1)30,31,30                                               1650
   30 READ (LBN'KR) (ISATZ(II),II=1,NSZ)                               1660
      IS=KR+1                                                           1670
   31 DO 32 LS=1,NT                                                     1680
      IF(NUNA(2)-ISATZ(KW))33,34,33                                     1690
   33 KW=KW+7                                                           1700
      IF(KW-NSZ)32,32,35                                                1710
   35 READ (LBN'IS) (ISATZ(II),II=1,NSZ)                               1720
      IS=IS+1                                                           1730
      KW=KW-NSZ                                                         1740
   32 CONTINUE                                                          1750
      KONTR=0                                                           1760
      GO TO 24                                                          1770
   34 KW=KW+1                                                           1780
      DO 36 LS=1,6                                                      1790
      IF(KW-NSZ)37,37,38                                                1800
   38 READ (LBN'IS) (ISATZ(II),II=1,NSZ)                               1810
      IS=IS+1                                                           1820
      KW=1                                                              1830
   37 GO TO (39,40,40,41,42,43),LS                                      1840
   39 NNN=ISATZ(KW)                                                     1850
      GOTO 36                                                           1860
   40 NNAM(LS)=ISATZ(KW)                                                1870
      GOTO 36                                                           1880
   41 NWP=ISATZ(KW)                                                     1890
      GO TO 36                                                          1900
   42 IDR=ISATZ(KW)                                                     1910
      GO TO 36                                                          1920
   43 IDW=ISATZ(KW)                                                     1930
   36 KW=KW+1                                                           1940
      IF(KK-1)46,46,47                                                  1950
   46 NNAM(4)=0                                                         1960
   47 DO 80 LS=1,4                                                      1970
   80 NN(LS)=NNAM(LS)                                                   1980
      IF(NWN)384,384,49                                                 1990
   49 NNK=NWP                                                           2000
      NWR=IDR                                                           2010
      NWW=IDW                                                           2020
      IF(IS-NWR-1)44,45,44                                              2030
   44 READ (LBN'NWR) (IWNA(II),II=1,NSZ)                               2040
      NWR=NWR+1                                                         2050
      GO TO 62                                                          2060
   45 DO 61 LS=1,NSZ                                                    2070
   61 IWNA(LS)=ISATZ(LS)                                                2080
      NWR=NWR+1                                                         2090
   62 DO 68 N=1,NNK                                                     2100
      NKO=N                                                             2110
      NW=NWW                                                            2120
      KP=5                                                              2130
      JD=3                                                              2140
      DO 54 LS=1,NWN                                                    2150
      IF(IWNA(NWW)-MNAM(KP))58,55,56                                    2160
   56 KONTR=0                                                           2170
      IVY=1                                                             2180
      IF(KK-2)57,59,859                                                 2190
   59 INAM(KP)=IWNA(NWW)                                                2200
      GOTO 60                                                           2210
  859 INAM(JD)=IWNA(NWW)                                                2220
      GO TO 60                                                          2230
   57 DAT1(KP+2)=XWNA(NWW)                                              2240
      GOTO 60                                                           2250
   55 KONTR=1                                                           2260
   60 KP=KP+2                                                           2270
      JD=JD+1                                                           2280
      NWW=NWW+1                                                         2290
      IF(NWW-NSZ)54,54,64                                               2300
   64 READ (LBN'NWR) (IWNA(II),II=1,NSZ)                               2310
      NWR=NWR+1                                                         2320
      NWW=1                                                             2330
   54 CONTINUE                                                          2340
      GO TO 74                                                          2350
   58 NWW=NW+NWN+3                                                      2360
      IF(NWW-NSZ)68,68,70                                               2370
   70 READ (LBN'NWR) (IWNA(II),II=1,NSZ)                               2380
      NWR=NWR+1                                                         2390
   73 NWW=NWW-NSZ                                                       2400
```

```
   68 CONTINUE                                                          2410
      KONTR=0                                                           2420
      IF(KK.EQ.3)  GO TO 580                                            2430
      WRITE (NOUTP,2002) MNAM(5),(MNAM(II),II=1,4)                      2440
 2002 FORMAT(1HO/' ***WARNING NDF. 2 : THE FURTHER NAME ',E16.8,' IS GRE 2450
     1ATER THAN THE GREATEST FURTHER NAME '/' INCLUDED IN THE KEDAK LIBR 2460
     2ARY FOR',1X,2A4,1X,2A4)                                           2470
      GO TO 98                                                          2480
  580 WRITE (NOUTP,581) MNAM(5),(INAM(II),II=1,2)                       2490
  581 FORMAT(1HO/' ***WARNING NDF. 2 : THE FURTHER NAME',E16.8,' IS GREA 2500
     1TER THAN THE GREATEST FURTHER NAME'/' INCLUDED IN THE KEDAK LIBRAR 2510
     2Y FOR',2I10)                                                      2520
      GO TO 98                                                          2530
 1004 WRITE (NOUTP,1005)                                                2540
 1005 FORMAT(1HO/' ***ERROR NDF. 2 : AT FIRST THE --DFN - ROUTINE MUST B 2550
     1E CALLED')                                                        2560
      STOP                                                              2570
   74 NWP=IWNA(NWW)                                                     2580
      DO 75 LS=1,2                                                      2590
      NWW=NWW+1                                                         2600
      IF(NWW-NSZ)76,76,78                                               2610
   78 READ (LBN'NWR) (IWNA(II),II=1,NSZ)                                2620
      NWR=NWR+1                                                         2630
      NWW=1                                                             2640
   76 GO TO (81,82),LS                                                  2650
   81 IDR=IWNA(NWW)                                                     2660
      GOTO 75                                                           2670
   82 IDW=IWNA(NWW)                                                     2680
   75 CONTINUE                                                          2690
      NWW=NWW+1                                                         2700
   48 IF(NWN)384,384,383                                                2710
  384 IF(IS-IDR-1)83,385,83                                             2720
  383 IF(NWR-IDR-1)83,84,83                                             2730
  385 DO 386 L=1,NSZ                                                    2740
  386 JDAT(L)=ISATZ(L)                                                  2750
      IDR=IDR+1                                                         2760
      GO TO 388                                                         2770
   84 DO 85 L=1,NSZ                                                     2780
   85 JDAT(L)=IWNA(L)                                                   2790
      IDR=IDR+1                                                         2800
      GO TO 388                                                         2810
   83 READ (LBN'IDR) (JDAT(II),II=1,NSZ)                               2820
      IDR=IDR+1                                                         2830
  388 NPA=1                                                             2840
   86 JD=NNAM(2)+NNAM(3)                                                2850
      IF(KK-2)87,88,88                                                  2860
   87 LS=NNAM(1)*2+1                                                    2870
      GO TO 89                                                          2880
   88 LS=1                                                              2890
   89 DO 90 L=1,JD                                                      2900
      GO TO (91,92,92),KK                                               2910
   91 DAT1(LS)=XJDAT(IDW)                                               2920
      DAT1(LS+1)=0.                                                     2930
      LS=LS+2                                                           2940
      GO TO 93                                                          2950
   92 DAT2(LS)=XJDAT(IDW)                                               2960
      LS=LS+1                                                           2970
   93 IDW=IDW+1                                                         2980
      IF(IDW-NSZ) 90,90,94                                              2990
   94 READ(LBN'IDR) (JDAT(II),II=1,NSZ)                                3000
      IDR=IDR+1                                                         3010
      IDW=1                                                             3020
   90 CONTINUE                                                          3030
      IF(IVY)1003,1003,98                                               3040
 1003 KONTR=1                                                           3050
      GO TO 99                                                          3060
   24 WRITE(NOUTP,97)NUNA(1),NUNA(2)                                    3070
   97 FORMAT(1HO/' ***WARNING NDF. 3 : THE DATA FOR',2I9,' ARE NOT INCLU 3080
     1DED IN THE KEDAK LIBRARY')                                        3090
      IF(JJ-1)98,98,96                                                  3100
   96 RETURN 1                                                          3110
   98 RETURN                                                            3120
C                                                                       3130
C                                                                       3140
C     SUBROUTINES NDFNXT, LDFNXT , IDFNXT                               3150
C                                                                       3160
      ENTRY NDFNXT (KONTR,NNAM,DAT1,ID,KC)                              3170
      ID=0                                                              3180
      KC=0                                                              3190
      LL=1                                                              3200
      GO TO 101                                                         3210
C                                                                       3220
      ENTRY LDFNXT(KONTR,NNAM,INAM,DAT2)                                3230
      LL=2                                                              3240
      GOTO 101                                                          3250
C                                                                       3260
      ENTRY IDFNXT(KONTR,NNAM,INAM,DAT2)                                3270
      LL=3                                                              3280
  101 NPA=NPA+1                                                         3290
      IVY=0                                                             3300
      IF(NPA-NWP)102,102,103                                            3310
  103 KONTR=0                                                           3320
      IF (NWN)387,387,389                                               3330
  389 NKO=NKO+1                                                         3340
      IF(NKO-NNK)391,391,387                                            3350
  387 RETURN                                                            3360
  102 KONTR=1                                                           3370
  391 DO 304 LS=1,3                                                     3380
  304 NNAM(LS)=NN(LS)                                                   3390
      IF(LL-2)105,124,106                                               3400
  105 NNAM(4)=0                                                         3410
      KDAT1(1)=MNAM(1)                                                  3420
      KDAT1(2)=MNAM(2)                                                  3430
      KDAT1(3)=IBEST(1)                                                 3440
      KDAT1(4)=IBEST(2)                                                 3450
      KDAT1(5)=MNAM(3)                                                  3460
      KDAT1(6)=MNAM(4)                                                  3470
      DO 401 II=1,6                                                     3480
  401 DAT1(II)=Z(II)                                                    3490
      GO TO 125                                                         3500
```

```
124 DO 126 LS=1,4                                                       3510
126 INAM(LS)=MNAM(LS)                                                   3520
    GO TO 125                                                           3530
106 DO 327 LS=1,2                                                       3540
327 INAM(LS)=NUNA(LS)                                                   3550
125 IF(NWN)86,86,390                                                    3560
390 IF(KONTR)108,108,86                                                 3570
108 KP=NWN+3                                                            3580
    IVY=1                                                               3590
    L=5                                                                 3600
    DO 109 LS=1,KP                                                      3610
    IF(NWW-NSZ)110,110,111                                              3620
111 READ (LBN'NWR) (IWNA(II),II=1,NSZ)                                  3630
    NWR=NWR+1                                                           3640
    NWW=1                                                               3650
110 IF(LS-NWN)112,112,113                                               3660
112 IF(LL-2)114,115,116                                                 3670
114 L=L+2                                                               3680
    KDAT1(L)=IWNA(NWW)                                                  3690
    KDAT1(L+1)=0                                                        3700
    DAT1(L)=Z(L)                                                        3710
    DAT1(L+1)=Z(L+1)                                                    3720
    GO TO 109                                                           3730
115 INAM(L)=IWNA(NWW)                                                   3740
    L=L+2                                                               3750
    GO TO 109                                                           3760
116 L=LS+2                                                              3770
    INAM(L)=IWNA(NWW)                                                   3780
113 L=LS-NWN                                                            3790
    GO TO (119,118,117),L                                               3800
119 NWP=IWNA(NWW)                                                       3810
    GOTO 109                                                            3820
118 IDR=IWNA(NWW)                                                       3830
    GOTO 109                                                            3840
117 IDW=IWNA(NWW)                                                       3850
109 NWW=NWW+1                                                           3860
    GO TO 388                                                           3870
    END                                                                 3880
```

```
    FUNCTION PHI(E)                                                     10
    PHI=1./E                                                            20
    RETURN                                                              30
    END                                                                 40
```

```
    SUBROUTINE DOPW(I,J)                                                10
    REAL*8 I,J                                                          20
    J=I                                                                 30
    RETURN                                                              40
    END                                                                 50
```

```
      REAL FUNCTION DPHI*8(E)                                           10
      REAL*8 E                                                          20
      LOGICAL*4 ORIFUN                                                  30
      COMMON/CFSMEL/ ORIFUN                                             40
C     THE STATEMENT "ORIFUN=.TRUE." MUST ONLY BE USED FOR THE ORIGINAL  50
C     FUNCTION, BUT NOT FOR A FUNCTION LINKED TO THE PROGRAM BY THE     60
C     USER.                                                             70
      ORIFUN=.TRUE.                                                     80
      DPHI=1.0D+0/E                                                     90
      RETURN                                                           100
      END                                                              110
```

```
      SUBROUTINE FSPIE                                                  10
C   FSPIE IS A SPECIAL ERROR-DETECTING SUBROUTINE ,WHICH IN CASE        20
C   OF AN ABNORMAL END  DETERMINS THE PSW  AND PRINTS THIS PSW +        30
C   A TRACE-BACK + THE REGISTER CONTENTS + THE SYSTEM COMPLETION        40
C   CODE..    FOR  FSPIE IS INSTALATION DEPENDENT ITS CODE IS NOT       50
C   DISTRIBUTED HERE                                                    60
      RETURN                                                            70
      END                                                               80
```

```
      SUBROUTINE FGEM(NS,SIGO,NE,ENG,NEF,ES,F,NT,TEMP,PR,AMR,NFST,SUM,  10
     1SUC,IRE,IREP,ER,L,GJ,GAT,GAN,GAG,GAF,ISTE,ISTEP,STE,STE1)         20
      REAL*8 MATN,FEST,IFEST,NN,MM,III                                  30
      DIMENSION ENG(NE),ES(NEF),F(NEF),TEMP(NT),SIGO(NS),IFEST(20),     40
     1FEST(20),                                                         50
     2        NN(4),IZAHL(4),SUMO(3),SUM(NS,7),STE(5,ISTE),SLO(NE,3),   60
     3ER(IRE),L(IRE),GJ(IRE),GAT(IRE),GAN(IRE),GAG(IRE),GAF(IRE),       70
     4STE1(ISTE)                                                        80
      COMMON MATN,ISTRUK,ISPA,NOUTP,LZWF,IR(2),KL                       90
      EQUIVALENCE (FEST(1),IFEST(1))                                   100
      WRITE (NOUTP,9000)                                               110
 9000 FORMAT(1H0/1HO/' PROGRAMM KENNZIFFER 1')                         120
      WRITE (NOUTP,9001)                                               130
 9001 FORMAT(' PROGRAMM ZUR BERECHNUNG VON RESONANZSELBSTABSCHIRMFAKTORE 140
     1N VON AUFGELOESTEN RESONANZPARAMETERN'/)                         150
      CALL FSPIE                                                       160
      CALL DOPW (8HBEST    ,NN(1))                                     170
      CALL DOPW (8HISOT1   ,NN(2))                                     180
      CALL DOPW (8HISOT2   ,NN(3))                                     190
      CALL DOPW (8HRES     ,NN(4))                                     200
      CALL DOPW (8HMIGR    ,MM)                                        210
      IREP=0                                                           220
      IREF=0                                                           230
      ISTEP=0                                                          240
```

```
      ISTEF=0                                                           250
      CALL EXPPX(X,X,X,X)                                               260
      NEFE=NEF                                                          270
      IF(NEF.NE.1) GOTO 411                                             280
      NEFE=0                                                            290
  411 PI=3.14159                                                        300
      NE1=NE-1                                                          310
   12 IZAHL(1)=3                                                        320
      IFEST(1)=MATN                                                     330
      IFEST(2)=NN(1)                                                    340
      IFEST(3)=NN(2)                                                    350
      CALL NDFLOC(IDD,IZAHL,FEST,IDAT,ICOD)                             360
      IF(IDD)110,111,110                                                370
  110 A=FEST(4)                                                         380
      IFEST(3)=NN(3)                                                    390
      CALL NDFLOC(IDD,IZAHL,FEST,IDAT,ICOD)                             400
      IF(IDD)115,111,115                                                410
  115 RLA=FEST(4)                                                       420
      R=FEST(5)                                                         430
      SICP=4.*PI*R**2                                                   440
      IFEST(3)=NN(4)                                                    450
      NR=1                                                              460
      CALL NDFLOC(IDD,IZAHL,FEST,IDAT,ICOD)                             470
      IF(IDD)112,111,112                                                480
  112 ER(NR)=FEST(4)                                                    490
      L(NR)=IFEST(5)                                                    500
      GJ(NR)=FEST(7)                                                    510
      GAT(NR)=FEST(8)                                                   520
      GAN(NR)=FEST(9)                                                   530
      GAG(NR)=FEST(10)+FEST(12)+FEST(13)                                540
      GAF(NR)=FEST(11)                                                  550
      NR=NR+1                                                           560
      IF(NR.LE.IRE)  GO TO 200                                          570
      NR=1                                                              580
      IREF=IREF+1                                                       590
  200 CALL NDFNXT(IDD,IZAHL,FEST,IDAT,ICOD)                             600
      IF(IDD)112,113,112                                                610
  113 NR=NR-1                                                           620
      IF(IREF.EQ.0)  GO TO 5                                            630
      IREP=(IREF-1)*IRE+NR+1                                            640
      RETURN                                                            650
    5 IF(NMR.EQ.-1)  NMR=NR                                             660
      NMIN=NMR                                                          670
      DO 63 IE=1,NE1                                                    680
      IF(ENG(IE+1)-ER(NR))63,63,64                                      690
   63 CONTINUE                                                          700
      NLAST=NE1                                                         710
      GOTO 66                                                           720
   64 NLAST=IE-1                                                        730
      IF(NLAST)65,65,66                                                 740
   65 NFST=1                                                            750
      GOTO 3                                                            760
   66 NFST     =NLAST+1                                                 770
    4 NANF=NE-IR(1)                                                     780
      IF(NANF-NLAST)510,510,3                                           790
  510 NEND=NE-IR(2)                                                     800
  502 IF(NEND-NLAST)503,503,505                                         810
  503 NLAST=NEND                                                        820
      NFST=0                                                            830
  505 DO 60 IT=1,NT                                                     840
      T=TEMP(IT)                                                        850
      NR1=1                                                             860
      DO 10 IE=NANF,NLAST                                               870
      DO 36 ISO=1,3                                                     880
   36 SUMC(ISO)=.0                                                      890
      DO 37 ISO=1,NS                                                    900
      DO 37 J1=1,7                                                      910
   37 SUM(ISO,J1)=.0                                                    920
      SUME=.0                                                           930
      K=1                                                               940
      STE(1,K)=ENG(IE)                                                  950
      DO 15 INR=NR1,NR                                                  960
      IF(ENG(IE)-ER(INR))16,15,15                                       970
   16 IF(ENG(IE+1)-ER(INR))18,18,17                                     980
   17 K=K+1                                                             990
      IF(K.LE.ISTE)  GO TO 201                                         1000
      K=1                                                              1010
      ISTEF=ISTEF+1                                                    1020
  201 STE(1,K)=ER(INR)                                                 1030
   15 CONTINUE                                                         1040
   18 K=K+1                                                            1050
      IF(K.LE.ISTE)  GO TO 202                                         1060
      K=1                                                              1070
      ISTEF=ISTEF+1                                                    1080
  202 STE(1,K)=ENG(IE+1)                                               1090
      KMAX=K                                                           1100
      IF(ISTEF.EQ.0)  GO TO 250                                        1110
      ISTEP=(ISTEF-1)*ISTE+K+50                                        1120
      RETURN                                                           1130
  250 NR1=INR                                                          1140
      KS=KMAX                                                          1150
      DO 2002 K=1,KS                                                   1160
 2002 STE1(K)=STE(1,K)                                                 1170
C     DO 2011 K=1,KS                                                   1180
C2011 WRITE(NOUTP,1050) K,STE1(K)                                      1190
 1050 FORMAT(' K=',I10,'STE1(K)=',E14.6)                               1200
      DO 19 K=1,KMAX                                                   1210
      CALL WIRQU(NR1,STE(1,K),STE(2,K),STE(3,K),STE(5,K),NR,IRE,ER,GJ, 1220
     1GAN,GAT,GAF,L,GAG,T,A,R,RLA,NMIN)                                1230
C     WRITE(NOUTP,1000) KMAX,K,STE(1,K),STE(3,K)                       1240
 1000 FORMAT(' KMAX=',I10,'K=',I10,'STE1=',E16.8,'STE3=',E16.8)        1250
   19 STE(4,K)=STE(5,K)-STE(3,K)-STE(2,K)                              1260
   22 KMX=KMAX+1                                                       1270
      KMX1=KMAX-1                                                      1280
      IF(KMX1)33,34,33                                                 1290
   33 IF(KMX.LE.ISTE)  GO TO 833                                       1300
      ISTEP=50                                                         1310
      RETURN                                                           1320
  833 DO 20 K=1,KMX1                                                   1330
      K1=KMX-K                                                         1340
```

```
      DO 20 J1=1,5                                                      1350
   20 STE(J1,K1+1)=STE(J1,K1)                                           1360
      IABF=0                                                            1370
      DO 2000 K=1,KS                                                    1380
      IF(STE(1,1).EQ.STE1(K)) IABF=1                                    1390
      IF(STE(1,3).EQ.STE1(K)) GO TO 2001                                1400
      GO TO 2000                                                        1410
 2001 IF(IABF.EQ.1) IST=0                                               1420
 2000 CONTINUE                                                          1430
      KMAX=KMAX+1                                                       1440
   35 STE(1,2)=(STE(1,3)+STE(1,1))/2.                                   1450
      CALL WIRQU(NR1,STE(1,2),STE(2,2),STE(3,2),STE(5,2),NR,IRE,ER,GJ,  1460
     1GAN,                                                              1470
     1GAT,GAF,L,GAG,T,A,R,RLA,NMIN)                                     1480
C     WRITE(NOUTP,1007) STE(1,2),STE(3,2)                               1490
 1007 FORMAT (' ERGEBNIS VON WIRQU:STE(1,2)=',E14.6,'STE(3,2)=',E14.6)  1500
      STE(4,2)=STE(5,2)-STE(3,2)-STE(2,2)                               1510
      DST=STE(1,2)-STE(1,1)                                             1520
C     WRITE(NOUTP,1006) STE(1,1),STE(1,2),STE(1,3),IST                  1530
 1006 FORMAT (' STE(1,1)=',E16.8,'STE(1,2)=',E16.8,'STE(1,3)=',E16.8,   1540
     1'IST=',I5)                                                        1550
      CALL STOSS(STE(1,1),STE(1,2),STE(1,3),F1,F2,F3,NEF,ES,F)          1560
      DO 21 J1=2,4                                                      1570
      FLC1=(3.*STE(J1,1)*F1+STE(J1,3)*F3)*DST*.25                       1580
      FLC2=(STE(J1,1)*F1+STE(J1,2)*F2)*DST*.5                           1590
      IF(FLC1)45,21,45                                                  1600
   45 AFL=ABS((FLC1-FLC2)/AMIN1(FLC1,FLC2))                             1610
C     WRITE(NOUTP,1001) J1,FLC1,FLC2,AFL                                1620
 1001 FORMAT(' J1=',I10,'FLC1=',E16.8,'FLC2=',E16.8,'AFL=',E16.8)       1630
      IF(AFL-PR     ) 1021,1021,1022                                    1640
 1021 IF(ISI.NE.1) GO TO 1010                                           1650
      GO TO 21                                                          1660
 1010 ISI=1                                                             1670
      GO TO 22                                                          1680
 1022 ISI=0                                                             1690
      GO TO 22                                                          1700
   21 CONTINUE                                                          1710
      DO 24 J1=1,3                                                      1720
   24 SUMO(J1)=(STE(J1+1,1)*F1+STE(J1+1,2)*F2)*DST*.5+SUMO(J1)          1730
      SUME=SUME+(F1+F2)*DST*.5                                          1740
C     WRITE(NOUTP,1002) SUMO(2),SUME                                    1750
      DO 25 ISO=1,NS                                                    1760
      SIG1=STE(5,1)*SIGO(ISO)                                           1770
      SIG2=STE(5,2)*SIGO(ISC)                                           1780
      SIG3=SIG1*SIG1                                                    1790
      SIG4=SIG2*SIG2                                                    1800
      SUM(ISO,5)=(F1/SIG3+F2/SIG4)*DST*.5+SUM(ISC,5)                    1810
      SUM(ISO,1)=(F1/SIG1+F2/SIG2)*DST*.5+SUM(ISO,1)                    1820
      DO 325 J1=6,7                                                     1830
  325 SUM(ISO,J1)=(STE(J1-2,1)*F1/SIG3+STE(J1-2,2)*F2/SIG4)*DST*.5      1840
     1+SUM(ISO,J1)                                                      1850
      DO 25 J1=2,4                                                      1860
   25 SUM(ISO,J1)=(STE(J1,1)*F1/SIG1+STE(J1,2)*F2/SIG2)*DST*.5+SUM(ISO,J 1870
     11)                                                                1880
      DO 27 J1=2,4                                                      1890
      FLC1=(STE(J1,1)*F1+3.*STE(J1,3)*F3)*DST*.25                       1900
      FLC2=(STE(J1,2)*F2+STE(J1,3)*F3)*DST*.5                           1910
      IF(FLC1)46,27,46                                                  1920
   46 AFL=ABS((FLC1-FLC2)/AMIN1(FLC1,FLC2))                             1930
C     WRITE(NOUTP,1001) J1,FLC1,FLC2,AFL                                1940
      IF(AFL-PR     )27,27,28                                           1950
   27 CONTINUE                                                          1960
      DO 29 J1=1,3                                                      1970
   29 SUMO(J1)=(STE(J1+1,2)*F2+STE(J1+1,3)*F3)*DST*.5+SUMO(J1)          1980
      SUME=SUME+(F2+F3)*DST*.5                                          1990
C     WRITE(NOUTP,1002) SUMO(2),SUME                                    2000
 1002 FORMAT(' SUMO(2)=',E16.8,'SUME=',E16.8)                           2010
      DO 30 ISO=1,NS                                                    2020
      SIG1=STE(5,2)*SIGO(ISO)                                           2030
      SIG2=STE(5,3)*SIGO(ISC)                                           2040
      SIG3=SIG1*SIG1                                                    2050
      SIG4=SIG2*SIG2                                                    2060
      SUM(ISO,5)=SUM(ISO,5)+(F2/SIG3+F3/SIG4)*DST*.5                    2070
      SUM(ISO,1)=SUM(ISO,1)+(F2/SIG1+F3/SIG2)*.5*DST                    2080
      DO 330 J1=6,7                                                     2090
  330 SUM(ISO,J1)=SUM(ISO,J1)+(STE(J1-2,2)*F2/SIG3+STE(J1-2,3)*F3/      2100
     1SIG4)*DST*.5                                                      2110
      DO 30 J1=2,4                                                      2120
   30 SUM(ISO,J1)=SUM(ISO,J1)+(STE(J1,2)*F2/SIG1+STE(J1,3)*F3/SIG2)*DST* 2130
     1.5                                                                2140
      DO 31 K=3,KMAX                                                    2150
      DO 31 J1=1,5                                                      2160
   31 STE(J1,K-2)=STE(J1,K)                                             2170
      KMAX=KMAX-2                                                       2180
      GOTO 22                                                           2190
   28 DO 32 J1=1,5                                                      2200
   32 STE(J1,1)=STE(J1,2)                                               2210
      GOTO 35                                                           2220
   34 IF(IT.EQ.1.AND.IE.EQ.NANF)  GO TO 935                             2230
      GO TO 934                                                         2240
  935 INDEX=0                                                           2250
      WRITE (LZWF) INDEX,MM                                             2260
  934 INDEX=6                                                           2270
      WRITE(LZWF)INDEX,MATN     ,TEMP(IT),IE,ENG(IE),ENG(IE+1)          2280
      DO 38 ISO=1,3                                                     2290
   38 SUMC(ISO)=SUMC(ISO)/SUME                                          2300
      INDEX=5                                                           2310
      SGT1=SUMO(1)+SUMO(2)+SUMO(3)                                      2320
      WRITE(LZWF)INDEX,SUMO(2),SUMC(3),SUMC(1),SUMO(3),SGT1             2330
      INDEX=6                                                           2340
      WRITE(NOUTP,957)                                                  2350
  957 FORMAT(1HO,18X,8HMATERIAL,3X,10HTEMPERATUR,2X,6HGRUPPE,7X,7HGRENZE 2360
     1N)                                                                2370
      IV=NE-IE                                                          2380
      WRITE(NOUTP,958)MATN     ,TEMP(IT),IV,ENG(IE),ENG(IE+1)           2390
  958 FORMAT(1H ,18X,A8,F11.2,6X,I2,1X,2E12.4/1X)                       2400
      WRITE(NOUTP,950)                                                  2410
  950 FORMAT(1HO,21X,7HSIGMA G,9X,7HSIGMA N,9X,7HSIGMA F,9X,7HSIGMAN1,  2420
     19X,7HSIGMAT1)                                                     2430
      WRITE (NOUTP,951) SUMO(2),SUMO(3),SUMO(1),SUMO(3),SGT1            2440
```

```
951 FORMAT(1H ,15X,5E16.8)                                              2450
    WRITE(NOUTP,952)                                                    2460
952 FORMAT(1HO,6X,7HSIGMA 0,11X,2HFG,14X,2HFN,14X,2HFF,14X,3HFN1,       2470
   113X,3HFT1/1X)                                                       2480
    DO 39 ISO=1,NS                                                      2490
    DO 40 J1=2,4                                                        2500
    IF(SUMO(J1-1))420,421,420                                           2510
421 SUM(ISO,J1)=1.                                                      2520
    GOTO 40                                                             2530
420 SUM(ISO,J1)=SUM(ISO,J1)/(SUM(ISO,1)*SUMO(J1-1))                     2540
 40 CONTINUE                                                            2550
    SUM(ISO,6)=SUM(ISO,6)/(SUM(ISO,5)*SUMO(3))                          2560
    SUM(ISO,7)=SUM(ISO,7)/(SUM(ISO,5)*(SUMO(1)+SUMO(2)+SUMO(3)))        2570
    WRITE (NOUTP,953)SIGO(ISO),SUM(ISO,3),SUM(ISO,4),SUM(ISO,2)         2580
   1,SUM(ISO,6),SUM(ISO,7)                                              2590
 39 WRITE(LZWF) INDEX,SIGO(ISO),SUM(ISO,3),SUM(ISO,4),SUM(ISO,2)        2600
   1,SUM(ISO,6),SUM(ISO,7)                                              2610
953 FORMAT(6E16.8)                                                      2620
 10 CONTINUE                                                            2630
 60 CONTINUE                                                            2640
  3 CONTINUE                                                            2650
111 KL=KL+1                                                             2660
    RETURN                                                              2670
    END                                                                 2680
```

```
    SUBROUTINE WIRQ (INR,E,SF,SG,ST,IRE,                                10
   1                                ER,GJ,GAN,GAT,GAF,L,GAG,T,A,R,RLA)  20
    REAL*8 MAT                                                          30
    DIMENSION ER(IRE),GJ(IRE),GAN(IRE),GAT(IRE),GAF(IRE),L(IRE),GAG(IR  40
   1E)                                                                  50
    COMMON MAT,ISTRUK,ISPA,NOUTP                                        60
    PI=3.14159                                                          70
    XKC=8.6165E-5                                                       80
    ERI=ER(INR)                                                         90
    ELA=RLA/SQRT(E)                                                    100
    PHIO=R/ELA                                                         110
    IF(ERI.LE.0.)  GN=GAN(INR)*SQRT(E)*(PHIO*PHIO)**L(INR)             120
    IF(ERI.GT.0.)  GN=GAN(INR)*SQRT(E/ERI)*(E/ERI)**L(INR)             130
    GT=GN+GAG(INR)+GAF(INR)                                            140
    SOC=4.*PI*ELA**2*GJ(INR)*GN/GT                                     150
    X=2.*(E-ER(INR))/GT                                                160
    IT=T                                                               170
    IF(IT)4,5,4                                                        180
  5 PSI=1./(1.+X*X)                                                    190
    CHI=X*PSI                                                          200
    GOTO 6                                                             210
  4 DELTA=SQRT(4.*XKO*T*E/A)                                           220
    TETA=(DELTA/GT)**2                                                 230
    CALL PSIXI(X,TETA,PSI,CHI)                                         240
  6 IF(L(INR)-1)1,1,2                                                  250
  2 SG=.0                                                              260
    SF=.0                                                              270
    ST=.0                                                              280
    GOTO 3                                                             290
  1 SG=SOC*GAG(INR)*PSI/GT                                             300
    SF=SOC*GAF(INR)*PSI/GT                                             310
    PHIL=PHIO-ATAN(PHIO*FLOAT(L(INR)))                                 320
    PHI2=2.*PHIL                                                       330
    ST=SOC*(PSI*COS(PHI2)+CHI*SIN(PHI2))                               340
    SIGP=4.*PI*ELA**2*FLOAT(2*L(INR)+1)*SIN(PHIL)**2                   350
    IF(ST+SIGP)10,10,3                                                 360
 10 WRITE(NOUTP,900)ER(INR),E,ST,SIGP                                  370
900 FORMAT(1HO,77H***WARNING 1.01 : THE CONTRIBUTION OF THE RESONANCE  380
   1WITH THE RESONANCE ENERGY,E13.6,3H EV/1H ,18X,13HAT THE ENERGY,E14 390
   2.6,13H IS NEGATIVE,,E14.6,22H BARNS, AND ITS ABSOLUT/1H ,18X,46HVAL 400
   3UE LARGER THAN THE POTENTIAL CROSS SECTION,F14.6,7H BARNS.)         410
  3 RETURN                                                             420
    END                                                                430
```

```
    SUBROUTINE WIRQU(NR1,E,SIFG,SIGG,SIGT,NR,IRE,                       10
   1                                ER,GJ,GAN,GAT,GAF,L,GAG,            20
   1T,A,R,RLA,NMIN)                                                     30
    REAL*8 MAT                                                          40
    DIMENSION ER(IRE),GJ(IRE),GAN(IRE),GAT(IRE),GAF(IRE),L(IRE),GAG(IR  50
   1E)                                                                  60
    COMMON MAT,ISTRUK,ISPA,NOUTP                                        70
    PI=3.14159                                                          80
    ELA=RLA/SQRT(E)                                                     90
    PHIO=R/ELA                                                         100
    PHI1=PHIO-ATAN(PHIO)                                               110
    SIGP=4.*PI*ELA**2*(SIN(PHIO)**2+3.*SIN(PHI1)**2)                   120
    NR2=NR1+1                                                          130
    DO 1 I=1,NR1                                                       140
    NR3=NR2-I                                                          150
    IF(E-ER(NR3))1,2,2                                                 160
  1 CONTINUE                                                           170
  2 SIFG=0.                                                            180
    SIGG=.0                                                            190
    SIGT=SIGP                                                          200
    IA=NR3-NMIN                                                        210
    IF(IA)3,3,4                                                        220
  3 IA=1                                                               230
  4 IE=NR3+NMIN                                                        240
    IF(IE-NR)5,6,6                                                     250
  6 IE=NR                                                              260
  5 DO 7 INR=IA,IE                                                     270
    CALL WIRQ(INR,E,SF,SG,ST,IRE,                                      280
   1                        ER,GJ,GAN,GAT,GAF,L,GAG,T,A,R,RLA)         290
    SIFG=SIFG+SF                                                       300
    SIGG=SIGG+SG                                                       310
    SIGT=SIGT+ST                                                       320
  7 CONTINUE                                                           330
    IF(SIGT)10,10,11                                                   340
 10 WRITE(NOUTP,900)SIGT,E                                             350
```

```
   11 CONTINUE                                                          360
  900 FORMAT(1HO,'***WARNING 1.02 : THE TOTAL CROSS SECTION IS NEGATIVE,  370
     1',E14.6,' BARNS, AT THE ENERGY'/19X,E14.8,' EV. THE TOTAL CROSS SE  380
     2CTION HAS BEEN SET EQUAL TO .1 BARN')                              390
      SING=SIGT-SIGG-SIFG                                                400
      IF(SING-0.1)12,13,13                                               410
   12 SING=0.1                                                           420
      SIGT=SING+SIGG+SIFG                                                430
   13 RETURN                                                             440
      END                                                                450
```

```
      SUBROUTINE STOSS(E1,E2,E3,F1,F2,F3,NFE ,ES,F)                      10
      DIMENSION F(NFE ),ES(NFE )                                         20
      NEFE=NFE                                                           30
      IF(NFE.EQ.1)  NEFE=0                                               40
      IF(NEFE)1,2,1                                                      50
    2 F1=PHI(E1)                                                         60
      F2=PHI(E2)                                                         70
      F3=PHI(E3)                                                         80
      GOTO 3                                                             90
    1 E=E1                                                              100
      IND=1                                                             110
    9 DO 4 I=1,NEFE                                                     120
      IF(E-ES(I))5,5,4                                                  130
    4 CONTINUE                                                          140
      I=NEFE                                                            150
    5 FF=F(I)-(ES(I)-E)*(F(I)-F(I-1))/(ES(I)-ES(I-1))                   160
      GOTO(6,7,8),IND                                                   170
    6 F1=FF                                                             180
      IND=2                                                             190
      E=E2                                                              200
      GOTO 9                                                            210
    7 F2=FF                                                             220
      IND=3                                                             230
      E=E3                                                              240
      GOTO 9                                                            250
    8 F3=FF                                                             260
    3 RETURN                                                            270
      END                                                               280
```

```
      SUBROUTINE PSIXI(X,T,U,V)                                          10
C                                                                        20
C     GENAU EINMAL IST IN EINEM PROGRAMM, DAS PSIXI AUFRUFT,             30
C     VOR DIESEM AUFRUF DAS STATEMENT                                    40
C                                                                        50
C     CALL EXPPX(X,X,X,X)                                                60
C                                                                        70
```

```
C     H SETZEN                                                           80
C                                                                        90
      DIMENSION D(8),C(8)                                               100
      XX=X*X                                                            110
      BB=1.+XX                                                          120
      U=HORP/BB                                                         130
      V=X*U                                                             140
      DO 1 N=1,8                                                        150
      AA=4.*T*C(N)                                                      160
      CC=2.*HORP*D(N)                                                   170
      ALPHA=1.-XX+AA                                                    180
      DIV=1./(ALPHA*ALPHA+4.*XX)                                        190
      U=U+CC*(BB+AA)*DIV                                                200
    1 V=V+CC*X*(BB-AA)*DIV                                              210
      IF(T.LE.8)GOTO 2                                                  220
      RT=SQRT(T)                                                        230
      ETA=PI/(H*RT)                                                     240
      EXPO=(XX-1.)/(4.*T)+ETA                                           250
      IF(EXPO.GT.25.)GOTO 2                                             260
      XI=X/(2.*T)                                                       270
      ZETA=X*ETA                                                        280
      ACOS=COS(XI)                                                      290
      BSIN=SIN(XI)                                                      300
      CCOS=EXP(-ETA)-COS(ZETA)                                          310
      DSIN=SIN(ZETA)                                                    320
      BOT=1./(CCOS*CCOS+DSIN*DSIN)                                      330
      REAL=BOT*(ACOS*CCOS-BSIN*DSIN)                                    340
      AMAG=BOT*(BSIN*CCOS+ACOS*DSIN)                                    350
      EXIT=RTPI*EXP(-EXPO)/RT                                           360
      U=U+EXIT*REAL                                                     370
      V=V-EXIT*AMAG                                                     380
    2 RETURN                                                            390
      ENTRY EXPPX                                                       400
      PI=3.141593                                                       410
      RTPI=SQRT(PI)                                                     420
      H=0.7                                                             430
      HORP=H/RTPI                                                       440
      B=H*H/(4.*PI*PI)                                                  450
      DO 3 N=1,8                                                        460
      ENN=N*N                                                           470
      C(N)=ENN*H*H                                                      480
    3 D(N)=EXP(-C(N))                                                   490
      RETURN                                                            500
      END                                                               510
```

```
      SUBROUTINE EZZ (E,NS,EZG,EZC,EZF,DRSG,DRFS,    CHI,XNYN,FXNYN,GN,    10
     1RQU,XL,XA,GG,NEY,EY,GF)                                            20
      REAL*8 MAT                                                         30
      DIMENSION CHI(25,4),XNYN(10),FXNYN(10),GN(10),XL(10),GG(10)        40
     1,EY(199),GF(10,199),X(2),Y(2)                                      50
      COMMON MAT,ISTRUK,ISPA,NOUTP                                       60
      GNN=GAMN(E,NS,GN,RQU,XL,XA)                                        70
```

```
      GNF=GAFM(E,NS,NEY,EY,GF)                                          80
      GNG=GAMG(E,NS,GG)                                                 90
      NY=XNYN(NS)                                                      100
      NFY=FXNYN(NS)                                                    110
      IF(NY.GT.4.OR.NFY.GT.4) GO TO 4                                  120
      GO TO 8                                                          130
    4 WRITE(NOUTP,100) NY,NFY,E,NS                                     140
  100 FORMAT(/' ***ERROR 2.01 : THE HIGHEST NUMBER OF EXIT CHANNELS IN N 150
     1EUTRON ELASTIC SCATTERING,NUEN,OR IN FISSION,NUEF,THAT CAN BE TREA 160
     2TED,IS 4'/' ***NUEN=',I4,'NUEF=',I4,'AT ENERGY',E12.5,'EV IN SERIE 170
     3S',I4)                                                           180
    8 DO 1 I=1,2                                                       190
      X(I)=.0                                                          200
    1 Y(I)=.0                                                          210
      IF (ISPA.EQ.0.OR.GNF    .LT.1.E-30) GO TO 6                      220
    5 NN=25                                                            230
      NF=25                                                            240
      XFN=625.                                                         250
    7 DO 2 I=1,NN                                                      260
      DO 2 J=1,NF                                                      270
      X1=((GNN*CHI(I,NY))**2)/(GNN*CHI(I,NY)+GNG+GNF*CHI(J,NFY))       280
      Y1=GNN*CHI(I,NY)/(GNN*CHI(I,NY)+GNG+GNF*CHI(J,NFY))              290
      X(1)=X(1)+X1                                                     300
      Y(1)=Y(1)+Y1                                                     310
      X(2)=X(2)+X1*GNF*CHI(J,NFY)                                      320
    2 Y(2)=Y(2)+Y1*GNF*CHI(J,NFY)                                      330
      EZG=X(1)/(Y(1)*GNN)                                              340
      EZC=1.+2./XNYN(NS)                                               350
      EZF=X(2)/(Y(2)*GNN)                                              360
      DRSG=Y(1)*GNG/(GNN*XFN)                                          370
      DRFS=Y(2)/(GNN*XFN)                                              380
      GO TO 10                                                         390
    6 NN=25                                                            400
      XFN=25.                                                          410
      DO 3 I=1,NN                                                      420
      X1=((GNN*CHI(I,NY))**2)/(GNN*CHI(I,NY)+GNG)                      430
      Y1=GNN*CHI(I,NY)/(GNN*CHI(I,NY)+GNG)                             440
      X(1)=X(1)+X1                                                     450
    3 Y(1)=Y(1)+Y1                                                     460
      EZG=X(1)/(Y(1)*GNN)                                              470
      EZC=1.+2./XNYN(NS)                                               480
      EZF=.0                                                           490
      DRSG=Y(1)*GNG/(GNN*XFN)                                          500
      DRFS=.0                                                          510
   10 CONTINUE                                                         520
      RETURN                                                           530
      END                                                              540
```

```
      FUNCTION DMIT(E,NS,DN,EBI)                                        10
      DIMENSION DN(10)                                                  20
      DMIT=DN(NS)*((EBI+E)/EBI)**2*EXP(-SQRT(89.72E-6)*(SQRT(EBI+E)-    30
     1SQRT(EBI)))                                                       40
      RETURN                                                            50
      END                                                               60
```

```
      FUNCTION DELTA(E,T,NS,DEL)                                        10
      DELTA=SQRT(DEL*T*E)                                               20
      RETURN                                                            30
      END                                                               40
```

```
      FUNCTION EPSI(E,T,NS,DN,EBI,DEL)                                  10
      DIMENSION EP(21),EPP(21),X1(2),FX1(2),DN(10)                      20
      DATA EP/0.,1.,1.5,2.,2.5,3.,3.5,4.,5.,7.,10.,14.,20.,30.,40.,     30
     X50.,60.,70.,80.,90.,100./,EPP/2.5066,1.7241,1.3705,1.0661,        40
     X0.82,0.6291,0.4845,0.3758,0.23261,0.10002,0.03577,0.012276,       50
     X0.003647,8.523E-4,2.8817E-4,1.2683E-4,5.979E-5,3.694E-5,2.5643E-5, 60
     X1.8679E-5,8.733E-6/                                               70
      X=DMIT(E,NS,DN,EBI)/DELTA(E,T,NS,DEL)                             80
      DO 1 I=2,21                                                       90
      IF(X-EP(I))4,4,1                                                 100
    1 CONTINUE                                                         110
    4 DO 5 K=1,2                                                       120
      II=I+K-2                                                         130
      X1(K)=EP(II)                                                     140
    5 FX1(K)=EPP(II)                                                   150
      EPSI=POL(X,X1,FX1)/X                                             160
      RETURN                                                           170
      END                                                              180
```

```
      FUNCTION GAMN(E,NS,GN,RQU,XL,XA)                                  10
      DIMENSION GN(10),XL(10)                                           20
      GAMN=GN(NS)*SQRT(E)*(E*RQU+(1.-XL(NS))*XA)/(E*RQU+XA)             30
      RETURN                                                            40
      END                                                               50
```

```
      FUNCTION GAMG(E,NS,GG)                                            10
      DIMENSION GG(10)                                                  20
      GAMG=GG(NS)                                                       30
      RETURN                                                            40
      END                                                               50
```

```
      FUNCTION GAFM(E,NS,NEY,EY,GF)                                     10
      REAL*8 MAT                                                        20
      DIMENSION EY(199),GF(10,199),X1(2),FX1(2)                         30
      COMMON MAT,ISTRUK,ISPA                                            40
      IF(ISPA     )2,2,3                                                50
    3 CALL SUCH (E,NSU,NEY,EY)                                          60
      DO 1 J=1,2                                                        70
      NSU1=NSU+J                                                        80
      X1(J)=EY(NSU1)                                                    90
    1 FX1(J)=GF(NS,NSU1)                                               100
      GAFM=POL(E,X1,FX1)                                               110
      GO TO 4                                                          120
    2 GAFM=0.                                                          130
    4 RETURN                                                           140
      END                                                              150
```

```
      FUNCTION POL(X,X1,FX1)                                            10
      DIMENSION X1(2),FX1(2)                                            20
      IF(X1(2)-X1(1))1,2,1                                              30
    2 POL=FX1(1)                                                        40
      GO TO 3                                                           50
    1 POL=FX1(1)+(FX1(2)-FX1(1))*(X-X1(1))/(X1(2)-X1(1))                60
    3 RETURN                                                            70
      END                                                               80
```

```
      SUBROUTINE SUCH (E,NSU,NEY,EY)                                    10
      DIMENSION EY(199)                                                 20
      DO 14 K=2,NEY                                                     30
      IF(EY(K)-E)14,13,13                                               40
   14 CONTINUE                                                          50
   13 NSU=K-2                                                           60
      RETURN                                                            70
      END                                                               80
```

```
      FUNCTION SIGC(E,NS,XA,GI,DN,EBI,GN,RQU,XL)                        10
      DIMENSION GI(10),DN(10),GN(10),XL(10)                             20
      SIGC=19.73921*XA*GI(NS)*GAMN(E,NS,GN,RQU,XL,XA)/(E*DMIT(E,NS,DN,  30
     1EBI))                                                             40
      RETURN                                                            50
      END                                                               60
```

```
      FUNCTION PHASE(E,NS,XA,RQU,XL)                                    10
      DIMENSION XL(10)                                                  20
      B=SQRT(RQU*E/XA)                                                  30
      PHASE=COS(2.*(B-XL(NS)*ATAN(B)))                                  40
      RETURN                                                            50
      END                                                               60
```

```
      SUBROUTINE FSTAT (MI,SIGO,J,ENG,NFE,REFE,EFE,MT,TEMP,SE,SM,       10
     1XEUGZ)                                                            20
      REAL*8 X,IX,MAT,NN                                                30
     1,MM                                                               40
      DIMENSION ENG(J),EFE(NFE),REFE(NFE),TEMP(MT),SIGO(MI),NADAT(2),   50
     2EY(199),NN(5),NAME(4),X(20) ,IX(20) ,CHI(25,4),GF(10,199),        60
     3       GN(10),XL(10),DN(10),GI(10),XNYN(10),FXNYN(10),GG(10),     70
     4SE(3,5,MI),SM(3,5,MI),          E(3),XEUGZ(5,MI),XSUGI(5),SU(5)   80
     5,EF(3)                                                            90
      COMMON MAT,ISTRUK,ISPA,NOUTP,LIZ,NANF,NENC,KL                    100
      EQUIVALENCE (X(1),IX(1))                                         110
      DATA CHI/8.383E-4,5.8607E-3,1.595668E-2,3.122396E-2,5.182214E-2,  120
     X7.796678E-2,0.1110434,0.14875186,0.19382632,0.2462014,0.3066044,  130
     X0.37595912,0.45541448,0.5464511,0.65097026,0.7714919,0.9114051,   140
     X1.075423,1.2703559,1.5065244,1.8006327,2.1822634,2.7109872,       150
     X3.5798648,5.9721596,2.0273E-2,6.195225E-2,0.1054415,0.15091425,   160
     X0.198549,0.2485715,0.301227,0.35680875,0.41567075,0.47820725,     170
     XC.544925,0.61641525,0.693415,0.77684375,0.867878,0.968046,        180
     X1.0793867,1.2047147,1.3480617,1.5155082,1.716864,1.9695355,       190
     X2.309333,2.832582,4.2188757,5.9001333E-2,0.1333242,0.19497146,    200
     X0.251645,0.3074142,0.36262126,0.4181491,0.4746072,0.53251576,     210
     XC.5965109,0.65162876,0.7165988,0.78492293,0.8682213,0.94071066,   220
     X1.0257787,1.118885,1.2221354,1.3385186,1.4725188,1.6312598,       230
     X1.8271452,2.0844432,2.4887964,3.497654,0.10176025,0.196785,       240
     XC.26520225,0.32682625,0.3842565,0.43967925,0.49512475,0.545537,   250
     X0.6059465,0.659715,0.717307,0.77698,0.8393075,0.90493675,         260
     X0.97467075,1.049486,1.1306795,1.2199627,1.3197665,1.4337535,      270
     X1.567579,1.7310672,1.9429085,2.2805085,3.089838/                  280
      WRITE (NOUTP,9000)                                               290
 9000 FORMAT(1HO/1HC/' PROGRAMM KENNZIFFER 2')                         300
      WRITE (NOUTP,9001)                                               310
 9001 FORMAT(' PROGRAMM ZUR BERECHNUNG VON RESONANZSELBSTABSCHIRMFAKTORE  320
     1N VON STATISTISCHEN RESONANZPARAMETERN'/)                         330
      IYDIM=199                                                        340
      IYDIM1=0                                                         350
      ISS=ISPA                                                         360
      NLS=0                                                            370
      NLS1=0                                                           380
      NEFE=NFE                                                         390
      IF(NFE.EQ.1)  NEFE=0                                             400
      ISIG=0                                                           410
      IF(SIGO(MI).GE.1.E6)  GO TO 260                                  420
      MI=MI+1                                                          430
      SIGO(MI)=1.E6                                                    440
      ISIG=1                                                           450
```

```
 260 CALL DOPW (8HFSTAT   ,MM)                                          460
     CALL DOPW (8HBEST    ,NN(1))                                       470
     CALL DOPW (8HISOT1   ,NN(2))                                       480
     CALL DOPW (8HISOT2   ,NN(3))                                       490
     CALL DOPW (8HST      ,NN(4))                                       500
     CALL DOPW (8HSTGF    ,NN(5))                                       510
     I=0                                                                520
     WRITE (LIZ)I,MM                                                    530
     NGR=J-NANF                                                         540
     NEN=J+1-NEND                                                       550
     IX(1)=MAT                                                          560
     IX(2)=NN(1)                                                        570
     IX(3)=NN(2)                                                        580
     NAME(1)=3                                                          590
     CALL NDFLOC (KONTR,NAME,X,NUDAT,IS)                                600
     IF(KONTR)51,51,62                                                  610
  51 WRITE(NOUTP,153)KONTR                                              620
 153 FORMAT(1HO,3X,7HKONTR =I3)                                         630
     GO TO 1000                                                         640
  62 DEL=344.489/X(4)                                                   650
     SPIN=DABS(X(6))                                                    660
     IX(3)=NN(3)                                                        670
     CALL NDFLOC(KONTR,NAME,X,NUDAT,IS)                                 680
     IF(KONTR)51,51,63                                                  690
  63 XA=X(4)*X(4)                                                       700
     RQU=X(5)*X(5)                                                      710
     EBI=X(6)                                                           720
     IX(3)=NN(4)                                                        730
     IT=1                                                               740
     CALL NDFLOC(KONTR,NAME,X,NUDAT,IS)                                 750
     IF(KONTR)51,51,28                                                  760
  28 IF(X(4)  -5.E-5.LE.1.)  GO TO 3000                                 770
     WRITE (NOUTP,9004)                                                 780
9004 FORMAT(//' ***WARNING 2.07 : CONTRIBUTIONS,THAT CORRESPOND TO L.GT 790
    1.1 (L=ANGULAR MOMENTUM) ARE NEGLECTED')                            800
     NLS=NLS+1                                                          810
     NLS1=NLS                                                           820
     IT=IT-1                                                            830
     GO TO 3005                                                         840
3000 XL(IT)=IX(4)                                                       850
     GG(IT)=X(6)*1.E3                                                   860
     DN(IT)=X(7)*1.E3                                                   870
     GN(IT)=X(8)*1.E3                                                   880
     GI(IT)=(2.*X(5)+1.)/(4.*SPIN+2.)                                   890
     EXNYN(IT)=IX(10)*1.0001                                            900
     XNYN(IT)=IX(11)*1.0001                                             910
3005 CALL NDFNXT(KONTR,NAME,X,NUDAT,IS)                                 920
     IF(KONTR)3006,3006,66                                              930
  66 IT=IT+1                                                            940
     GO TO 28                                                           950
3006 WRITE(NOUTP,9005) IT                                               960
9005 FORMAT(' NUMBER OF SERIES,TAKEN INTO ACCOUNT IS IT=',I6)           970
 404 NAME(1)=3                                                          980
     IX(1)=MAT                                                          990
     IX(2)=NN(1)                                                       1000
     IX(3)=NN(5)                                                       1010
     IY=1                                                              1020
     KI=1                                                              1030
     CALL NDFLOC(KONTR,NAME,X,NUDAT,IS)                                1040
     IF(KONTR)128,128,74                                               1050
  128 ISPA1=0                                                          1060
     IF(ISPA.NE.ISPA1) GO TO 132                                       1070
     GO TO 201                                                         1080
  132 ISPA=ISPA1                                                       1090
C     WRITE(NOUTP,9006) MAT,ISPA                                       1100
C9006 FORMAT(/' FOR MATERIAL ',A8,' THE DATA TYPE STGF IS NOT AVAILABLE 1110
C    1ON THE NUCLEAR DATA LIBRARY.ISPA IS SET ',I4,' INTERNALLY')      1120
     GO TO 201                                                         1130
   74 ISPA1=1                                                          1140
     IF(ISPA.NE.ISPA1) GO TO 129                                       1150
     GO TO 131                                                         1160
  129 ISPA=ISPA1                                                       1170
C     WRITE(NOUTP,9007) MAT,ISPA                                       1180
C9007 FORMAT(/' FOR MATERIAL ',A8,'THE DATA TYPE STGF IS AVAILABLE ON TH 1190
C    1E NUCLEAR DATA LIBRARY.ISPA IS SET',I4,' INTERNALLY')            1200
  131 IF(X(4).LT.ENG(NGR+1))  GO TO 75                                 1210
     WRITE(NOUTP,9002)ENG(NGR),ENG(NGR+1)                              1220
 9002 FORMAT(1HO,37H***ERROR 2.02 : THE ENERGY GROUP FROM,E16.8,6H EV TO 1230
    1,E16.8,22H EV IS NOT POSSIBLE IN/15X,67HTHIS MODULE,BECAUSE NO STA 1240
    2TISTICAL INFORMATION IS AVAILABLE IN THIS/19X,21HENERGYRANGE ON KE 1250
    3DAK.)                                                             1260
     NGR=NGR+1                                                         1270
     IF(NGR-NEN)131,1000,1000                                          1280
   75 IF(X(4).LE.ENG(NGR))  GO TO 76                                   1290
     IF ((IY+1).LE.IYDIM) GO TO 72                                     1300
     IYDIM1=1                                                          1310
     GO TO 79                                                          1320
   72 EY(IY)=ENG(NGR)                                                  1330
     GF(KI,IY)=X(8)*1.E3                                               1340
     EY(IY+1)=X(4)                                                     1350
     GF(KI,IY+1)=X(8)*1.E3                                             1360
   78 KI=KI+1                                                          1370
     IF(KI.GT.IT.AND.NLS.EQ.0) GO TO 92                                1380
     IF(KI.GT.IT) GO TO 81                                             1390
     CALL NDFNXT(KONTR,NAME,X,NUDAT,IS)                                1400
     IF(KONTR)201,201,131                                              1410
   81 CALL NDFNXT(KONTR,NAME,X,NUDAT,IS)                               1420
     IF(KONTR) 201,201,77                                              1430
   77 NLS=NLS-1                                                        1440
     GO TO 78                                                          1450
   92 KI=1                                                             1460
     IY=IY+1                                                           1470
     IF (IY.GT.IYDIM) IYDIM1=1                                         1480
     NEY=IY-1                                                          1490
     NLS=NLS1                                                          1500
   79 CALL NDFNXT(KONTR,NAME,X,NUDAT,IS)                               1510
     IF(KONTR)201,201,91                                               1520
   76 IF (IY.LT.IYDIM) GO TO 205                                       1530
     IYDIM1=1                                                          1540
     GO TO 78                                                          1550
```

```
  205 EY(IY)=X(4)                                                          1560
      GF(KI,IY)=X(8)*1.E3                                                  1570
      GO TO 78                                                             1580
   91 IF (IYDIM1.EQ.1) GO TO 71                                            1590
      EY(IY)=X(4)                                                          1600
      GF(KI,IY)=X(8)*1.E3                                                  1610
   71 KI=KI+1                                                              1620
      IF(KI.GT.IT.AND.NLS.EQ.0) GO TO 92                                   1630
      IF(KI.GT.IT) GO TO 81                                                1640
      GO TO 79                                                             1650
  201 IF(IYDIM1.EQ.1) GO TO 202                                            1660
      GO TO 204                                                            1670
  202 WRITE(NOUTP,9003) IYDIM,IY                                           1680
 9003 FORMAT(' &&&&&IYDIM TOO SMALL,IYDIM=',I6,' ACTUAL DIMENSION OF EY    1690
     1IS IY=',I6)                                                          1700
      GO TO 1000                                                           1710
  204 DO 7  I=1,MT                                                         1720
      TT=TEMP(I)                                                           1730
      IF(TT.EQ.0)  GO TO 700                                               1740
      K=NGR-1                                                              1750
      N=1                                                                  1760
      IF(K+1-NEN)4,1000,1000                                               1770
    4 K=K+1                                                                1780
      E(N)=ENG(K)                                                          1790
   16 IF(N.NE.1) GO TO 21                                                  1800
      INEXT=1                                                              1810
      NEXTGR=0                                                             1820
      ENEXT=E(N)                                                           1830
      SSSSNE=0.                                                            1840
   21 CONTINUE                                                             1850
      CALL QUER(E(N),TT,N,SE        ,SM        ,XNYN,FXNYN,DEL,RQU,CHI,   1860
     1DN,EBI,XA,XL,GN,GG,NEY,EY,GF,GI,IT,MI,SIGC,NEXTGR,ENEXT,INEXT,       1870
     2SSSSNE)                                                              1880
      GO TO (23,24,25),N                                                   1890
   23 IF(K+1-NEN)6,6,7                                                     1900
    6 IF(ISPA.EQ.0)  GO TO 4000                                            1910
      IF(EY(NEY).LT.ENG(K+1))  GO TO 7                                     1920
 4000 N=2                                                                  1930
      E(N)=(ENG(K)+ENG(K+1))*0.5                                           1940
      GO TO 16                                                             1950
   24 N=3                                                                  1960
      GO TO 4                                                              1970
   25 LIJ=5                                                                1980
      IF(NEFE)300,301,300                                                  1990
  301 DO 1 IST=1,3                                                         2000
    1 EF(IST)=PHI(E(IST))                                                  2010
      GO TO 27                                                             2020
  300 L=2                                                                  2030
      DO 5 IST=1,3                                                         2040
      DO 12  KK=L,NEFE                                                     2050
      IF(REFE(KK)-E(IST))12,38,213                                         2060
   12 CONTINUE                                                             2070
      KK=NEFE                                                              2080
  213 EF(IST)=EFE(KK-1)+(EFE(KK)-EFE(KK-1))/(REFE(KK)-REFE(KK-1))*(E(IST   2090
     1)-REFE(KK-1))                                                        2100
      GO TO 26                                                             2110
   38 EF(IST)=EFE(KK)                                                      2120
   26 L=KK                                                                 2130
    5 CONTINUE                                                             2140
   27 H=(E(3)-E(2))*3.333333E-1                                            2150
      DO 29 KI=1,MI                                                        2160
      DO 29  IS=1,LIJ                                                      2170
      IF(SE(1,IS,KI).NE.-99999..AND.SE(2,IS,KI).NE.-99999..AND.SE(3,IS,    2180
     1KI).NE.-99999.)  GO TO 2000                                          2190
      XEUGZ(IS,KI)=-99999.                                                 2200
      GO TO 29                                                             2210
 2000 XEUGZ(IS,KI)=H*(SE(1,IS,KI)*EF(1)+4.*SE(2,IS,KI)*EF(2)+SE(3,IS,KI)   2220
     1*EF(3))                                                              2230
   29 CONTINUE                                                             2240
      DO 30  IS=1,LIJ                                                      2250
C     WRITE(NOUTP,5000) IS,SM(1,IS,1),SM(2,IS,1),SM(3,IS,1)                2260
      IF(SM(1,IS,1).NE.-99999..AND.SM(2,IS,1).NE.-99999..AND.SM(3,IS,1)    2270
     1.NE.-99999.)  GO TO 2001                                             2280
      SU(IS)=-99999.                                                       2290
      GO TO 2002                                                           2300
 2001 SU(IS)=H*(SM(1,IS,1)*EF(1)+4.*SM(2,IS,1)*EF(2)+SM(3,IS,1)*EF(3))     2310
 2002 IF(SE(1,IS,MI).NE.-99999..AND.SE(2,IS,MI).NE.-99999..AND.SE(3,IS,    2320
     1MI).NE.-99999.)  GO TO 2004                                          2330
      XSUGL(IS)=-99999.                                                    2340
      GO TO 30                                                             2350
 2004 XSUGL(IS)=H*(SE(1,IS,MI)*EF(1)+4.*SE(2,IS,MI)*EF(2)+SE(3,IS,MI)*EF   2360
     1(3))                                                                 2370
   30 CONTINUE                                                             2380
      XNE=H*(EF(1)+4.*EF(2)+EF(3))                                         2390
      DO 32  KI=1,MI                                                       2400
      DO 32  IS=1,LIJ                                                      2410
      IF(XEUGZ(IS,KI).NE.-99999..AND.XSUGL(IS).NE.-99999.)  GO TO 2003     2420
      XEUGZ(IS,KI)=-99999.                                                 2430
      GO TO 32                                                             2440
 2003 XEUGZ(IS,KI)=XEUGZ(IS,KI)/XSUGL(IS)                                  2450
   32 CONTINUE                                                             2460
      DO 31  IS=1,LIJ                                                      2470
      IF(SU(IS).EQ.-99999.)  GO TO 31                                      2480
      SU(IS)=SU(IS)/XNE                                                    2490
   31 CONTINUE                                                             2500
      KI=K-1                                                               2510
      IS=J-KI                                                              2520
      WRITE (NOUTP,130) MAT    ,TT,IS,ENG(KI),ENG(K)                       2530
  130 FORMAT(1HO,16X,8HMATERIAL,2X,10HTEMPERATUR,2X,6HGRUPPE,8X,7HGRENZE   2540
     1N/1H ,16X,A9,1X,F8.2,5X,I3,2E12.4)                                   2550
      IA=6                                                                 2560
      WRITE (LIZ)IN,MAT    ,TT,KI,ENG(KI),ENG(K)                           2570
      WRITE(NOUTP,37)(SU(IS),IS=1,LIJ)                                     2580
   37 FORMAT(1HO,20X,7HSIGMA G,9X,7HSIGMA N,9X,7HSIGMA F,9X,7HSIGMAN1,     2590
     19X,7HSIGMAT1/1H ,14X,5E16.8)                                         2600
      IA=LIJ                                                               2610
      WRITE(LIZ)IN,(SU(IS),IS=1,LIJ)                                       2620
      WRITE(NOUTP,138)                                                     2630
  138 FORMAT(1HO,5X,7HSIGMA 0,11X,2HFG,14X,2HFN,14X,2HFF,14X,3HFN1,13X,    2640
     13HFT1/1X)                                                            2650
```

```
      DO 139  KK=1,MI                                                   2660
      WRITE(NOUTP,36)SIGO(KK),(XEUGZ(IS,KK),IS=1,LIJ)                   2670
   36 FORMAT(1X,E15.8,5E16.8)                                           2680
      IN=LIJ+1                                                          2690
  139 WRITE(LIZ)IN,SIGO(KK),(XEUGZ(IS,KK),IS=1,LIJ)                     2700
   40 DO 70  KK=1,MI                                                    2710
      DO 70  IN=1,LIJ                                                   2720
      SE(1,IN,KK)=SE(3,IN,KK)                                           2730
   70 SM(1,IN,KK)=SM(3,IN,KK)                                           2740
      E(1)=E(3)                                                         2750
      GO TO 23                                                          2760
  700 WRITE (NOUTP,701)                                                 2770
  701 FORMAT(1HO,93H***ERROR 2.03 : A CALCULATION OF RESONANCE SELF SHIE 2780
     1LDING FACTORS AT ZERO TEMPERATURE (DEGREE/17X,39HKELVIN) IS NOT PO 2790
     2SSIBLE IN THIS MODULE,)                                           2800
    7 CONTINUE                                                          2810
 1000 IF(ISIG.EQ.1)  MI=MI-1                                            2820
      BACKSPACE LIZ                                                     2830
      READ(LIZ) I,NN(1)                                                 2840
      IF(I.EQ.0.AND.NN(1).EQ.MM)  BACKSPACE LIZ                         2850
      KL=KL+1                                                           2860
      ISPA=ISS                                                          2870
      RETURN                                                            2880
      END                                                               2890
```

```
      SUBROUTINE QUER (E,TT,A,SE,SM,XNYN,FXNY,DEL,RQU,CHI,    DN,EBI,XA,    10
     1XL,GN,GG,NEY,EY,GFA,GI,IT,MI,SIGO,NEXTGR,ENEXT,INEXT,SSSSNE)          20
      REAL*8 MAT                                                        30
      DIMENSION                                SIGO(MI),A(5),B(5),ACI(10),    40
     1PH(10),AC(10),GFF(25),TERM(5),CHI(25,4),XNYN(10),FXNY(10),GNN(25),     50
     2SE(3,5,MI),SM(3,5,MI),DN(10),XL(10),GN(10),GG(10),EY(199),             60
     3GFA(10,199),GI(10)                                                     70
      COMMON MAT,ISTRUK,ISPA,NOUTP,LIZ,NANF,NEND,KL                          80
      TEST=0.0                                                               90
      C=0.5                                                                 100
      DO 25 K=1,MI                                                          110
      SE(N,1,K)=0.                                                          120
      SE(N,2,K)=12.566371*RQU                                               130
      IF(ISPA    .EQ.1)  GO TO 41                                           140
      SE(N,3,K)=1.                                                          150
      GO TO 40                                                              160
   41 SE(N,3,K)=0.                                                          170
   40 SE(N,4,K)=SE(N,2,K)                                                   180
      SE(N,5,K)=SE(N,2,K)                                                   190
      SM(N,1,K)=0.                                                          200
      SM(N,2,K)=SE(N,2,K)                                                   210
      SM(N,3,K)=0.                                                          220
      SM(N,4,K)=SE(N,2,K)                                                   230
      SM(N,5,K)=SE(N,2,K)                                                   240
      ST=0.                                                                 250
      DO 1 I=1,IT                                                           260
      AC(I)=SIGC(E,I,XA,GI,DN,EBI,GN,RQU,XL)                                270
```

```
      PH(I)=PHASE(E,I,XA,RQU,XL)                                        280
      AC(I)=AC(I)*PH(I)                                                 290
    1 ST=ST+AC(I)                                                       300
      ST=ST+SIGO(K)+SE(N,2,K)                                           310
      DO 2 I=1,IT                                                       320
      ISE=0                                                             330
      IJ=1                                                              340
      KJ=3                                                              350
      CALL EZZ(E,I,EZG,EZC,EZF,DRSG,DRFS,    CHI,XNYN,FXNY,GN,RQU,XL,XA,    360
     1GG,NEY,EY,GFA)                                                    370
      D=EMIT(E,I,DN,EBI)                                                380
      DL=DELTA(E,TT,I,DEL)                                              390
      A(1)=AC(I)*DRSG                                                   400
      G=GAMN(E,I,GN,RQU,XL,XA)+GAMG(E,I,GG)+GAFM(E,I,NEY,EY,GFA)        410
      IF(G/DL-C)22,22,922                                               420

  922 TETA=G/DL                                                         430
      WRITE(NOUTP,923)TETA,I,TT,E                                       440
  923 FORMAT(1HO,31H***WARNING 2.04 : GAMMA/DELTA =,E14.6,11H FOR SERIES 450
     1,I3,19H AT THE TEMPERATURE,E14.6/19X,31HDEGREE KELVIN,AND AT THE E 460
     2NERGY,E14.6,4H EV.)                                               470
   22 XY=D*ACI(I)*EPSI(E,TT,I,DN,EBI,DEL)/(2.506628*DL*ST**2)           480
      SPI=ST                                                            490
      SSS=ST-ACI(I)                                                     500
      SSSS=-2.*SSS+SIGO(K)                                              510
      IF(ST-ACI(I)).GT.0)  GO TO 31                                     520
      GO TO 30                                                          530
   31 IF(N.EQ.3.AND.K.EQ.1.AND.ISE.EQ.1.AND.I.EQ.INEXT) NEXTGR=0        540
      IF(NEXTGR.EQ.1) GO TO 33                                          550
      GO TO 23                                                          560
   33 IF(N.EQ.2.AND.NEXTGR.EQ.1.AND.K.EQ.1)                    GO TO 32 570
      GO TO 23                                                          580
   32 WRITE(NOUTP,43) ENEXT,SSSSNE                                     590
   43 FORMAT(//////' ***WARNING 2.05 : THE THEORY APPLIED FOR THE CALCULA 600
     1TION OF THE CURRENT WEIGHTED SELF-SHIELDING FACTORS IS NOT VALID'/   610
     2' ***FOR ALL VALUES OF SIGO AT ENERGY',E12.5,'EV.AT THIS ENERGY SI   620
     3GC HAS TO BE GREATER THAN',E12.5,'.'/' ***FOR MORE DETAILED INFORM   630
     4ATION COMPARE WARNING 2.05 FOR THE ENERGY GROUP,CALCULATED BEFORE.   640
     5')                                                                  650
      NEXTGR=0                                                          660
      SSSSNE=0.                                                         670
      GO TO 23                                                          680
C     DO 26 L=IJ,5                                                      690
C     SE(N,L,K)=-99999.                                                 700
C  26 SM(N,L,K)=-99999.                                                 710
   30 WRITE (NOUTP,42)SIGO(K),I,SSS,E,SSSS                              720
   42 FORMAT(/' ***WARNING 2.05 : CONCERNS CALCULATION OF **FNI** AND ** 730
     1FTI**.FOR SIGO=',E12.5,'SPEFF* IS NEGATIVE IN THE SERIES',I4/' *** 740
     2SPEFF*=',E12.5,'AT ENERGY',E12.5,'EV.'/' ***ACCORDING TO KFK 1784,  750
     3APPENDIX II,FORMULA 25, THE THEORY DEVELOPED THERE IS NOT VALID IN  760
     4 THIS CASE.'/' ***AT THIS ENERGY AND IN THIS SERIES THE THEORY IS   770
     5VALID FOR SIGO GREATER THAN',F12.5)                               780
      IF(N.EQ.3.AND.K .EQ.1) GO TO 28                                   790
      GO TO 23                                                          800
   28 NEXTGR=1                                                          810
      ENEXT=E                                                           820
```

```
      SSSSNE=AMAX1(SSSS,SSSSNE)                                          830
      INEXT=I                                                            840
C     GO TO 25                                                           850
   22 A(3)=0.                                                            860
      B(3)=0.                                                            870
      AA=0.398942*ACI(I)*D*EZC/(DL*SPI)                                  880
C     WRITE (NOUTP,500) AA                                               890
  500 FORMAT (' AA=',E14.6)                                              900
      IF(AA-TEST)3,3,4                                                   910
    3 BT=(1.-AA)*D*ACI(I)/SPI                                            920
      B(1)=(1.-AA*EZG/EZC)*D*A(1)/SPI                                    930
      IF(ISPA    )5,5,6                                                  940
    6 A(3)=AC(I)*DRFS                                                    950
      B(3)=(1.-AA*EZF/EZC)*D*A(3)/SPI                                    960
    5 A(2)=ACI(I)-A(3)-A(1)                                              970
      B(2)=BT-B(1)-B(3)                                                  980
C     IF(ISE.EQ.0) GO TO 2000                                            990
C     QF=1.+ACI(I)/(SPI+ACI(I))                                         1000
C     GO TO 2001                                                        1010
 2000 QF=1.+ACI(I)/SPI                                                   1020
 2001 BT=QF*BT                                                           1030
      B(1)=QF*B(1)                                                       1040
      B(2)=QF*B(2)                                                       1050
      B(3)=QF*B(3)                                                       1060
      IF(ISE.EQ.0)  GO TO 27                                             1070
      A(4)=A(2)                                                          1080
      A(5)=ACI(I)                                                        1090
      B(4)=B(2)                                                          1100
      B(5)=BT                                                            1110
   27 XNEN=1./(1.-BT/D+XY*ACI(I))                                        1120
      IF(XNEN.GT.0)  GO TO 202                                           1130
      WRITE (NOUTP,203)                                                  1140
  203 FORMAT(1HO,52H***WARNING 2.06 : INACCURATE OVERLAPPING CORRECTION.  1150
     1)                                                                  1160
  202 CONTINUE                                                           1170
      DO 57 L=IJ,KJ                                                      1180
      TERM(L)=(ST-ACI(I))*XNEN*(B(L)/D-XY*A(L))                          1190
      SE(N,L,K)=SE(N,L,K)+TERM(L)                                        1200
    7 SM(N,L,K)=SM(N,L,K)+A(L)                                           1210
   57 CONTINUE                                                           1220
      GO TO 20                                                           1230
    4 GO=GAMN(E,I,GN,RQU,XL,XA)                                          1240
      CI=SPI*GO*1.5707963/(ACI(I)*D)                                     1250
      IF(ISPA    )8,8,9                                                  1260
    8 GF=0.                                                              1270
      NF=1                                                               1280
      NN=25                                                              1290
      GFF(1)=0.                                                          1300
      NL=XNYN(I)                                                         1310
      DO 10 M=1,NN                                                       1320
   10 GNN(M)=GO*CHI(M,NU)                                                1330
   11 GAX=GAMG(E,I,GG)                                                   1340
      BT=0.                                                              1350
      B(1)=0.                                                            1360
      B(2)=0.                                                            1370
      LG=1                                                               1380
      DO 12 M=1,NN                                                       1390
      GNX=GNN(M)                                                         1400
      DO 12 NI=1,NF                                                      1410
      GFX=GFF(NI)                                                        1420
      GTX=GAX+GNX+GFX                                                    1430
      XK=1.442695*ALOG(1.E5*CI*GTX/GNX)                                  1440
      XT=GTX/DL                                                          1450
      CALL FSPIE                                                         1460
      CALL TAB (XT,XK,LG,DSJ,XABCJ,DJK)                                  1470
      CALL FSPIE                                                         1480
C     WRITE(NOUTP,1000) XT,XK,XABCJ                                      1490
 1000 FORMAT(' XT=',G16.8,'XK=',G16.8,'XABCJ=',G16.8)                    1500
      B(3)=B(3)+GFX*XABCJ                                                1510
      B(1)=B(1)+XABCJ                                                    1520
   12 BT=BT+GTX*XABCJ                                                    1530
      AZ=NN                                                              1540
      BZ=NF                                                              1550
      FK=AZ*BZ                                                           1560
      B(1)=B(1)*GAX/(PH(I)*FK)                                           1570
      B(3)=B(3)/(PH(I)*FK)                                               1580
      BT=BT/FK                                                           1590
      GO TO 5                                                            1600
    9 NL=XNYN(I)                                                         1610
      A(3)=AC(I)*DRFS                                                    1620
      NN=25                                                              1630
      NF=25                                                              1640
      DO 200 M=1,NN                                                      1650
  200 GNN(M)=GO*CHI(M,NU)                                                1660
      GF=GAFM(E,I,NEY,EY,GFA)                                            1670
      NL=FXNY(I)                                                         1680
      DO 201 M=1,NF                                                      1690
  201 GFF(M)=GF*CHI(M,NU)                                                1700
      GO TO 11                                                           1710
   20 IF(ISE.EQ.1)  GO TO 21                                             1720
      ISE=1                                                              1730
      FT=ST                                                              1740
      ST=ST*0.5                                                          1750
      IJ=4                                                               1760
      KJ=5                                                               1770
      GO TO 22                                                           1780
   21 ST=FT                                                              1790
    2 CONTINUE                                                           1800
   25 CONTINUE                                                           1810
      RETURN                                                             1820
      END                                                                1830
```

```
      SUBROUTINE TAB(XT,XK,LG,DSJ,XABCJ,DJK)                              10
      DIMENSION XXK(20),XXT(33),XJ(660)                                   20
      DIMENSION T01(20),T02(20),T03(20),T04(20),T05(20),T06(20),T07(20),  30
     1T08(20),T09(20),T10(20),T11(20),T12(20),T13(20),T14(20),T15(20),    40
     2T16(20),T17(20),T18(20),T19(20),T20(20),T21(20),T22(20),T23(20),    50
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2T24(20),T25(20),T26(20),T27(20),T28(20),T29(20),T30(20),T31(20),
4T32(20),T33(20)
 EQUIVALENCE (XXK(1),R),(XXT(1),T),(XJ(1),L),
1            (A,C,Y),(B,D,Y1,W0),(T2,Y5,P,EAXG,XKC5,XXXK),
2(T4,Y6,XKO6,J),(DK,R1),(XK1,SJ0),(XK2,SJ1),(DKA,R1,V1),(DKB,R2,V2)
3,(DKC,R3,V3),(SV,N),(AB1,TD,M),(BB2,AXG),(SY1,XXXT,S1),
4(XKO2,XJA2,S2),(SXM,XKC3,XJA3,S3),(XKO4,XJB1),(R1K,XJB2),
5(R2K,XJB3),(R3K,XJC1),(BETA,XJC3),(K,SG,SJ3),(Y2,ZZK,XJ1),(Y3,
6WG),(XJ3,Y4),          (SY,I),(XJC2,SJ2),(XJA1,SJ4)
 EQUIVALENCE (XJ(1),TO1(1)),(XJ(21),TO2(1)),(XJ(41),TO3(1)),
1(XJ(61),TO4(1)),(XJ(81),TO5(1)),(XJ(101),TO6(1)),(XJ(121),TO7(1)),
2(XJ(141),TO8(1)),(XJ(161),TO9(1)),(XJ(181),T10(1)),(XJ(201),T11(1)
3),(XJ(221),T12(1)),(XJ(241),T13(1)),(XJ(261),T14(1)),(XJ(281),T15(
41)),(XJ(301),T16(1)),(XJ(321),T17(1)),(XJ(341),T18(1)),(XJ(361),T1
59(1)),(XJ(381),T20(1)),(XJ(401),T21(1)),(XJ(421),T22(1)),
6(XJ(441),T23(1)),(XJ(461),T24(1)),(XJ(481),T25(1)),(XJ(501),T26(1)
7),(XJ(521),T27(1)),(XJ(541),T28(1)),(XJ(561),T29(1)),(XJ(581),T30(
81)),(XJ(601),T31(1)),(XJ(621),T32(1)),(XJ(641),T33(1))
 DATA XXK/ 5.2, 5.6, 6.0, 6.4, 6.8, 7.2, 7.6, 8.0, 8.4, 8.8, 9.2,
X 9.6,10.0,10.4,10.8,11.2,11.6,12.0,12.4,12.8/
 DATA XXT/0.01,0.02,0.03,0.04,0.05,0.06,0.07,0.08,0.09,0.10,0.11,
X0.12,0.13,0.14,0.15,0.16,0.17,0.18,0.19,0.20,0.26,0.32,0.38,0.44,
X0.50,0.56,0.62,0.68,0.74,0.80,0.86,0.92,0.98/
 DATA T01/348.3270,329.0620,309.3460,289.0880,268.2430,246.8240,
X224.91800,202.69300,180.40300,158.38700,137.04200,116.78800,
X 98.01930, 81.05280, 66.09140, 53.20820, 42.35590, 33.39130,
X 26.11050, 20.28100/
 DATA T02/205.0000,194.1000,183.5000,173.0000,162.5000,151.9000,
X141.20000,130.20000,119.10000,107.80000, 96.43000, 85.17000,
X 74.17000, 63.64000, 53.78000, 44.78000, 36.74000, 29.75000,
X 23.80000, 18.85000/
 DATA T03/154.4000,145.3000,136.9000,128.9000,121.2000,113.7000,
X106.30000, 98.80000, 91.28000, 83.67000, 75.99000, 68.28000,
X 60.61000, 53.09000, 45.83000, 38.98000, 32.65000, 26.95000,
X 21.95000, 17.65000/
 DATA T04/129.5430,120.8780,113.1000,105.9960, 98.3851, 93.1199,
X 87.07990, 81.16910, 75.31440, 69.46550, 63.59470, 57.69990,
X 51.80430, 45.95800, 40.23460, 34.72510, 29.52760, 24.73430,
X 20.41850, 16.62540/
 DATA T05/115.3000,106.6000, 99.0000, 92.2100, 86.0500, 80.3700,
X 75.03000, 69.93300, 64.97000, 60.10000, 55.26000, 50.43000,
X 45.60000, 40.81000, 36.08000, 31.47000, 27.06000, 22.93000,
X 19.14000, 15.75000/
 DATA T06/106.4000, 97.5700, 89.9000, 83.1800, 77.2000, 71.8000,
X 66.84000, 62.19000, 57.76000, 53.47000, 49.27000, 45.13000,
X 41.00000, 36.91000, 32.86000, 28.89000, 25.06000, 21.43000,
X 18.05000, 14.98000/
 DATA T07/100.5080, 91.4730, 83.6906, 76.9337, 71.0030, 65.7266,
X 60.95750, 56.57200, 52.46730, 48.56010, 44.78500, 41.09360,
X 37.45480, 33.85470, 30.29690, 26.80240, 23.40750, 20.15950,
X 17.11060, 14.31030/
 DATA T08/ 96.4200, 87.1900, 79.2700, 72.4300, 66.4800, 61.2400,
X 56.58000, 52.35000, 48.45000, 44.79000, 41.30000, 37.93000,
X 34.64000, 31.40000, 28.21000, 25.07000, 22.02000, 19.08000,
X 16.29000, 13.72000/
 DATA T09/ 93.4900, 84.0900, 76.0200, 69.0800, 63.0800, 57.8400,
X 53.22000, 49.07000, 45.30000, 41.82000, 38.53000, 35.39000,
X 32.36000, 29.39000, 26.48000, 23.62000, 20.83000, 18.14000,
X 15.58000, 13.19000/
 DATA T10/ 91.3415, 81.7729, 73.5745, 66.5357, 60.4667, 55.1985,
X 50.58150, 46.48530, 42.79780, 39.42410, 36.28530, 33.31770,
X 30.47200, 27.71280, 25.01900, 22.38310, 19.81150, 17.32270,
X 14.94500, 12.71180/
 DATA T11/ 89.7100, 80.0100, 71.6900, 64.5600, 58.4200, 53.1100,
X 48.48000, 44.40000, 40.76000, 37.47000, 34.43000, 31.59000,
X 28.89000, 26.30000, 23.78000, 21.32000, 18.92000, 16.60000,
X 14.38000, 12.28000/
 DATA T12/ 88.4600, 78.6400, 70.2200, 62.9900, 56.7800, 51.4200,
X 46.77000, 42.70000, 39.09000, 35.84000, 32.88000, 30.14000,
X 27.55000, 25.09000, 22.70000, 20.39000, 18.14000, 15.97000,
X 13.88000, 11.90000/
 DATA T13/ 87.4785, 77.5623, 69.0480, 61.7399, 55.4611, 50.0523,
X 45.37000, 41.28650, 37.68900, 34.47960, 31.57410, 28.90220,
X 26.40610, 24.04060, 21.77230, 19.58010, 17.45450, 15.39730,
X 13.42070, 11.54430/
 DATA T14/ 86.7000, 76.7000, 68.1000, 60.7200, 54.3800, 48.9200,
X 44.21000, 40.11000, 36.51000, 33.32000, 30.46000, 27.84000,
X 25.41000, 23.13000, 20.96000, 18.86000, 16.84000, 14.89000,
X 13.01000, 11.22000/
 DATA T15/ 86.0600, 75.9900, 67.3300, 59.8900, 53.4900, 47.9800,
X 43.23000, 39.11000, 35.51000, 32.34000, 29.49000, 26.92000,
X 24.55000, 22.33000, 20.24000, 18.23000, 16.29000, 14.43000,
X 12.64000, 10.93000/
 DATA T16/ 85.5500, 75.4200, 66.6900, 59.1900, 52.7400, 47.1900,
X 42.41000, 38.26000, 34.66000, 31.48000, 28.66000, 26.12000,
X 23.79000, 21.63000, 19.60000, 17.66000, 15.80000, 14.01000,
X 12.29000, 10.66000/
 DATA T17/ 85.1184, 74.9383, 66.1636, 58.6102, 52.1123, 46.5214,
X 41.70360, 37.53840, 33.91760, 30.74480, 27.93540, 25.41610,
X 23.12450, 21.00880, 19.02780, 17.15060, 15.35620, 13.63380,
X 11.98190, 10.40740/
 DATA T18/ 84.7600, 74.5400, 65.7200, 58.1200, 51.5800, 45.9500,
X 41.10000, 36.91000, 33.28000, 30.10000, 27.30000, 24.80000,
X 22.53000, 20.45000, 18.52000, 16.69000, 14.95000, 13.29000,
X 11.70000, 10.18000/
 DATA T19/ 84.4600, 74.2000, 65.3400, 57.7000, 51.1200, 45.4600,
X 40.58000, 36.37000, 32.72000, 29.53000, 26.73000, 24.25000,
X 22.00000, 19.96000, 18.06000, 16.28000, 14.59000, 12.97000,
X 11.43000,  9.96300/
 DATA T20/ 84.2023, 73.9074, 65.0142, 57.3417, 50.7292, 45.0336,
X 40.12650, 35.89180, 32.22580, 29.03470, 26.23560, 23.75540,
X 21.53060, 19.50740, 17.64160, 15.89810, 14.25100, 12.68360,
X 11.18790,  9.76410/
 DATA T21/ 83.2433, 72.8209, 63.7912, 55.9766, 49.2205, 43.3851,
X 38.34820, 34.00070, 30.24480, 26.99280, 24.16570, 21.69310,
X 19.51260, 17.56960, 15.81730, 14.21660, 12.73650, 11.35310,
X 10.05070,  8.82059/
 DATA T22/ 82.7808, 72.2943, 63.1948, 55.3048, 48.4693, 42.5527,
X 37.43530, 33.01150, 29.18750, 25.87920, 23.01150, 20.51690,
X 18.33520, 16.41300, 14.70340, 13.16620, 11.76780, 10.48140,
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     X  9.28662,  8.16990/                                                  1160
      DATA T23/ 82.5236, 72.0012, 62.8617, 54.9281, 48.0456, 42.0794,       1170
     X 36.91100, 32.43670, 28.56450, 25.21300, 22.30950, 19.78900,          1180
     X 17.59340, 15.67080, 13.97510, 12.46640, 11.11010,  9.87782,          1190
     X  8.74691,  7.70062/                                                  1200
      DATA T24/ 82.3662, 71.8216, 62.6574, 54.6965, 47.7842, 41.7860,       1210
     X 36.58420, 32.07560, 28.16950, 24.78600, 21.85410, 19.31000,          1220
     X 17.09880, 15.16850, 13.47470, 11.97790, 10.64360,  9.44274,          1230
     X  8.35127,  7.35063/                                                  1240
      DATA T25/ 82.2628, 71.7037, 62.5233, 54.5442, 47.6121, 41.5923,       1250
     X 36.36750, 31.83500, 27.90470, 24.49750, 21.54360, 18.98080,          1260
     X 16.75420, 14.81430, 13.11730, 11.62440, 10.30150,  9.11911,          1270
     X  8.05277,  7.08266/                                                  1280
      DATA T26/ 82.1914, 71.6222, 62.4304, 54.4388, 47.4928, 41.4579,       1290
     X 36.21670, 31.66690, 27.71890, 24.29400, 21.32300, 18.74490,          1300
     X 16.50530, 14.55600, 12.85400, 11.36100, 10.04260,  8.87225,          1310
     X  7.82223,  6.87307/                                                  1320
      DATA T27/ 82.1399, 71.5634, 62.3636, 54.3629, 47.4068, 41.3608,       1330
     X 36.10770, 31.54510, 27.58380, 24.14540, 21.16120, 18.57060,          1340
     X 16.32020, 14.36230, 12.65480, 11.16000,  9.84471,  8.67993,          1350
     X  7.64071,  6.70620/                                                  1360
      DATA T28/ 82.1016, 71.5197, 62.3138, 54.3063, 47.3427, 41.2885,       1370
     X 36.02630, 31.45410, 27.48250, 24.03370, 21.03500, 18.43850,          1380
     X 16.17910, 14.21370, 12.50080, 11.00330,  9.68843,  8.52743,          1390
     X  7.49539,  6.57129/                                                  1400
      DATA T29/ 82.0723, 71.4863, 62.2758, 54.2631, 47.2937, 41.2331,       1410
     X 35.96400, 31.38430, 27.40480, 23.94770, 20.94470, 18.33610,          1420
     X 16.06920, 14.09740, 12.37950, 10.87900,  9.56256,  8.40460,          1430
     X  7.37737,  6.46077/                                                  1440
      DATA T30/ 82.0494, 71.4602, 62.2461, 54.2293, 47.2554, 41.1898,       1450
     X 35.91530, 31.32960, 27.34380, 23.88010, 20.87040, 18.25520,          1460
     X 15.98200, 14.00470, 12.28240, 10.77890,  9.46232,  8.30433,          1470
     X  7.28033,  6.36920/                                                  1480
      DATA T31/ 82.0311, 71.4394, 62.2224, 54.2024, 47.2249, 41.1553,       1490
     X 35.87640, 31.28600, 27.29510, 23.82600, 20.81080, 18.19010,          1500
     X 15.91170, 13.92970, 12.20340, 10.69720,  9.37921,  8.22151,          1510
     X  7.19965,  6.29253/                                                  1520
      DATA T32/ 82.0164, 71.4226, 62.2032, 54.1806, 47.2002, 41.1274,       1530
     X 35.84490, 31.25060, 27.25560, 23.78210, 20.76240, 18.13710,          1540
     X 15.85430, 13.86820, 12.13850, 10.62960,  9.31019,  8.15236,          1550
     X  7.13192,  6.22775/                                                  1560
      DATA T33/ 82.0042, 71.4088, 62.1875, 54.1628, 47.1800, 41.1045,       1570
     X 35.81900, 31.22160, 27.22310, 23.74590, 20.72250, 18.09340,          1580
     X 15.80680, 13.81720, 12.08440, 10.57320,  9.25227,  8.09408,          1590
     X  7.07449,  6.17256/                                                  1600
      N=20                                                                  1610
      M=33                                                                  1620
      DO 1 IB=1,N                                                           1630
      I=IB                                                                  1640
      IF(XK-XXK(IB))2,3,1                                                   1650
    1 CONTINUE                                                              1660
    3 IF(I-2)9,33,23                                                        1670
   23 IF(I-N+1)33,33,9                                                      1680
   33 XXXK=XK                                                               1690
      GO TO 12                                                              1700
      2 IF(I-2)9, 5,24                                                      1710
     24 IF(I-N+1)32,32,9                                                    1720
     32 A=ABS (XK-XXK(I))                                                   1730
        B=XK-XXK(I-1)                                                       1740
        IF(B-A)4,4,5                                                        1750
      4 XXXK=XXK(I-1)                                                       1760
        I=I-1                                                               1770
        GO TO 12                                                            1780
      5 XXXK=XXK(I)                                                         1790
     12 IF(XT-XXT(M-1))499,499,9                                            1800
    499 DO 6 JB=1,M                                                         1810
        J=JB                                                                1820
        IF(XT-XXT(JB))7,8,6                                                 1830
      6 CONTINUE                                                            1840
      8 IF(J-2)9,18,28                                                      1850
     28 IF(J-M+1)18,18,9                                                    1860
     18 XXXT=XT                                                             1870
        GO TO 13                                                            1880
      7 IF(J-2)9,11,29                                                      1890
     29 IF(J-M+1)17,17,9                                                    1900
     17 C=ABS (XT-XXT(J))                                                   1910
        D=XT-XXT(J-1)                                                       1920
        IF(D-C)10,10,11                                                     1930
     10 XXXT=XXT(J-1)                                                       1940
        J=J-1                                                               1950
        GO TO 13                                                            1960
     11 XXXT=XXT(J)                                                         1970
     13 K=(J-1)*N+I                                                         1980
        XJB2=XJ(K)                                                          1990
        XJA2=XJ(K-1)                                                        2000
        XJC2=XJ(K+1)                                                        2010
        K=K-N                                                               2020
        XJB1=XJ(K)                                                          2030
        XJA1=XJ(K-1)                                                        2040
        XJC1=XJ(K+1)                                                        2050
        K=K+2*N                                                             2060
        XJB3=XJ(K)                                                          2070
        XJA3=XJ(K-1)                                                        2080
        XJC3=XJ(K+1)                                                        2090
        DK=XXXK-XXK(I-1)                                                    2100
        AB1=XXT(J+1)-XXXT                                                   2110
        AB2=XXXT-XXT(J-1)                                                   2120
        AB1=AB1/AB2                                                         2130
        IF(LG-2)157,800,157                                                 2140
    157 IF(XK-XXXK)159,159,70                                               2150
    159 XK1=(XXXK-XK)/DK                                                    2160
        XK2=(XK-XXK(I-1))/DK                                                2170
        XJ1=XK1*XJA1+XK2*XJB1                                               2180
        XJ2=XK1*XJA2+XK2*XJB2                                               2190
        XJ3=XK1*XJA3+XK2*XJB3                                               2200
        GO TO 71                                                            2210
     70 XK1=(XXK(I+1)-XK)/DK                                                2220
        XK2=(XK-XXXK)/DK                                                    2230
        XJ1=XK1*XJB1+XK2*XJC1                                               2240
        XJ2=XK1*XJB2+XK2*XJC2                                               2250
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      XJ3=XK1*XJB3+XK2*XJC3                                                    2260
   71 DSJ=(AB1+1.)/(AB1*(XT-XXT(J-1))/(XJ3-XJ2)+(XT-XXT(J+1))/(XJ1-XJ2))      2270
      IF(LG)222,111,222                                                        2280
  222 XABCJ=XJ2+(XT-XXXT)*DSJ                                                  2290
      IF(LG)800,800,221                                                        2300
  221 IF(LG-1)111,111,800                                                      2310
  800 XK1=XT-XXT(J-1)                                                          2320
      XK2=XT-XXT(J+1)                                                          2330
      XJ1=AB1/(AB1+1.)                                                         2340
      DKA=XJ1*(XK1/(XJA3-XJA2)+XK2/(XJA1-XJA2))                                2350
      DKB=XJ1*(XK1/(XJB3-XJB2)+XK2/(XJB1-XJB2))                                2360
      DKC=XJ1*(XK1/(XJC3-XJC2)+XK2/(XJC1-XJC2))                                2370
      XK1=XT-XXXT                                                              2380
      XJ1=XJA2+XK1/DKA                                                         2390
      XJ2=XJB2+XK1/DKB                                                         2400
      XJ3=XJC2+XK1/DKC                                                         2410
      DJK=(0.5*(XJ3-XJ1)+(XK-XXXK)/DK*(XJ3-2.*XJ2+XJ1))/DK                     2420
      GO TO 111                                                                2430
    9 AXG=XT*XT                                                                2440
      IF(LG)19,1119,19                                                         2450
   19 IF(XT-6.)1119,2229,2229                                                  2460
 1119 TD=1./AXG                                                               2470
      EAXG=EXP (0.25*AXG)                                                      2480
      XA=XT*0.8862269*(1.-ERF (0.5*XT))*EAXG                                   2490
      XM=1.253314*XT*(1.-ERF(7.071067E-1*XT))*EAXG*EAXG                        2500
      XKC4=SQRT (XA)                                                           2510
      WG=SQRT (((1.+2.*TD)*XA-1.)/(8.*XA*TD*TD))                               2520
      BETA=2.**XK*1.E-5                                                        2530
      Y=XA/BETA                                                                2540
C     WRITE(6,7000) XA,XM,XKC4,BETA,Y                                          2550
 7000 FORMAT(' XA=',G16.8,'XM=',G16.8,'XKC4=',G16.8,                           2560
     1'BETA=',G16.8,'Y=',G16.8)                                               2570
      IF(LG)995,995,50                                                         2580
   50 IF(LG-1)995,700,995                                                      2590
  995 SV=2.*TD                                                                 2600
      T2=1./SV                                                                 2610
      T4=T2*T2                                                                 2620
      SXA=(-T4-T2)*XA+T4                                                       2630
      SXM=((-2.)*T4-T2)*XM+2.*T4                                               2640
      DK=SV*XA                                                                 2650
      SG=(0.5*TD*DK*(SXA+2.*XA+SV*SXA)-((1.+SV)*XA-1.)*(DK+TD*TD*SXA))/        2660
     1(SV*DK*DK*TD)                                                            2670
      XKC1=SXA*0.5/XKC4                                                        2680
      XKC2=(XA*SXM-SXA*XM)/(XA*XA)                                             2690
      XKC3=(SXA*WG-XA*SG*0.5/WG)/(WG*WG)                                       2700
      R1=(-17.)*XKC1-16.*XKC2+XKC3                                             2710
      R2=5.3333333*(8.*XKC1+11.*XKC2-XKC3)                                     2720
      R3=5.3333333*((-5.)*XKC1-8.*XKC2+XKC3)                                   2730
      XKC5=XM/XA                                                               2740
      XKC6=XA/WG                                                               2750
      R1K=32.-17.*XKC4-16.*XKC5+XKC6                                           2760
      R2K=5.3333333*(-18.+8.*XKC4+11.*XKC5-XKC6)                               2770
      R3K=5.3333333*(12.-5.*XKC4-8.*XKC5+XKC6)                                 2780
      SY=SXA/BETA                                                              2790
      IF(Y-0.3)900,25,25                                                       2800

   25 SV=1./(1.+Y)                                                             2810
      XJC=SQRT (SV)                                                            2820
      Y1=1./Y                                                                  2830
      XJ1=(1.-XJ0)*Y1                                                          2840
      XJ2=(0.5-XJ1)*Y1                                                         2850
      XJ3=(0.375-XJ2)*Y1                                                       2860
      XJ4=(0.3125-XJ3)*Y1                                                      2870
      SJ0=SY*XJ0*SV*(-0.5)                                                     2880
      SY1=SY*Y1                                                                2890
      SJ1=(-SJ0)*Y1-XJ1*SY1                                                    2900
      SJ2=(-SJ1)*Y1-XJ2*SY1                                                    2910
      SJ3=(-SJ2)*Y1-XJ3*SY1                                                    2920
      SJ4=(-SJ3)*Y1-XJ4*SY1                                                    2930
      GO TO 1000                                                               2940
  900 XJ5=((((((((((0.1444644*Y-0.1494459)*Y+0.1549810)*Y-0.1611802)*Y         2950
     1+0.1681880)*Y-0.1761970)*Y+0.1854705)*Y-0.1963806)*Y+0.2094726)*Y        2960
     2-0.2255859)*Y+0.2460937                                                  2970
      XJ4=0.2734375-Y*XJ5                                                      2980
      XJ3=0.3125-Y*XJ4                                                         2990
      XJ2=0.375-Y*XJ3                                                          3000
      XJ1=0.5-Y*XJ2                                                            3010
      XJ0=1.-Y*XJ1                                                             3020
      SJ5=((((((((((1.444644*Y-1.3450131)*Y+1.239848)*Y-1.1282614)*Y           3030
     1+1.009128)*Y-0.880985)*Y+0.741882)*Y-0.5891418)*Y+0.4189452)*Y-          3040
     20.2255859)*SY                                                            3050
      SJ4=-(SY*XJ5+Y*SJ5)                                                      3060
      SJ3=-(SY*XJ4+Y*SJ4)                                                      3070
      SJ2=-(SY*XJ3+Y*SJ3)                                                      3080
      SJ1=-(SY*XJ2+Y*SJ2)                                                      3090
      SJ0=-(SY*XJ1+Y*SJ1)                                                      3100
 1000 DSJ=(-3.1415926)/(BETA*AXG  *XT)*(XKC1*XJ0+R1*(-XJ1+2.*XJ2)+XKC4        3110
     1*SJ0+R1K*(-SJ1+2.*SJ2)+R2*((-3.)*XJ2+4.*XJ3)+R2K*((-3.)*SJ2+4.*         3120
     2SJ3)+R3*((-5.)*XJ3+6.*XJ4)+R3K*((-5.)*SJ3+6.*SJ4))                      3130
      IF(LG)60,111,49                                                          3140
   49 IF(LG-1)111,111,60                                                       3150
   60 IF(XT-6.)700,220,220                                                     3160
  700 ZZK=XM/XA                                                                3170
      S1=1.-XKC4                                                               3180
      S2=4.-2.*XKC4-2.*ZZK                                                     3190
      S3=1.+0.08333333*(XA/WG-5.*XKC4-8.*ZZK)                                  3200
C     WRITE(6,7001) ZZK,S1,S2,S3                                               3210
 7001 FORMAT(' ZZK=',G16.8,'S1=',G16.8,'S2=',G16.8,'S3=',G16.8)                3220
 6669 RI=1.+Y                                                                 3230
      V0=1./SQRT (RI)                                                          3240
      Y2=Y*Y                                                                   3250
      Y3=Y2*Y                                                                  3260
      Y4=Y2*Y2                                                                 3270
      IF(Y-0.2)55,66,66                                                        3280
   55 V1=(-Y+8.)*Y/(16.*RI)                                                    3290
      IF(Y.GE.1.E-10) V1=V1+(Y3*Y3-16.*Y2*Y3+64.*Y4)/(4096.*((Y+2.)*Y+1.       3300
     1))                                                                       3310
C     WRITE(6,7002) V1                                                         3320
 7002 FORMAT(' V1=',G16.8)                                                     3330
      GO TO 77                                                                 3340
   66 V1=(8.-((-Y+4.)*Y+8.)*V0)/Y2                                             3350
```

```
   77 IF(Y-2.)88,99,99                                                  3360
   88 SV=RI*RI                                                          3370
      Y5=2.+Y                                                           3380
      Y6=Y5*Y5*Y5                                                       3390
      V2=Y/(2.*Y5*RI)-Y3*Y2/(128.*Y6*SV)                                3400
      P=(3.*Y+16.)*Y+16.                                                3410
      V3=3.*Y2/(RI*P)                                                   3420
C     WRITE(6,7005) V3                                                  3430
 7005 FORMAT('VV=',G16.8)                                               3440
      IF(Y4.LT.1.E-30) GO TO 44                                         3450
      V3=V3          -3.*Y4*Y4/(16.*SV*P*P*P)                           3460
C     WRITE(6,7003) V3                                                  3470
 7003 FORMAT('V3=',G16.8)                                               3480
      GO TO 44                                                          3490
   99 V2=(-8.-4.*Y+((Y+8.)*Y+8.)*V0)*4./Y3                              3500
      V3=(((-6.)*Y-32.)*Y-32.+(((Y+18.)*Y+48.)*Y+32.)*VC)*12./Y4        3510
   44 XABCJ=(V0-S1*V1+S2*V2+S3*V3)*1.5707963/BETA                       3520
      IF(LG)220,111,1111                                                3530
 1111 IF(LG-2)111,220,111                                               3540
  220 DJK=-0.69315*XABCJ-1.088797*Y/SXA*(XKC4*SJ0+R1K*(-SJ1+2.*SJ2)     3550
     1+R2K*(-3.*SJ2+4.*SJ3)+R3K*(-5.*SJ3+6.*SJ4))                       3560
      GO TO 111                                                         3570
 2229 BETA=2.**XK*1.E-5                                                 3580
      XABCJ=1.5707963/(BETA*SQRT (1.+1./BETA-6./AXG))                   3590
      IF(LG)1119,111,34                                                 3600
   34 IF(LG-1)111,111,1119                                              3610
  111 RETURN                                                            3620
      END                                                               3630
```

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      SUBROUTINE FSTRUK(MI,SIGO,NE,ENG,NFE,REFE,EFE,NENBER,ENBER,NWFUN,    10
     *CONWFU,EPSROM,DRINWA,ITEST,IZPUMS,ITUMS,ISPATE,MIBER,GIBER,MIBERP,   20
     *IIBER,CIBER,FFAKT,MABWF,ABWF,MABWFP,MXINT,XINT,MXINTP,               30
     *MABQ1,ABQ1,MABQ1P,MABQ2,ABQ2,MABC2P,MABQ3,ABQ3,MABC3P,               40
     *KMROM,AUXROM,KMROMP,RF,MRF,RFL,MRFP)                                 50
      LOGICAL*4 TEST1,TEST2,TEST3,LERMSG,LFAR(2,3),LFARA(2,3)              60
      REAL*8 MAT,RESULT,RF,RFL,RPHI,RABS,RELA,RTOT,RFISS,RELFL,            70
     * RPHIL,RABSL,RELAL,RTOTL,RFISSL,RELFLL                              80
      DIMENSION SIGO(1),ENG(1),REFE(1),EFE(1),FMAT(2),ENBER(1),NWFUN(1),   90
     *CONWFU(1),GIBER(1),IIBER(1),CIBER(1),FFAKT(MI,6),ABWF(MABWF,4),     100
     *XINT(1),ABQ1(MABC1,4),ABQ2(MABC2,4),ABQ3(MABQ3,4),AUXROM(1),        110
     *RF(MI,MRF),RFL(MI,MRF),FARIN(2,3,2),FARAN(2,3),IFUNAR(2,3),         120
     *ITTF(3),ITTFU(3)                                                    130
      EQUIVALENCE (MAT,EMAT(1))                                           140
      COMMON MAT,NR3(2),NOUTP,JA,NANF,NEND,KL                             150
      COMMON/CFSTRU/ TEST1,TEST2,TEST3,LERMSG,GLSCH,MAFTYP,NFTYP,ITYP,    160
     *ITYPFU,UGR,OGR,CONST,NR1(8),BSIGC                                   170
      COMMON/CFSDUR/ IDUR                                                 180
C     PROGRAMM KENNZIFFER 3.                                              190
C     BERECHNUNG VON RESONANZSELBSTABSCHIRMFAKTOREN VON                   200
C     PUNKTWEISE GEGEBENEN WIRKUNGSQUERSCHNITTEN.                         210
C     B E D E U T U N G   D E R   E I N G A B E G R O E S S E N .         220
C     MI        ZAHL DER SIGO-WERTE.                                      230
C     SIGO      SIGO(I),I=1,MI    SIGO-WERTE.                             240
C     NE        ZAHL DER GRUPPENGRENZEN.                                  250
C     ENG       ENG(I),I=1,NE     GRUPPENGRENZEN.                         260
C     NFE       ZAHL DER PUNKTE DES WICHTUNGSSPEKTRUMS.                   270
C               NFE<=1 SPEKTRUM  N I C H T  PUNKTWEISE GEGEBEN.           280
C               NFE> 1 SPEKTRUM PUNKTWEISE GEGEBEN.                       290
C     REFE      REFE(I),I=1,NFE   ABSZISSENWERTE DES SPEKTRUMS.           300
C     EFE       EFE(I),I=1,NFE    ORDINATENWERTE DES SPEKTRUMS.           310
C     NENBER    ZAHL DER ENERGIEBEREICHE FUER DIE VERSCHIEDENEN SPEKTREN  320
C     ENBER(I-1) ... ENBER(I)  GUELTIGKEITSBEREICH DER ANZUWENDENDEN      330
C                              WICHTUNGSFUNKTION NWFUN(I).                340
C                              I LAEUFT VON 1 BIS NENBER.                 350
C                              DEFINITION: ENBER(0)=1.0E-5 .              360
C                              SONDERFALL: ENBER(1)=-1.0 GLEICH           370
C                                          GESAMTEN ENERGIEBEREICH.       380
C                              ES MUSS GELTEN:                            390
C                              1.0E-5 <= ENBER(I) <= 20.0E+6 .            400
C     NWFUN(I)  =NFTYP. TYP DER I-TEN WICHTUNGSFUNKTION, DIE ZUR ANWEN-   410
C                       DUNG KOMMT, SOWIE ART DER AUSZUFUEHRENDEN         420
C                       INTEGRATION. I=1,NENBER.                          430
C                       ( MOEGLICHE WERTE FUER NFTYP SIEHE UNTEN.)        440
C     CONWFU(I) NORMIERUNGSKONSTANTE DER FUNKTION IM I-TEN                450
C               WICHTUNGSBEREICH. I=1,NENBER.                             460
C     MOEGLICHE WERTE VON NFTYP.                                          470
C     NFTYP  <= 0   REIN NUMERISCHE INTEGRATION.                          480
C            > 0   ANALYTISCHE INTEGRATION.                               490
C     |NFTYP|   = 0   BELIEBIGE FUNKTION PHI.                            500
C                 1   PUNKTWEISE WICHTUNGSFUNKTION                        510
C                 2   CONWFU(I)/X                                         520
C     DIE FAELLE NFTYP<=-2 WERDEN WIE DER FALL NFTYP=0 BEHANDELT.         530
C     NFTYP=1 IST NUR DANN MOEGLICH, WENN NFE>1 IST.                      540
C     EPSROM   GENAUIGKEITSSCHRANKE FUER ROMBERGINTEGRATION.              550
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C      KMROM    2**(KMROM-1) GLEICH MAXIMALE INTERVALLZAHL FUER              560
C               ROMBERGINTEGRATION.                                          570
C      DRINWA   WARNUNGSAUSDRUCK IN NUMERISCHER INTEGRATION.                 580
C               AUSDRUCK ERFOLGT, WENN GEWUENSCHTER RELATIVER FEHLER         590
C               UM MEHR ALS DAS DRINWA-FACHE UEBERSCHRITTEN WIRD.            600
C      ITEST    STEUERUNG FUER AUSDRUCK DER MELDUNGEN.                       610
C           =0  NORMALER AUSDRUCK FUER PRODUKTIONSLAEUFE.                    620
C           UNGLEICH 0  ERWEITERTER AUSDRUCK FUER TESTLAEUFE.                630
C      F I L E S F E L D E R                                                 640
C      GIBER(I),I=1,NIBER    INTEGRATIONSBEREICHE INNERHALB EINER GRUPPE.    650
C      IIBER(I),I=1,NIBER    WICHTUNGSFUNKTION(EN) UND ART(EN) DER           660
C                            INTEGRATION INNERHALB EINER GRUPPE ( NWFUN).    670
C      CIBER(I),I=1,NIBER    NORMIERUNGSKONSTANTE(N) FUER DIE FUNKTION(EN)   680
C                            INNERHALB EINER GRUPPE ( CONWFU ) .             690
C      NIBER    MAXIMALER WERT FUER NIBER.                                   700
C      NIBERP   ZAHL DER ZUSAETZLICH BENOETIGTEN WORTE IN ALLEN MIT          710
C               NIBER DIMENSIONIERTEN FELDERN.                               720
C      ((FFAKT(I,J),I=1,MI),J=1,6)  F-FAKTOREN FUER EINE GRUPPE.             730
C      DAS FELD ABWF IST NUR FUER NFE>1 VON BEDEUTUNG.                       740
C      ABWF     FELD ZUR DARSTELLUNG DER PUNKTWEISEN WICHTUNGSFUNKTION       750
C               ALS GERADENSTUECKE.                                          760
C      ABWF(I,1)  ENERGIEWERT DES INTERVALLENDES ZU DEM DIE NACHFOLGENDEN    770
C                 A UND B WERTE GEHOEREN.                                    780
C      ABWF(I,2) UND ABWF(I,3)   A UND B WERT DES GERADENSTUECKES Y=AX+B.    790
C      ABWF(I,4)   SIEHE ELEMENT (I,4) WEITER UNTEN.                         800
C      MABWF    MAXIMALER WERT FUER I.                                       810
C      MABWFP   ZUSAETZLICH BENOETIGTE WORTE IN DEN MIT MABWF                820
C               DIMENSIONIERTEN FELDERN.                                     830
C      ACHTUNG: ABWF(I,2), ABWF(I,3) UND ABWF(I,4) SIND OHNE BEDEUTUNG.      840
C      XINT(I),I=1,NXINT  FELD ZUR ABSPEICHERUNG DER INTEGRATIONS            850
C         INTERVALLE INNERHALB EINES INTEGRATIONSBEREICHES.                  860
C      MXINT    MAXIMALES NXINT.                                             870
C      MXINTP   ZUSAETZLICH BENOETIGTE WORTE IN ALLEN MIT MXINT              880
C               DIMENSIONIERTEN FELDERN.                                     890
C      ABQ1     FELD ZUR DARSTELLUNG DES 1. QUERSCHNITTES ALS GERADENST.     900
C      ABQ2     FELD ZUR DARSTELLUNG DES 2. QUERSCHNITTES ALS GERADENST.     910
C      ABQ3     FELD ZUR DARSTELLUNG DES 3. QUERSCHNITTES ALS GERADENST.     920
C      FUER ABQ1, ABQ2 UND ABQ3 GILT:                                        930
C      ELEMENT (I,1)  ENERGIEWERT DES INTERVALLENDES ZU DEM DIE              940
C                     NACHFOLGENDEN WERTE A UND B GEHOEREN.                  950
C      ELEMENT (I,2)  A WERT DES GERADENSTUECKES Y=A*X+B.                    960
C      ELEMENT (I,3)  B WERT DES GERADENSTUECKES Y=A*X+B.                    970
C      ELEMENT (I,4)  =0:  A=B=0.                                           980
C                     <0:  NULLDURCHGANG IM INTERVALL.                      990
C                     >0:  KEIN NULLDURCHGANG UND A ODER B UNGLEICH 0.     1000
C      DIE ELEMENTE (I,2), (I,3) UND (I,4) SIND OHNE BEDEUTUNG.            1010
C      MABQ1    DIMENSION VON ABQ1.                                        1020
C      MABQ1P   ZAHL DER WORTE UM DEN MABQ1 VERGROESSERT WERDEN MUSS.      1030
C      MABQ2    DIMENSION VON ABQ2.                                        1040
C      MABQ2P   ZAHL DER WORTE UM DEN MABQ2 VERGROESSERT WERDEN MUSS.      1050
C      MABQ3    DIMENSION VON ABQ3.                                        1060
C      MABQ3P   ZAHL DER WORTE UM DIE MABQ3 VERGROESSERT WERDEN MUSS.      1070
C      AUXROM   HILFSFELD BEI ROMBERG-INTEGRATION.                         1080
C      KMROM    DIMENSION VON AUXROM.                                      1090
C      KMROMP   ZAHL DER WORTE UM DIE KMROM VERGROESSERT WERDEN MUSS.      1100
C      RF       HILFSFELD ZUR SPEICHERUNG DER SIGO-ABHAENGIGEN             1110
C               INTEGRALRESULTATE.                                         1120
C      ELEMENT  INTEGRAL VON                                               1130
C      RF(MI,1)  F(E)/(SGT+SIGO)                                           1140
C      RF(MI,2)  F(E)/((SGT+SIGO)**2)                                      1150
C      RF(MI,3)  F(E)*SGN*MUEL/(SGT+SIGO)                                  1160
C      RF(MI,4)  F(E)*SGT/((SGT+SIGO)**2)                                  1170

C      RF(MI,5)  F(E)*SGN*MUEL/((SGT+SIGO)**2)                             1180
C      RF(MI,6)  F(E)*SGA/(SGT+SIGO)                                       1190
C      RF(MI,7)  F(E)*SGN/(SGT+SIGO)                                       1200
C      RF(MI,8)  F(E)*SGF/(SGT+SIGO)   NUR FUER ISPATE=1 VORHANDEN         1210
C      RFL      LOKALE SPEICHERUNG DER RF-WERTE.                           1220
C      MRFP     NORMAL = 0 . =1 NUR DANN, WENN FESTGESTELLT WURDE,         1230
C               DASS MRF VERAENDERT WERDEN MUSS.                           1240
C      ITYPFU DIENT BEI ITYP=2 ODER ITYP=6 ZUR GENAUEREN SPEZIFIZIERUNG    1250
C      DER IM NENNER STEHENDEN ZU INTEGRIERENDEN FUNKTION ZUM ZWECKE       1260
C      BESSERER FEHLERAUSDRUCKE.                                           1270
C      ES BEDEUTET:                                                        1280
C      ITYPFU  BEDEUTUNG                                                   1290
C         0    KEINE BEDEUTUNG                                           1300
C         1    SGT                                                       1310
C         2    SGA                                                       1320
C         3    SGN                                                       1330
C         4    SGF                                                       1340
       GOTO 3                                                            1350
C      PUNKTEGITTER VON WICHTUNGSFUNKTION IN XINT BRINGEN.               1360
  100 CALL FSXIIN(NXINT,MXINT,XINT,UGR,OGR)                              1370
C      FUER |NFTYP| UNGLEICH 1 WIRD NICHTS WEITER GEMACHT, DA UGR UND OGR 1380
C      SCHON IN XINT STEHEN. FUER |NFTYP|=1 WIRD ABWF(,1) IN XINT         1390
C      EINGEFUEGT.                                                       1400
       IF(IABS(NFTYP).EQ.1) CALL FSXINT(NXINT,MXINT,XINT,MXINTP,         1410
      *NABWF,ABWF,MABWF,4,8445)                                          1420
       GOTO LABXIN,(13,21,27,31,37)                                      1430
C      INTEGRALBERECHNUNG                                                1440
  101 CALL FSGRAL(RESULT,NXINT,XINT,                                     1450
      *        NABWF,ABWF,MABWF,                                         1460
      *        NABQ1,ABQ1,MABQ1,NABQ2,ABQ2,MABQ2,NABQ3,ABQ3,MABQ3,       1470
      *        KMROM,AUXROM,KMROMP,EPSROM,DRINWA,                        1480
      *        IFAR,LFAR,LFARA,FARIN,FARAN,IFUNAR,8445,8446)             1490
       GOTO LABGRA,(14,16,18,22,24,25,26,28,29,32,34,35,38,39)           1500
  102 DO 5 K=1,3                                                         1510
       LFAR(1,K)=.FALSE.                                                 1520
       LFAR(2,K)=.FALSE.                                                 1530
       LFARA(1,K)=.FALSE.                                                1540
    5  LFARA(2,K)=.FALSE.                                                1550
       GOTO LABFEL,(41,42,43,44,45)                                      1560
  103 K=1                                                                1570
    8  IF(.NOT.LFARA(K,IFAR)) GOTO 6                                     1580
       LFAR(K,IFAR)=.FALSE.                                              1590
       LFARA(K,IFAR)=.FALSE.                                             1600
       CALL FSWR04(1008,ITTF(IFAR),ITTFU(IFAR),FARAN(K,IFAR),BSIGO)      1610
       CALL FSWR02(-2005,FARIN(K,IFAR,1),FARIN(K,IFAR,2))                1620
       IF(K.EQ.1) CALL FSWR02(-2007,IFUNAR(1,IFAR),ITTF(IFAR))           1630
       IF(K.EQ.2) CALL FSWR02(-2008,IFUNAR(2,IFAR),ITTF(IFAR))           1640
    6  IF(K.EQ.2) GOTO 7                                                 1650
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      K=2                                                                1660
      GOTO 8                                                             1670
    7 GOTO LABPRI,(17,50,51,23,30,52,33,40,60)                           1680
  104 DO 9 L=1,3                                                         1690
      IF(LFAR(1,L)) LFARA(1,L)=.TRUE.                                    1700
      IF(LFAR(2,L)) LFARA(2,L)=.TRUE.                                    1710
    9 CONTINUE                                                           1720
      ASSIGN 60 TO LABPRI                                                1730
      DO 60 IFAR=1,3                                                     1740
      IF(LFARA(1,IFAR).OR.LFARA(2,IFAR)) GOTO 103                        1750
   60 CONTINUE                                                           1760
      GOTO LABPEN,(53,54,55,56,36)                                       1770
    3 IF(IDUR.NE.0) GOTO 46                                              1780
      TEST1=.FALSE.                                                      1790
      TEST2=.FALSE.                                                      1800
      TEST3=.FALSE.                                                      1810
      LERMSG=.FALSE.                                                     1820
      IF(ITEST.LT.10) GOTO 4                                             1830
      LERMSG=.TRUE.                                                      1840
      ITEST=ITEST-10                                                     1850
    4 IF(ITEST.GE.1) TEST1=.TRUE.                                        1860
      IF(ITEST.GE.2) TEST2=.TRUE.                                        1870
      IF(ITEST.GE.3) TEST3=.TRUE.                                        1880
C     INITIALISIERUNG VON FEHLERARRAY.                                   1890
      CALL FSWR00(1)                                                     1900
C     NULLSETZEN VON ALLEN ERWEITERUNGSGROESSEN (.....P) .               1910
   46 MIBERP=0                                                           1920
      MABWFP=0                                                           1930
      MXINTP=0                                                           1940
      MABQ1P=0                                                           1950
      MABQ2P=0                                                           1960
      MABQ3P=0                                                           1970
      KMROMP=0                                                           1980
      MRFP=0                                                             1990
C     IDUR GIBT AM PROGRAMMENDE BZW. PROGRAMMANFANG DIE ZAHL DER         2000
C     GRUPPEN AN, FUER DIE BEREITS WERTE BERECHNET WURDEN.               2010
C     D.H. IDUR LIEGT ZWISCHEN 0 UND NANF-NEND. (GRUPPENZAHL-1)          2020
C     BEIM ERSTEN ANLAUF FUER EINE REIHE VON GRUPPEN IST IDUR=0.         2030
C     NACH ERFOLGREICHEM PROGRAMMENDE WIRD IDUR WIEDER GLEICH NULL       2040
C     GESETZT. DIES GILT AUCH FUER EINEN ABBRUCH DES PROGRAMMS, OHNE     2050
C     DASS EIN WEITERER ANLAUF MOEGLICH IST.                             2060
C     SCHREIBEN DER UEBERSCHRIFT.                                        2070
      IF(IDUR.EQ.0) WRITE(NOUTP,1000)                                    2080
 1000 FORMAT('1')                                                        2090
      IF(IDUR.EQ.0) CALL FSWR02(1001,EMAT(1),EMAT(2))                    2100
C     MAXIMALER BETRAG FUER NFTYP: MNFTYP                                2110
      MNFTYP=2                                                           2120
C     GLSCH  SCHRANKE FUER TOLERANZ VON ZWEI GLEITKOMMAZAHLEN.           2130
C            ( SIEHE LOGICAL FUNCTION FSTOLE )                           2140
      GLSCH=1.0E-6                                                       2150
C     1. GRUPPE FUER DIE BERECHNUNGEN ERFOLGEN.                          2160
      IGR=NANF-IDUR                                                      2170
C     PRUEFUNG UND AUSDRUCK EINIGER GROESSEN.                            2180
      CALL FSTRUO(NE,ENG,NANF,NEND,NFE,REFE,EFE,NENBER,ENBER,            2190
     *NWFUN,CONWFU,EPSROM,KMROM,DRINWA,ISPATE,MIBER,MABWF,MXINT,MABQ1,   2200
     *MABQ2,MABQ3,MRF,MRFP,&446,&445)                                    2210
C     SIND ALLE QUERSCHNITTSTYPEN VORHANDEN ?                            2220
      IF(IDUR.EQ.0) CALL FSTRU1(&446)                                    2230
C     LOOP FUER ALLE GRUPPEN                                             2240
    1 CONTINUE                                                           2250
C     EVENTUELLE UMSCHALTUNG VON TEST1, TEST2, TEST3 UND LERMSG.         2260
      IF(IZPUMS.LE.-1) GOTO 61                                           2270
      IF(IZPUMS.NE.IGR.OR.ITUMS.LT.0) GOTO 61                            2280
      IITUMS=ITUMS                                                       2290
      LERMSG=.FALSE.                                                     2300
      IF(IITUMS.LT.10) GOTO 62                                           2310
   63 IITUMS=IITUMS-10                                                   2320
      LERMSG=.TRUE.                                                      2330
   62 TEST1=.FALSE.                                                      2340
      TEST2=.FALSE.                                                      2350
      TEST3=.FALSE.                                                      2360
      IF(IITUMS.GE.1) TEST1=.TRUE.                                       2370
      IF(IITUMS.GE.2) TEST2=.TRUE.                                       2380
      IF(IITUMS.GE.3) TEST3=.TRUE.                                       2390
   61 CONTINUE                                                           2400
C     AUSDRUCK VON MATERIALNAME, GRUPPENNUMMER, GRUPPENGRENZEN,          2410
C     WICHTUNGSFUNKTIONSBEREICH(E), -TYP(EN) UND ART(EN) DER             2420
C     INTEGRATION.                                                       2430
C     VOR DEM AUSDRUCK DER LETZTEN DREI GROESSEN: BESTIMMUNG DER         2440
C     INTEGRATIONSBEREICHE INNERHALB EINER GRUPPE. GIBER(I), I=1,NIBER   2450
C     GIBER(1)=GRUPPENANFANG.  GIBER(NIBER)=GRUPPENENDE.                 2460
C     ES WERDEN AUCH IIBER(I),I=1,NIBER UND  CIBER(I),I=1,NIBER GESETZT. 2470
      CALL FSTRU2(IGR,NE,ENG,NIBER,MIBER,GIBER,MIBERP,IIBER,CIBER,       2480
     *NENBER,ENBER,NWFUN,CONWFU,&445)                                    2490
C     NULLSETZEN DER GRUPPENMITTELWERTE.                                 2500
C     (AN DIESE STELLE KANN GESPRUNGEN WERDEN, WENN DIE ZAHL DER         2510
C     INTEGRATIONSBEREICHE INNERHALB EINER GRUPPE ERWEITERT WURDE.)      2520
    2 CONTINUE                                                           2530
C     LOOP UEBER ALLE INTEGRATIONSBEREICHE                               2540
      RPHI=0.0                                                           2550
      RABS=0.0                                                           2560
      RELA=0.0                                                           2570
      RTOT=0.0                                                           2580
      RFISS=0.0                                                          2590
      RELFL=0.0                                                          2600
      RPHIL=0.0                                                          2610
      RABSL=0.0                                                          2620
      RFLAL=0.0                                                          2630
      RTOTL=0.0                                                          2640
      RFISSL=0.0                                                         2650
      RELFLL=0.0                                                         2660
      DO 19 I=1,MI                                                       2670
      DO 19 J=1,MRF                                                      2680
      RF(I,J)=0.0                                                        2690
   19 RFL(I,J)=0.0                                                       2700
      DO 10 IB=2,NIBER                                                   2710
      UGR=GIBER(IB-1)                                                    2720
      OGR=GIBER(IB)                                                      2730
      NFTYP=IIBER(IB)                                                    2740
      CONST=CIBER(IB)                                                    2750
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      IF(IABS(NFTYP).GT.MNFTYP.OR.UGR.GT.OGR) CALL FSWR03(3001,'FSTR',
     *'UK  ',1)
C     WENN |NFTYP|=1 MUESSEN A UND B FLER DAS PUNKTWEISE WICHTUNGS
C     SPEKTRUM BERECHNET WERDEN.
      IF(IABS(NFTYP).NE.1) GOTO 11
      CALL FSTRU3(NFE,REFF,EFE,NABWF,MABWF,ABWF,MABWFP,&445,&446)
   11 CONTINUE
      ASSIGN 13 TO LABXIN
      GOTO 100
C     I N T E G R A L   V O N   F(E)DE  VON UGR BIS OGR.
   13 ITYP=1
      ITYPFU=0
      ASSIGN 14 TO LABGRA
      GOTO 101
   14 RPHIL=RESULT
C     INTEGRAL VON SGA*PHI VON UGR BIS OGR
      CALL FSQUER('SGA     ',UGR,OGR,NABQ1,MABQ1,ABQ1,MABQ1P,&445,&446)
      CALL FSXINT(NXINT,MXINT,XINT,MXINTP,NABQ1,ABQ1,MABQ1,4,&445)
      ITYP=2
      ITYPFU=2
      ASSIGN 16 TO LABGRA
      GOTO 101
   16 RABSL=RESULT
C     INTEGRAL VON SGA*F(E)/(SGT+SIGO)    RF(MI,6)   ITYP=6  ITYPFU=2
      CALL FSQUER('SGT     ',UGR,OGR,NABQ3,MABQ3,ABQ3,MABQ3P,&445,&446)
      CALL FSXINT(NXINT,MXINT,XINT,MXINTP,NABQ3,ABQ3,MABQ3,4,&445)
      ITYP=6
      ITYPFU=2
      ITTF(1)=ITYP
      ITTFU(1)=ITYPFU
      ASSIGN 18 TO LABGRA
      IF(LERMSG) GOTO 41
      IFAR=1
      ASSIGN 41 TO LABFEL
      GOTO 102
   41 DO 17 I=1,MI
      BSIGO=SIGO(I)
      GOTO 101
   18 RFL(I,6)=RESULT
      IF(LERMSG) GOTO 17
      ASSIGN 17 TO LABPRI
      GOTO 103
   17 CONTINUE
      IF(LERMSG) GOTO 53
      ASSIGN 53 TO LABPEN
      GOTO 104
C     INTEGRALE VON
C     F(E)*SGT                          ITYP=2  ITYPFU=1
C     F(E)/(SGT+SIGO)          RF(MI,1) ITYP=4  ITYPFU=0
C     F(E)/((SGT+SIGO)**2)     RF(MI,2) ITYP=5  ITYPFU=0
C     F(E)*SGT/((SGT+SIGO)**2) RF(MI,4) ITYP=7  ITYPFU=0
C
   53 ASSIGN 21 TO LABXIN
      GOTO 100
   21 CALL FSTRU5(ABQ3,NABQ3,MABQ3,ABQ1,NABQ1,MABQ1,MABQ1P,&445)
      CALL FSXINT(NXINT,MXINT,XINT,MXINTP,NABQ1,ABQ1,MABQ1,4,&445)
      ITYP=2
      ITYPFU=1
      ASSIGN 22 TO LABGRA
      GOTO 101
   22 RTOTL=RESULT
      IF(LERMSG) GOTO 42
      ASSIGN 42 TO LABFEL
      GOTO 102
   42 DO 23 I=1,MI
      BSIGO=SIGO(I)
      ITYP=4
      ITYPFU=0
      ITTF(1)=ITYP
      ITTFU(1)=ITYPFU
      ASSIGN 24 TO LABGRA
      IFAR=1
      GOTO 101
   24 RFL(I,1)=RESULT
      IF(LERMSG) GOTO 50
      ASSIGN 50 TO LABPRI
      GOTO 103
   50 ITYP=5
      ITYPFU=0
      ITTF(2)=ITYP
      ITTFU(1)=ITYPFU
      ASSIGN 25 TO LABGRA
      IFAR=2
      GOTO 101
   25 RFL(I,2)=RESULT
      IF(LERMSG) GOTO 51
      ASSIGN 51 TO LABPRI
      GOTO 103
   51 ITYP=7
      ITYPFU=0
      ITTF(3)=ITYP
      ITTFU(3)=ITYPFU
      ASSIGN 26 TO LABGRA
      IFAR=3
      GOTO 101
   26 RFL(I,4)=RESULT
      IF(LERMSG) GOTO 23
      ASSIGN 23 TO LABPRI
      GOTO 103
   23 CONTINUE
      IF(LERMSG) GOTO 54
      ASSIGN 54 TO LABPEN
      GOTO 104
C     INTEGRAL VON F(E)*SGN   ITYP=2  ITYPFU=3
   54 ASSIGN 27 TO LABXIN
      GOTO 100
   27 CALL FSQUER('SGN     ',UGR,OGR,NABQ1,MABQ1,ABQ1,MABQ1P,&445,&446)
      CALL FSXINT(NXINT,MXINT,XINT,MXINTP,NABQ1,ABQ1,MABQ1,4,&445)
      ITYP=2
      ITYPFU=3
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      ASSIGN 28 TO LABGRA                                                    3860
      GOTO 101                                                               3870
   28 RELAL=RESULT                                                           3880
C     INTEGRAL VON F(E)*SGN/(SGT+SIGO)   RF(MI,7)   ITYP=6  ITYPFU=3         3890
      CALL FSXINT(NXINT,MXINT,XINT,MXINTP,NABQ3,ABQ3,MABQ3,4,&445)           3900
      ITYP=6                                                                 3910
      ITYPFU=3                                                               3920
      ITTF(1)=ITYP                                                           3930
      ITTFU(1)=ITYPFU                                                        3940
      ASSIGN 29 TO LABGRA                                                    3950
      IF(LERMSG) GOTO 43                                                     3960
      ASSIGN 43 TO LABFEL                                                    3970
      GOTO 102                                                               3980
   43 DO 30 I=1,MI                                                           3990
      BSIGO=SIGO(I)                                                          4000
      IFAR=1                                                                 4010
      GOTO 101                                                               4020
   29 RFL(I,7)=RESULT                                                        4030
      IF(LERMSG) GOTO 30                                                     4040
      ASSIGN 30 TO LABPRI                                                    4050
      GOTO 103                                                               4060
   30 CONTINUE                                                               4070
      IF(LERMSG) GOTO 55                                                     4080
      ASSIGN 55 TO LABPEN                                                    4090
      GOTO 104                                                               4100
C     INTEGRAL VON F(E)*SGN*MUEL   ITYP=3  ITYPFU=0                          4110
   55 ASSIGN 31 TO LABXIN                                                    4120
      GOTO 100                                                               4130
   31 CALL FSXINT(NXINT,MXINT,XINT,MXINTP,NABQ1,ABQ1,MABQ1,4,&445)           4140
      CALL FSQUER('MUEL    ',UGR,CGR,NABQ2,MABQ2,ABQ2,MABQ2P,&445,&446)      4150
      CALL FSXINT(NXINT,MXINT,XINT,MXINTP,NABQ2,ABQ2,MABQ2,4,&445)           4160
      ITYP=3                                                                 4170
      ITYPFU=0                                                               4180
      ASSIGN 32 TO LABGRA                                                    4190
      GOTO 101                                                               4200
   32 RELFLL=RESULT                                                          4210
C     INTEGRALE VON                                                          4220
C     F(E)*SGN*MUEL/(SGT+SIGO)        RF(MI,3)   ITYP=8  ITYPFU=0            4230
C     F(E)*SGN*MUEL/((SGT+SIGO)**2)   RF(MI,5)   ITYP=5  ITYPFL=0            4240
      CALL FSXINT(NXINT,MXINT,XINT,MXINTP,NABQ3,ABQ3,MABQ3,4,&445)           4250
      IF(LERMSG) GOTO 44                                                     4260
      ASSIGN 44 TO LABFEL                                                    4270
      GOTO 102                                                               4280
   44 DO 33 I=1,MI                                                           4290
      BSIGO=SIGO(I)                                                          4300
      ITYP=8                                                                 4310
      ITYPFU=0                                                               4320
      ITTF(1)=ITYP                                                           4330
      ITTFU(1)=ITYPFU                                                        4340
      ASSIGN 34 TO LABGRA                                                    4350
      IFAR=1                                                                 4360
      GOTO 101                                                               4370
   34 RFL(I,3)=RESULT                                                        4380
      IF(LERMSG) GOTO 52                                                     4390
      ASSIGN 52 TO LABPRI                                                    4400
      GOTO 103                                                               4410
   52 ITYP=9                                                                 4420
      ITYPFU=0                                                               4430
      ITTF(2)=ITYP                                                           4440
      ITTFU(2)=ITYPFU                                                        4450
      ASSIGN 35 TO LABGRA                                                    4460
      IFAR=2                                                                 4470
      GOTO 101                                                               4480
   35 RFL(I,5)=RESULT                                                        4490
      IF(LERMSG) GOTO 33                                                     4500
      ASSIGN 33 TO LABPRI                                                    4510
      GOTO 103                                                               4520
   33 CONTINUE                                                               4530
      IF(LERMSG) GOTO 56                                                     4540
      ASSIGN 56 TO LABPEN                                                    4550
      GOTO 104                                                               4560
C     NUR FUER ISPATE=1 BERECHNUNG VON SIGF UND FF.                          4570
   56 IF(ISPATE.NE.1) GOTO 36                                                4580
C     INTEGRAL VON F(E)*SGF   ITYP=2  ITYPFU=4                               4590
      ASSIGN 37 TO LABXIN                                                    4600
      GOTO 100                                                               4610
   37 CALL FSQUER('SGF     ',UGR,CGR,NABQ1,MABQ1,ABQ1,MABQIP,&445,&446)      4620
      CALL FSXINT(NXINT,MXINT,XINT,MXINTP,NABQ1,ABQ1,MABQ1,4,&445)           4630
      ITYP=2                                                                 4640
      ITYPFU=4                                                               4650
      ASSIGN 38 TO LABGRA                                                    4660
      GOTO 101                                                               4670
   38 RFISSL=RESULT                                                          4680
C     INTEGRAL VON F(E)*SGF/(SGT+SIGO)   RF(MI,8)   ITYP=6  ITYPFU=4         4690
      CALL FSXINT(NXINT,MXINT,XINT,MXINTP,NABQ3,ABQ3,MABQ3,4,&445)           4700
      ITYP=6                                                                 4710
      ITYPFU=4                                                               4720
      ITTF(1)=ITYP                                                           4730
      ITTFU(1)=ITYPFU                                                        4740
      ASSIGN 39 TO LABGRA                                                    4750
      IF(LERMSG) GOTO 45                                                     4760
      ASSIGN 45 TO LABFEL                                                    4770
      GOTO 102                                                               4780
   45 DO 40 I=1,MI                                                           4790
      BSIGO=SIGO(I)                                                          4800
      IFAR=1                                                                 4810
      GOTO 101                                                               4820
   39 RFL(I,8)=RESULT                                                        4830
      IF(LERMSG) GOTO 40                                                     4840
      ASSIGN 40 TO LABPRI                                                    4850
      GOTO 103                                                               4860
   40 CONTINUE                                                               4870
      IF(LERMSG) GOTO 36                                                     4880
      ASSIGN 36 TO LABPEN                                                    4890
      GOTO 104                                                               4900
   36 RFHI=RPHI+RPHIL                                                        4910
      RABS=RABS+RABSL                                                        4920
      RELA=RELA+RELAL                                                        4930
      RTOT=RTOT+RTOTL                                                        4940
      RFISS=RFISS+RFISSL                                                     4950
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      RELFL=RELFL+RELFLL                                                4960
      DO 20 I=1,MI                                                      4970
      DO 20 J=1,MRF                                                     4980
   20 RF(I,J)=RF(I,J)+RFL(I,J)                                          4990
   10 CONTINUE                                                          5000
      CALL FSTRU4(ENG,NE,IGR,FFAKT,MI,SIGO,RPHI,RABS,FELA,RTCT,RFISS,   5010
     *RELFL,RF,MRF,ISPATE)                                              5020
C     NAECHSTE GRUPPE                                                   5030
      IGR=IGR-1                                                         5040
      IF(IGR.GE.NEND) GOTO 1                                            5050
C     PROGRAMMENDE NACH ERFOLGREICHEM DURCHLAUF.                        5060
  444 KL=KL+1                                                           5070
      IDUR=0                                                            5080
      CALL FSWR01(1002,KL)                                              5090
C     UEBERSICHT UEBER DIE GEDRUCKTEN FEHLER- UND WARNUNGS              5100
C     MELDUNGEN.                                                        5110
      CALL FSWRS9                                                       5120
  333 RETURN                                                            5130
C     PROGRAMMENDE MIT ERNEUTEM PROGRAMMANLAUF MIT VERGROESSERTEM (N)   5140
C                                DATENFELD (ERN) .                      5150
  445 CALL FSWR00(1003)                                                 5160
      IF(MXINTP.EQ.0) MXINTP=MAX0(MXINT,MABQ1+MABQ1P,MABQ2+MABQ2P,MABQ3+ 5170
     *                        MABQ3P)-MXINT                             5180
      IDUR=NANF-IGR                                                     5190
      GOTO 333                                                          5200
C     ABBRUCH DES PROGRAMMS KENNZIFFER 3, DA DATEN ( PROGRAMMSTEUER     5210
C             KERNDATEN ODER SPEKTRUMSDATEN ) DIE DURCHFUEHRUNG         5220
C             DER RECHNUNG NICHT ZULIESSEN.                             5230
  446 CALL FSWR00(3002)                                                 5240
      IDUR=0                                                            5250
      KL=KL+1                                                           5260
      GOTO 333                                                          5270
      END                                                               5280
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      SUBROUTINE FSTRUC(NE,ENG,NANF,NEND,NFE,REFE,EFE,NENBER,            10
     *ENBER,NWFUN,CONWFU,EPSROM,KMROM,DRINWA,ISPATE,MIBER,MABWF,MXINT,   20
     *MABQ1,MABQ2,MABQ3,MRF,MRFP,*,*)                                    30
C     PRUEFUNG UND AUSDRUCK EINIGER GROESSEN.                            40
      DIMENSION ENG(1),ENBER(1),NWFUN(1),CONWFU(1),IH(3),RH1(3),RH2(3),  50
     *REFE(1),EFE(1),IARG2(4)                                            60
      LOGICAL*4 FEHLER,TEST1,TEST2,TEST3,LERMSG,FSTOLE,ORIFUN            70
      REAL*8 MAT,BEST,SGF,ARG3(5)                                        80
      DATA BEST,SGF/'BEST    ','SGF     '/                               90
      COMMON MAT,NR1(2),NC                                              100
      COMMON/CFSTRU/ TEST1,TEST2,TEST3,LERMSG,GLSCH,MATTYP,NFTYP        110
      COMMON/CFSDUR/IDUR                                                120
      COMMON/CFSMEL/ ORIFUN                                             130
      FEHLER=.FALSE.                                                    140
C     NE >= 1 ?                                                         150
      IF(NE.GE.1) GOTO 18                                               160
      FEHLER=.TRUE.                                                     170
      CALL FSWR06(3009,'NE  ','    ',NE,'.GE.','THAN',1)                180
C     NANF >= 1 ?                                                       190
   18 IF(NANF.GE.1) GOTO 19                                             200
      FEHLER=.TRUE.                                                     210
      CALL FSWR06(3009,'NANF','    ',NANF,'.GE.','THAN',1)              220
C     NEND >= 1 ?                                                       230
   19 IF(NEND.GE.1) GOTO 20                                             240
      FEHLER=.TRUE.                                                     250
      CALL FSWR06(3009,'NEND','    ',NEND,'.GE.','THAN',1)              260
C     NENBER >= 1 ?                                                     270
   20 IF(NENBER.GE.1) GOTO 21                                           280
      FEHLER=.TRUE.                                                     290
      CALL FSWR06(3009,'NENB','ER  ',NENBER,'.GE.','THAN',1)            300
   21 CONTINUE                                                          310
C     MIBER >= 5                                                        320
      IF(MIBER.GE.5) GOTO 43                                            330
      FEHLER=.TRUE.                                                     340
      CALL FSWR06(3009,'MIBE','R   ',MIBER,'.GE.','THAN',5)             350
   43 CONTINUE                                                          360
      IF(NFE.LE.1.OR.MABWF.GE.50) GOTO 44                               370
      FEHLER=.TRUE.                                                     380
      CALL FSWR06(3009,'MABW','F   ',MABWF,'.GE.','THAN',50)            390
   44 CONTINUE                                                          400
      IF(MXINT.GE.100) GOTO 45                                          410
      FEHLER=.TRUE.                                                     420
      CALL FSWR06(3009,'MXIN','T   ',MXINT,'.GE.','THAN',100)          430
   45 CONTINUE                                                          440
      IF(MABQ1.GE.100) GOTO 46                                          450
      FEHLER=.TRUE.                                                     460
      CALL FSWR06(3009,'MABQ','1   ',MABQ1,'.GE.','THAN',100)          470
   46 IF(MABQ2.GE.100) GOTO 47                                          480
      FEHLER=.TRUE.                                                     490
      CALL FSWR06(3009,'MABQ','2   ',MABQ2,'.GE.','THAN',100)          500
   47 IF(MABQ3.GE.100) GOTO 48                                          510
      FEHLER=.TRUE.                                                     520
      CALL FSWR06(3009,'MABQ','3   ',MABQ3,'.GE.','THAN',100)          530
   48 CONTINUE                                                          540
      IF(IDUR.NE.0) GOTO 3                                              550
C     SETZEN UND TEST VON ISPATE. IST SGF VORHANDEN, DANN MUSS ISPATE=1 560
C     SEIN. IST ES UNGLEICH 1, SO WIRD ES GLEICH 1 GESETZT.             570
C     IST SGF NICHT VORHANDEN, DANN MUSS ISPATE=0 SEIN.                 580
      IARG2(1)=3                                                        590
      ARG3(1)=MAT                                                       600
      ARG3(2)=BEST                                                      610
      ARG3(3)=SGF                                                       620
      IRC=0                                                             630
      CALL NDFLOC(IRC,IARG2,ARG3,ARG4,ARG5)                             640
      IF(IRC.EQ.1) GOTO 17                                              650
C     KEIN SGF VORHANDEN.                                               660
      IF(ISPATE.EQ.0) GOTO 3                                            670
      ISPATE=0                                                          680
      GOTO 3                                                            690
C     SGF VORHANDEN.                                                    700
   17 IF(ISPATE.EQ.1) GOTO 3                                            710
      ISPATE=1                                                          720
      GOTO 3                                                            730
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    3 CONTINUE                                                          740
C     TEST VON MRF. FUER ISPATE=0 MUSS ES 7, FUER ISPATE=1 MUSS         750
C                 ES 8 SEIN.                                            760
      IF((ISPATE.EQ.0.AND.MRF.NE.7).OR.(ISPATE.EQ.1.AND.MRF.NE.8))      770
     *GOTO 889                                                          780
C     TEST VON IDUR.                                                    790
   27 IF(IDUR.GE.0) GOTO 40                                             800
      FEHLER=.TRUE.                                                     810
      CALL FSWR06(3009,'IDUR','     ',IDUR,'.GE.','THAN',0)             820
   40 IF(IDUR.LE.(NE-2)) GOTO 41                                        830
      FEHLER=.TRUE.                                                     840
      CALL FSWR06(3009,'IDUR','     ',IDUR,'.LE.','THAN',NE-2)          850
   41 CONTINUE                                                          860
C     WENN NFE>1 TEST VON REFE.                                         870
      IF(NFE.LE.1) GOTO 50                                              880
      DO 51 I=2,NFE                                                     890
      IF(REFE(I).GT.REFE(I-1)) GOTO 51                                  900
      FEHLER=.TRUE.                                                     910
      CALL FSWR07(3012,'REFE','     ',I,REFE(I),'.GT.','THAN',REFE(I-1))  920
   51 CONTINUE                                                          930
   50 CONTINUE                                                          940
C     NANF >= END ?                                                     950
      IF(NANF.GE.NEND) GOTO 1                                           960
      FEHLER=.TRUE.                                                     970
      CALL FSWR02(3003,NANF,NEND)                                       980
    1 CONTINUE                                                          990
C     GRUPPENNUMMERN INNERHALB VON ENERGIEGRENZENSCHEMA?               1000
C     GRUPPE I GEHT VON ENG(NE-I) BIS ENG(NE-(I-1)) .                  1010
C     D.H. I MUSS IMMER KLEINER ALS NF SEIN                            1020
      IF(NANF.LT.NE) GOTO 2                                            1030
      IF(NANF.EQ.NE) CALL FSWR02(2001,NANF,NE-1)                       1040
      IF(NANF.GT.NE) CALL FSWR03(2002,NANF,NE,NE-1)                    1050
      NANF=NE-1                                                        1060
      IF(NANF.GE.NEND) GOTO 2                                          1070
      NEND=NANF                                                        1080
      CALL FSWR02(2003,NEND,NANF)                                      1090
    2 CONTINUE                                                         1100
C     IDUR MUSS KLEINER GLEICH NANF-NEND SEIN.                         1110
      IF(IDUR.LE.(NANF-NEND)) GOTO 42                                  1120
      FEHLER=.TRUE.                                                    1130
      CALL FSWR06(3009,'IDUR','     ',IDUR,'.LE.','THAN',NANF-NEND)    1140
   42 CONTINUE                                                         1150
      IF(IDUR.GT.0) GOTO 5                                             1160
C     AUSDRUCK DER ENERGIEGRUPPEN FUER WELCHE DIE BERECHNUNGEN ERFOLGEN. 1170
      IF(NANF.GT.NEND) GOTO 4                                          1180
      WRITE(NO,1000) NANF,ENG(NE-NANF),ENG(NE-(NANF-1))                1190
 1000 FORMAT('OTHE CALCULATIONS WILL BE DONE FOR GROUP',I5,            1200
     *', WHICH HAS THE BOUNDARIES ',1PE15.6,' EV  AND ',               1210
     *1PE15.6,' EV.')                                                  1220
      GOTO 5                                                           1230
    4 WRITE(NO,1001)                                                   1240
 1001 FORMAT('OTHE CALCULATIONS WILL BE DONE FOR THE FOLLOWING ENERGY GR 1250
     *OUPS.'/)                                                         1260
      NHELP=NANF-NEND                                                  1270
      IF(NHELP.EQ.1) WRITE(NO,1002)                                    1280
 1002 FORMAT(' ',2(' NUMBER      LOWER           UPPER     ')/         1290
     *       ' ',2('            LIMIT (EV)      LIMIT (EV)  ')/)      1300
      IF(NHELP.GT.1) WRITE(NO,1003)                                    1310
 1003 FORMAT(' ',3(' NUMBER      LOWER           UPPER     ')/         1320
     *       ' ',3(' LIMIT (EV)      LIMIT (EV)  ')/)                 1330
      NGRANZ=NANF-NEND+1                                               1340
      NHELP=(NGRANZ-1)/3+1                                             1350
      DO 10 J=1,NHELP                                                  1360
      I=NANF-3*(J-1)                                                   1370
      IH2=1                                                            1380
      IF((I-1).GE.NEND) IH2=2                                          1390
      IF((I-2).GE.NEND) IH2=3                                          1400
      DO 11 II=1,IH2                                                   1410
      IH(II)=I-II+1                                                    1420
      RH1(II)=ENG(NE-I+II-1)                                           1430
   11 RH2(II)=ENG(NE-I+II)                                             1440
      WRITE(NO,1004) (IH(II),RH1(II),RH2(II),II=1,IH2)                 1450
 1004 FORMAT(' ',3(2PI6,2X,1PE14.6,2X,1PE14.6,2X))                     1460
   10 CONTINUE                                                         1470
    5 CONTINUE                                                         1480
C     WENN ISPATE GLEICH 1 AUSDRUCK.                                   1490
      IF(IDUR.EQ.0.AND.ISPATE.EQ.1) WRITE(NO,1014)                     1500
 1014 FORMAT('OTHE MATERIAL IS  F I S S I O N A B L E .')              1510
C     WENN ISPATE GLEICH NULL AUSDRUCK.                                1520
      IF(IDUR.EQ.0.AND.ISPATE.EQ.0) WRITE(NO,1015)                     1530
 1015 FORMAT('OTHE MATERIAL IS  N O T   FISSIONABLE.')                 1540
C     ENG(I) MUESSEN >= 0 SEIN.                                        1550
      DO 22 I=1,NE                                                     1560
      IF(ENG(I).GT.0.0.OR.FSTOLE(ENG(I),0.0,GLSCH)) GOTO 22            1570
      FEHLER=.TRUE.                                                    1580
      CALL FSWR07(3012,'ENG ','     ',I,ENG(I),'.GE.','THAN',0.0)      1590
   22 CONTINUE                                                         1600
C     DRUCK VON DRINWA.                                                1610
      IF(IDUR.EQ.0) WRITE(NO,1016) DRINWA,EPSROW                       1620
 1016 FORMAT('OWARNING MESSAGES IN NUMERICAL INTEGRATION WILL BE PRINTED 1630
     *, IF THE ACTUAL RELATIVE ERROR'/                                 1640
     *' IS GREATER OR EQUAL THAN ',1PE12.4,' TIMES THE WISHED RELATIVE E 1650
     *RROR = ',1PE12.4,'.')                                            1660
C     UEBERPRUEFUNG DER GRUPPENGRENZEN.                                1670
      NGRANZ=NANF-NEND+1                                               1680
      DO 6 J=1,NGRANZ                                                  1690
      I=NANF-(J-1)                                                     1700
      IF(ENG(NE-I).LT.ENG(NE-(I-1))) GOTO 6                            1710
      FEHLER=.TRUE.                                                    1720
      CALL FSWR01(3005,I)                                              1730
    6 CONTINUE                                                         1740
C     AUSDRUCK UND UEBERPRUEFUNG DER BEREICHE FUER DIE INTERPOLATIONS  1750
C     FUNKTION.                                                        1760
      IF(IDUR.EQ.0) WRITE(NO,1005)                                     1770
 1005 FORMAT('OTHE FOLLOWING WEIGHTING SPECTRUM(S) IS (ARE) USED.'/    1780
     *       ' ',14X,'ENERGY RANGE',14X,7X,'WEIGHTING SPECTRUM',18X,   1790
     *'  TYP OF INTEGRATION'/)                                         1800
      DO 7 I=1,NENBER                                                  1810
C     ENERGIEBEREICH.                                                  1820
      IF(.NOT.FSTOLE(ENBER(I),-1.0,GLSCH)) GOTO 8                      1830
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      IF(IDUR.EQ.0) WRITE(NO,1006)                                      1840
 1006 FORMAT(' ',14X,'WHOLE RANGE')                                     1850
      GOTO 9                                                            1860
    8 IF(I.EQ.1.AND.IDUR.EQ.0) WRITE(NO,1007) ENBER(1)                  1870
 1007 FORMAT(' ',8X,'1.0E-5 EV  TO  ',1PE14.6,' EV')                    1880
      IF(I.GT.1.AND.IDUR.EQ.0) WRITE(NO,1008) ENBER(I-1),ENBER(I)       1890
 1008 FORMAT(' ',1PE14.6,' EV  TO  ',1PE14.6,' EV')                     1900
    9 CONTINUE                                                          1910
C     FUNKTIONSTYP UND ART DER INTEGRATION.                             1920
      NFTYP=NWFUN(I)                                                    1930
      IABSNF=IABS(NFTYP)                                                1940
      IF(IABSNF.LE.MNFTYP) GOTO 12                                      1950
      FEHLER=.TRUE.                                                     1960
      CALL FSWR03(3006,I,NFTYP,MNFTYP)                                  1970
      GOTO 7                                                            1980
   12 ISPRU=IABSNF+1                                                    1990
      IF(IDUR.NE.0)  GOTO 13                                            2000
      GOTO (14,15,16                                                    2010
     *),ISPRU                                                           2020
      CALL FSWR03(3001,'FSTR','UO  ',1)                                 2030
   14 ORIFUN=.FALSE.                                                    2040
      DPHITE=DPHI(1.0D+0)                                               2050
      IF(ORIFUN) WRITE(NO,1009)                                         2060
      IF(.NOT.ORIFUN) WRITE(NO,1017)                                    2070
 1009 FORMAT('+',40X,'  ORIGINAL FUNCTION DPHI=1.0D+0/E')               2080
 1017 FORMAT('+',40X,'  FUNCTION DPHI GIVEN BY THE USER')               2090
      GOTO 13                                                           2100
   15 WRITE(NO,1010)                                                    2110
 1010 FORMAT('+',40X,'  POINTWISE GIVEN WEIGHTING SPECTRUM')            2120
      GOTO 13                                                           2130
   16 WRITE(NO,1011) CONWFU(I)                                          2140
 1011 FORMAT('+',40X,2X,4X,1PE13.5,'/E')                                2150
      GOTO 13                                                           2160
   13 CONTINUE                                                          2170
C     INTEGRATIONSART.                                                  2180
      IF(IDUR.NE.0) GOTO 7                                              2190
      IF(NFTYP.LE.0) WRITE(NO,1012)                                     2200
 1012 FORMAT('+',85X,'      NUMERICAL')                                 2210
      IF(NFTYP.GT.0) WRITE(NO,1013)                                     2220
 1013 FORMAT('+',85X,'      ANALYTICAL')                                2230
    7 CONTINUE                                                          2240
C     WENN EIN PUNKTWEISES WICHTUNGSSPEKTRUM VERLANGT WIRD,             2250
C     MUSS NFE > 1 SEIN.                                                2260
      DO 23 I=1,NENBER                                                  2270
      IF(IABS(NWFUN(I)).NE.1.OR.NFE.GT.1) GOTO 23                       2280
      FEHLER=.TRUE.                                                     2290
      CALL FSWR01(3007,I)                                               2300
   23 CONTINUE                                                          2310
C     WEICHE FUER NENBER=1 UND NENBER > 1 .                             2320
      IF(NENBER.GT.1) GOTO 24                                           2330
C     ENBER(1)  MUSS ENTWEDER GLEICH -1.0 ODER GROESSER GLEICH          2340
C     ENG(NE-(NEND-1)) SEIN.                                            2350
      IF(FSTOLE(ENBER(1),-1.0,GLSCH).OR.ENBER(1).GE.ENG(NE-(NEND-1))    2360
     *.OR.FSTOLE(ENBER(1),ENG(NE-(NEND-1)),GLSCH)) GOTO 25              2370
      FEHLER=.TRUE.                                                     2380
      CALL FSWR02(3004,ENBER(1),ENG(NE-(NEND-1)))                       2390
      GOTO 25                                                           2400
C     WENN NENBER > 1 IST MUSS ENBER(NENBER) >= ENG(NE-(NEND-1)) SEIN.  2410
   24 IF(FSTOLE(ENBER(NENBER),ENG(NE-(NEND-1)),GLSCH).OR.               2420
     *ENBER(NENBER).GT.ENG(NE-(NEND-1))) GOTO 26                        2430
      FEHLER=.TRUE.                                                     2440
      CALL FSWR07(3012,'ENBE','R   ',NENBER,ENBER(NENBER),'.GE.',       2450
     *'THAN',ENG(NE-(NEND-1)))                                          2460
   26 CONTINUE                                                          2470
C     ENBER(I)  MUSS GROESSER SEIN ALS ENBER(I-1)                       2480
      DO 29 I=2,NENBER                                                  2490
      IF(ENBER(I).GT.ENBER(I-1)) GOTO 29                                2500
      FEHLER=.TRUE.                                                     2510
      CALL FSWR07(3012,'ENBE','R   ',I,ENBER(I),'.GT.','THAN',ENBER(I-1) 2520
     *)                                                                 2530
   29 CONTINUE                                                          2540
   25 CONTINUE                                                          2550
C     WENN |NWFUN(I)| >= 2 DANN MUSS CONWFU(I) UNGLEICH NULL SEIN.      2560
      DO 30 I=1,NENBER                                                  2570
      IF(IABS(NWFUN(I)).LT.2.OR..NOT.FSTOLE(CONWFU(I),0.0,GLSCH))       2580
     *GOTO 30                                                           2590
      FEHLER=.TRUE.                                                     2600
      CALL FSWR07(3012,'CONW','FU  ',I,CONWFU(I),'.NE.','THAN',0.0)     2610
   30 CONTINUE                                                          2620
C     TEST VON EPSROM UND KMROM.                                        2630
C     0.0 <= EPSROM <= 1.0                                              2640
C     10  <= KMROM  <= 40                                               2650
      IF(EPSROM.GT.0.0.OR.FSTOLE(EPSROM,0.0,GLSCH)) GOTO 31             2660
      FEHLER=.TRUE.                                                     2670
      CALL FSWR06(3010,'EPSR','OM  ',EPSROM,'.GE.','THAN',0.0)          2680
   31 IF(EPSROM.LT.1.0.OR.FSTOLE(EPSROM,1.0,GLSCH)) GOTO 32             2690
      FEHLER=.TRUE.                                                     2700
      CALL FSWR06(3010,'EPSR','OM  ',EPSROM,'.LE.','THAN',1.0)          2710
   32 IF(KMROM.GE.10) GOTO 33                                           2720
      FEHLER=.TRUE.                                                     2730
      CALL FSWR05(3009,'KMRO','M   ',KMROM,'.GE.','THAN',10)            2740
   33 IF(KMROM.LE.40) GOTO 34                                           2750
      FEHLER=.TRUE.                                                     2760
      CALL FSWR06(3009,'KMRO','M   ',KMROM,'.LE.','THAN',40)            2770
   34 CONTINUE                                                          2780
      IF(FEHLER) GOTO 898                                               2790
C     KEIN FEHLER FESTGESTELLT.                                         2800
      IF(TEST1) CALL FSWRCO(1004)                                       2810
  333 RETURN                                                            2820
C     STEUERDATEN LASSEN DURCHFUEHRUNG DER RECHNUNG NICHT ZU.           2830
  888 RETURN 1                                                          2840
  889 MREP=1                                                            2850
      RETURN 2                                                          2860
      END                                                               2870
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      SUBROUTINE FSTRU1(*)                                              10
C     PRUEFT OB DIE QUERSCHNITTSTYPEN SGA, SGN, SGT UND MUEL VORHANDEN  20
C     SIND.                                                             30
C                                                                       40
      LOGICAL*4 FEHLER,TEST1,TEST2,TEST3,LERMSG                         50
      REAL*8 ARG3(5),NAMES(4),MAT,TEXT                                  60
      DIMENSION IARG2(4),EMAT(2),TYP(2)                                 70
      DATA TEXT/'BEST    '/,NAMES/'SGA     ','SGN     ','SGT     ',    80
     *'MUEL    '/                                                      90
      EQUIVALENCE (MAT,EMAT(1)),(ARG3(3),TYP(1))                       100
      COMMON MAT                                                       110
      COMMON/CFSTRU/ TEST1,TEST2,TEST3,LERMSG                          120
      FEHLER=.FALSE.                                                   130
      IARG2(1)=3                                                       140
      ARG3(1)=MAT                                                      150
      ARG3(2)=TEXT                                                     160
      DO 1 I=1,4                                                       170
      ARG3(3)=NAMES(I)                                                 180
      IRC=0                                                            190
      CALL NDFLOC(IRC,IARG2,ARG3,ARG4,ARG5)                            200
      IF(IRC.EQ.1) GOTO 1                                              210
      FEHLER=.TRUE.                                                    220
      CALL FSWR04(3008,EMAT(1),EMAT(2),TYP(1),TYP(2))                  230
    1 CONTINUE                                                         240
      IF(FEHLER) RETURN 1                                              250
      IF(TEST1) CALL FSWR00(1006)                                      260
      RETURN                                                           270
      END                                                              280
```

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      SUBROUTINE FSTRU2(IGR,NE,ENG,NIBER,MIBER,GIBER,MIBERP,IIBER,CIBER,  10
     *                  NENBER,ENBER,NWFUN,CONWFU,*)                      20
C     AUSDRUCK VON MATERIALNAME, GRUPPENNUMMER UND GRUPPENGRENZEN.      30
C     BESTIMMUNG UND AUSDRUCK VON INTEGRATIONSBEREICH(E) ART(EN)        40
C     UND TYP(EN) DER INTEGRATION INNERHALB EINER GRUPPE.               50
      DIMENSION ENG(1),GIBER(1),IIBER(1),CIBER(1),ENBER(1),NWFUN(1),    60
     *          CONWFU(1)                                               70
      LOGICAL*4 FSTOLE,TEST1,TEST2,TEST3,LERMSG                         80
      REAL*8 MAT                                                        90
      COMMON/CFSTRU/ TEST1,TEST2,TEST3,LERMSG,GLSCH                    100
      COMMON MAT,NR1(2),NO                                             110
C                                                                      120
      WRITE(NO,1008)                                                   130
 1008 FORMAT('0')                                                      140
      WRITE(NO,1009)                                                   150
 1009 FORMAT(' ',126('*'))                                             160
      WRITE(NO,1000) MAT,IGR,ENG(NE-IGR),ENG(NE-(IGR-1))               170
 1000 FORMAT(' *',A8,'   GROUP=',I4,'  LOWER BOUNDARY=',1PE14.6,' EV   180
     *UPPER BOUNDARY=',1PE14.6,' EV.',32X,'*')                         190
C     SETZEN VON GIBER(1) UND GIBER(NIBER).                            200
      NIBER=2                                                          210
      IF(NIBER.GT.MIBER) CALL FSWRC3(3CC1,'FSTR','U2  ',1)             220
      GIBER(1)=ENG(NE-IGR)                                             230
      GIBER(NIBER)=ENG(NE-(IGR-1))                                     240
C     BESTIMMUNG DER DURCH WICHTUNGSFUNKTIONEN BEDINGTEN UNTERBEREICHE. 250
C     IIBER(1) UND CIBER(1) SIND OHNE BEDEUTUNG UND WERDEN DESHALB     260
C     GLEICH -999999 BZW. -999999.C GESETZT.                           270
      IIBER(1)=-999999                                                 280
      CIBER(1)=-999999.0                                               290
C     WENN NENBER GLEICH 1 IST, DANN GIBT ES KEINE UNTERBEREICHE.      300
      IF(NENBER.EQ.1) GOTO 1                                           310
C     SUCHE VON ENBER(I) MIT GIBER(NIBER-1)<ENBER(I)<GIBER(NIBER)      320
      DO 2 I=1,NIBER                                                   330
      IF(ENBER(I).LT.GIBER(NIBER-1).OR.FSTOLE(ENBER(I),GIBER(NIBER-1),GL 340
     *SCH)) GOTO 2                                                     350
      IF(ENBER(I).GT.GIBER(NIBER).OR.FSTOLE(ENBER(I),GIBER(NIBER),GLSCH) 360
     *) GOTO 3                                                         370
      NIBER=NIBER+1                                                    380
      IF(NIBER.GT.MIBER) GOTO 2                                        390
      GIBER(NIBER)=GIBER(NIBER-1)                                      400
      GIBER(NIBER-1)=ENBER(I)                                          410
    2 CONTINUE                                                         420
    3 IF(NIBER.LE.MIBER) GOTO 1                                        430
      MIBERP=NIBER-MIBER                                               440
      RETURN 1                                                         450
    1 CONTINUE                                                         460
C     SETZEN DER WICHTUNGSFUNKTIONSTYPEN UND INTEGRATIONSARTEN.        470
C     SETZEN DER NORMIERUNGSKONSTANTEN.                                480
      IF(NENBER.GT.1) GOTO 4                                           490
      IF(NIBER.GT.2) CALL FSWR03(3001,'FSTR','U2  ',2)                 500
      IIBER(2)=NWFUN(1)                                                510
      CIBER(2)=CONWFU(1)                                               520
      GOTO 10                                                          530
    4 CONTINUE                                                         540
      I=2                                                              550
    8 J=1                                                              560
    7 IF(.NOT.FSTOLE(GIBER(I),ENBER(J),GLSCH).AND.                     570
     *ENBER(J).LT.GIBER(I)) GOTO 5                                     580
      IIBER(I)=NWFUN(J)                                                590
      CIBER(I)=CONWFU(J)                                               600
      GOTO 6                                                           610
    5 J=J+1                                                            620
      IF(J.LE.NENBER) GOTO 7                                           630
      IF(I.NE.NIBER) CALL FSWRC3(3C01,'FSTR','U2  ',3)                 640
      IIBER(I)=NWFUN(NENBER)                                           650
      CIBER(I)=CONWFU(NENBER)                                          660
      GOTO 10                                                          670
    6 I=I+1                                                            680
      IF(I.LE.NIBER) GOTO 8                                            690
   10 CONTINUE                                                         700
C     AUSDRUCK DER INTEGRATIONSBEREICHE, TYPEN DER WICHTUNGSFUNKTION   710
C     UND ARTEN DER INTEGRATION.                                       720
      DO 11 I=2,NIBER                                                  730
      WRITE(NO,1001) GIBER(I-1),GIBER(I)                               740
 1001 FORMAT(' *',11X,'FROM ',1PE14.6,' EV  TO ',1PE14.6,' EV')        750
      IF(IIBER(I).LE.0) WRITE(NO,1002)                                 760
 1002 FORMAT('+',58X,'NUMERICAL')                                      770
      IF(IIBER(I).GT.0) WRITE(NO,1003)                                 780
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 1003 FORMAT('+',58X,'ANALYTICAL')                                      790
      WRITE(NO,1004)                                                    800
 1004 FORMAT('+',68X,' INTEGRATION IS USED.')                           810
      ISPRU=IABS(IIBER(I))+1                                            820
      GOTO (14,15,16                                                    830
     *),ISPRU                                                           840
      CALL FSWR03(3001,'FSTR','U2  ',4)                                 850
   14 WRITE(NO,1005)                                                    860
 1005 FORMAT('+',89X,' DPHI IS USED AS WEIGHTING SPECTRUM.*')           870
      GOTO 11                                                           880
   15 WRITE(NO,1006)                                                    890
 1006 FORMAT('+',89X,' POINTWISE GIVEN WEIGHTING SPECTRUM.*')           900
      GOTO 11                                                           910
   16 WRITE(NO,1007) CIBER(I)                                           920
 1007 FORMAT('+',89X,' FUNCTION ',1PE13.5,'/E  USED',5X,'*'/            930
     *' *',97X,'AS WEIGHTING SPECTRUM.',5X,'*')                         940
      GOTO 11                                                           950
   11 CONTINUE                                                          960
      WRITE(NO,1009)                                                    970
      IF(TEST1) CALL FSWR00(1007)                                       980
  333 RETURN                                                            990
      END                                                              1000
```

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      SUBROUTINE FSTRU3(NFE,REFE,EFE,NABWF,MABWF,ABWF,MABWFP,*,*)        10
C     DARSTELLUNG DER PUNKTWEISEN WICHTUNGSFUNKTION DURCH GERADENSTUECKE  20
C     NABWF IST DER INDEX BIS ZU DEM DAS FELD ABWF GEFUELLT IST.          30
      DIMENSION REFE(1),EFE(1),ABWF(MABWF,4)                              40
      LOGICAL*4 TEST1,TEST2,TEST3,LERMSG,FSTCLE,FINBED                    50
      COMMON NR1(4),NO                                                    60
      COMMON/CFSTRU/ TEST1,TEST2,TEST3,LERMSG,GLSCH,                      70
     *NR2(4),UGR,OGR                                                      80
      IF(NFE.LE.1) CALL FSWR03(3001,'FSTR','U3  ',1)                      90
      FINBED=.FALSE.                                                     100
C     VERGLEICH VON UGR MIT REFE(1).                                     110
C     UGR > REFE(1) ODER FSTCLE(UGR,REFE(1),GLSCH) GLEICH .TRUE.         120
C                   ABWF(1,1)=UGR  ; ABWF(1,2)=-999999.0 ;               130
C                                    ABWF(1,3)=-999999.0 ;               140
C                                    ABWF(1,4)=-999999.0;                150
C                   NABWF=1 ;                                           160
C                   I=2 SETZEN UND 1. REFE(I) SUCHEN, MIT UGR < REFE(I) 170
C     UGR < REFE(1) FEHLERAUSGANG.                                       180
      IF(UGR.GT.REFE(1).OR.FSTCLE(UGR,REFE(1),GLSCH)) GOTO 1             190
      CALL FSWR07(3015,'FIRS','T   ',REFE(1),'.GT.','LOWE','R   ',UGR)   200
  888 RETURN 2                                                           210
    1 ABWF(1,1)=UGR                                                      220
      ABWF(1,2)=-999999.0                                                230
      ABWF(1,3)=-999999.0                                                240
      ABWF(1,4)=-999999.0                                                250
      NABWF=1                                                            260
      NN=1                                                               270
      IF(TEST2) WRITE(NO,1000) NN,(ABWF(1,J),J=1,4)                      280
 1000 FORMAT(' ABWF: NABWF=',I5,' E=',1PE14.6,' A=',1PE14.6,' B=',       290
     *1PE14.6,' ABWF(NABWF,4)=',1PE12.4,'.')                            300
      I=2                                                                310
    2 IF(REFE(I).GT.UGR) GOTO 3                                          320
      I=I+1                                                              330
      IF(I.LE.NFE) GOTO 2                                                340
C     KEIN ENERGIEPUNKT DES SPEKTRUMS IST GROESSER ALS UGR.              350
      CALL FSWR02(3014,UGR,OGR)                                          360
      GOTO 888                                                           370
    3 CONTINUE                                                           380
C     LOOP SOLANGE DURCHFUEHREN, BIS (EINSCHLIESSLICH) 1. REFE(I)>=OGR   390
C     WIRD KEIN REFE(I)>=OGR, IST AUCH FSTOLE(REFE(NFE),OGR,GLSCH)       400
C     GLEICH .TRUE. ZUGELASSEN.                                          410
      IF(FINBED) GOTO 7                                                  420
    4 IF(REFE(I).LT.OGR) GOTO 8                                          430
      FINBED=.TRUE.                                                      440
    8 NABWF=NABWF+1                                                      450
C     A UND B DER GERADENSTUECKE BERECHNEN.                              460
      IF(NABWF.GT.MABWF) GOTO 5                                          470
      IF(REFE(I).LT.REFE(I-1)) CALL FSWR03(3001,'FSTR','U2  ',2)         480
      ABWF(NABWF,1)=REFE(I)                                              490
      Q=1.0/(REFE(I)-REFE(I-1))                                          500
      ABWF(NABWF,2)=(EFE(I)-EFE(I-1))*Q                                  510
      ABWF(NABWF,3)=(EFE(I-1)*REFE(I)-EFE(I)*REFE(I-1))*Q                520
      ABWF(NABWF,4)=1.0                                                  530
      IF(ABWF(NABWF,2).NE.0.0.OR.ABWF(NABWF,3).NE.0.0) GOTO 9            540
      ABWF(NABWF,4)=0.0                                                  550
      GOTO 10                                                            560
    9 Y1=EFE(I-1)                                                        570
      IF(NABWF.EQ.2) Y1=ABWF(2,2)*ABWF(1,1)+ABWF(2,3)                    580
      Y2=EFE(I)                                                          590
      IF(Y1*Y2.LT.0.0) ABWF(NABWF,4)=-1.0                                600
   10 IF(TEST2.AND..NOT.FINBED) WRITE(NO,1000) NABWF,(ABWF(NABWF,J),J=1,  610
     *4)                                                                 620
    5 IF(FINBED) GOTO 7                                                  630
      I=I+1                                                              640
      IF(I.LE.NFE) GOTO 4                                                650
C     KEIN REFE(I) WAR >= OGR.                                           660
C     FSTOLE(REFE(NFE),OGR,GLSCH) GLEICH .TRUE. WIRD ZUGELASSEN.         670
C     ANDERNFALLS FEHLER.                                                680
      IF(FSTCLE(REFE(NFE),OGR,GLSCH)) GOTO 7                             690
      CALL FSWR07(3015,'LAST','    ',REFE(NFE),'.LT.','UPPE','R   ',OGR)  700
      GOTO 888                                                           710
    7 IF(NABWF.LE.MABWF) GOTO 330                                        720
      MABWFP=NABWF-MABWF                                                 730
      RETURN 1                                                           740
  330 ABWF(NABWF,1)=OGR                                                  750
      ABWF(NABWF,4)=1.0                                                  760
      IF(ABWF(NABWF,2).EQ.0.0.AND.ABWF(NABWF,3).EQ.0.0)CALL FSWR03(3001, 770
     *'FSTR','U3  ',3)                                                   780
      Y1=ABWF(NABWF,2)*ABWF(NABWF-1,1)+ABWF(NABWF,3)                     790
      Y2=ABWF(NABWF,2)*ABWF(NABWF,1)  +ABWF(NABWF,3)                     800
      IF(Y1*Y2.LT.0.0) ABWF(NABWF,4)=-1.0                                810
      IF(TEST2) WRITE(NO,1000) NABWF,(ABWF(NABWF,J),J=1,4)               820
  333 RETURN                                                             830
      END                                                                840
```

```
      SUBROUTINE FSTRU4(ENG,NE,IGR,FFAKT,MI,SIGO,RPHI,RABS,RELA,RTOT,
     *RFISS,RELFL,RF,MRF,ISPATE)
      LOGICAL*4 TEST1,TEST2,TEST3,LERMSG,LFAR1(6),LFAR2(6),LFAR1A(6),
     *LFAR2A(6)
      REAL*8 MAT,STRK,RPHI,RABS,RELA,RTOT,RFISS,RELFL,RF,
     *SG8C,SG8A,SG8N,SG8N01,SG8N1,SG8T1,SG8F,HELP1,HELP2,HELP3,HELP23
      DIMENSION ENG(1),FFAKT(MI,6),SIGO(1),RF(MI,MRF),TF(7),FAR1AN(6),
     *FAR2AN(6)
      DATA STRK/'STRK    '/,TF/' FA ',' FN ',' FF ','FNC1','FN1 ','FTL '
     *,' FC '/
      COMMON MAT,NR1(2),NOUTP,JA,NANF,NEND
      COMMON/CFSDUR/ ICUR
      COMMON/CFSTRU/ TEST1,TEST2,TEST3,LERMSG
      UGR=ENG(NE-IGR)
      OGR=ENG(NE-(IGR-1))
      IF(.NOT.TEST2) GOTO 1
      CALL FSWR06(1010,'     ','FLUX',UGR,OGR,'PHI',RPHI)
      CALL FSWR06(-1010,'     ','FLUX',UGR,OGR,'SGA',RABS)
      CALL FSWR06(-1010,'     ','FLUX',UGR,OGR,'SGN',RELA)
      CALL FSWR06(-1010,'     ','FLUX',UGR,OGR,'SGT',RTOT)
      CALL FSWR06(-1010,'     ','FLUX',UGR,OGR,'SGF',RFISS)
      CALL FSWR06(-1010,'CUR ','REAT',UGR,OGR,'SGN',RELFL)
C     AUSDRUCK VON RF.
      WRITE(NOUTP,1005) MI,MRF
 1005 FORMAT('0AUSDRUCK VON RF. MI=',I4,'  MRF=',I2,'.')
      DO 11 I=1,MI
      WRITE(NOUTP,1006) (RF(I,J),J=1,MRF)
 1006 FORMAT(' ',1P8E13.6)
   11 CONTINUE
C     GRUPPENQUERSCHNITTE NULL UND F-FAKTOREN EINS SETZEN.
    1 CONTINUE
      SG8A=0.0
      SG8F=0.0
      SG8N=0.0
      SG8N01=0.0
      SG8N1=0.0
      SG8T1=0.0
      DO 2 I=1,MI
      DO 2 J=1,6
    2 FFAKT(I,J)=1.0
C     BERECHNUNG DER GRUPPENQUERSCHNITTE UND F-FAKTOREN.
      IF(RPHI.NE.0.0) GOTO 9
C     INTEGRAL UEBER PHI GLEICH 0.0. DANN MUESSEN RABS, RELA, RTOT,
C     (RFISS) UND RELFL AUCH GLEICH NULL SEIN.
      IF(RABS.NE.0.0.OR.RELA.NE.0.0.OR.RTOT.NE.0.0.OR.RELFL.NE.0.0.OR.
     *(ISPATE.EQ.1.AND.RFISS.NE.0.0)) CALL FSWR03(3001,'FSTR','U4  ',1)
      CALL FSWR00(-2012)
      GOTO 10
    9 SG8A=RABS/RPHI
      SG8N=RELA/RPHI
      SG8N01=RELFL/RPHI
      SG8N1=SG8N01
      SG8T1=RTOT/RPHI
      IF(ISPATE.EQ.1) SG8F=RFISS/RPHI
      SIGA=FSSNGL(SG8A)
      SIGN=FSSNGL(SG8N)
      SIGN01=FSSNGL(SG8N01)
      SIGN1=FSSNGL(SG8N1)
      SIGT1=FSSNGL(SG8T1)
      SIGF=FSSNGL(SG8F)
   10 CONTINUE
C     F-FAKTOREN BILDEN.
C     BEI VORKOMMENDEN DIVISIONEN DURCH NULL WIRD DER F-FAKTOR
C     GLEICH 1.0 GESETZT.
C
      IF(LERMSG) GOTO 34
      DO 33 J=1,6
      LFAR1(J)=.FALSE.
      LFAR2(J)=.FALSE.
      LFAR1A(J)=.FALSE.
      LFAR2A(J)=.FALSE.
   33 CONTINUE
   34 DO 12 I=1,MI
      J=0
   13 J=J+1
      IF(J.EQ.1.OR.LERMSG) GOTO 41
      IF(.NOT.LFAR1A(J-1)) GOTO 42
      CALL FSWR03(2017,HELP4,FAR1AN(J-1),SIGO(I-1))
      LFAR1(J-1)=.FALSE.
      LFAR1A(J-1)=.FALSE.
   42 IF(.NOT.LFAR2A(J-1)) GOTO 41
      CALL FSWR03(2018,HELP4,FAR2AN(J-1),SIGO(I-1))
      LFAR2(J-1)=.FALSE.
      LFAR2A(J-1)=.FALSE.
   41 IF(J.GT.6) GOTO 12
      IF(J.EQ.3.AND.ISPATE.NE.1) J=J+1
      HELP1=SG8A-SG8F
      IF(J.NE.1.OR.ISPATE.EQ.0) GOTO 14
      HELP4=TF(7)
      IF(HELP1.NE.0.0.AND.RF(I,1).NE.0.0) GOTO 15
      IF(LERMSG) GOTO 37
      IF(LFAR1(J)) GOTO 13
      LFAR1(J)=.TRUE.
      FAR1AN(J)=SIGO(I)
      GOTO 13
   37 CALL FSWR02(2014,HELP4,SIGO(I))
   18 CALL FSWR06(-1014,RF(I,6),RF(I,1),RF(I,8),RF(I,1),SIGA,SIGF)
      GOTO 13
   15 HELP2=RF(I,6)-RF(I,8)
      IF(.NOT.LERMSG.AND.LFAR1(J)) LFAR1A(J)=.TRUE.
      FFAKT(I,1)=FSSNGL((HELP2/RF(I,1))/HELP1)
      IF(HELP2.EQ.0.0) GOTO 45
      IF(.NOT.LERMSG.AND.LFAR2(J)) LFAR2A(J)=.TRUE.
      GOTO 13
   45 IF(LERMSG) GOTO 38
      IF(LFAR2(J)) GOTO 13
```

```
      LFAR2(J)=.TRUE.                                                   1070
      FAR2AN(J)=SIGO(I)                                                 1080
      GOTO 13                                                           1090
   38 CALL FSWR02(2016,HELP4,SIGO(I))                                   1100
      GOTO 18                                                           1110
   14 HELP4=TF(J)                                                       1120
      GOTO (21,22,23,24,25,26),J                                        1130
      CALL FSWR03(3001,'FSTR','U4  ',2)                                 1140
   21 HELP1=RF(I,6)                                                     1150
      HELP3=SG8A                                                        1160
      GOTO 16                                                           1170
   22 HELP1=RF(I,7)                                                     1180
      HELP3=SG8N                                                        1190
      GOTO 16                                                           1200
   23 HELP1=RF(I,8)                                                     1210
      HELP3=SG8F                                                        1220
      GOTO 16                                                           1230
   24 HELP1=RF(I,3)                                                     1240
      HELP3=SG8N01                                                      1250
   16 HELP2=RF(I,1)                                                     1260
      GOTO 30                                                           1270
   25 HELP1=RF(I,5)                                                     1280
      HELP3=SG8N1                                                       1290
      GOTO 17                                                           1300
   26 HELP1=RF(I,4)                                                     1310
      HELP3=SG8T1                                                       1320
   17 HELP2=RF(I,2)                                                     1330
   30 HELP23=HELP2*HELP3                                                1340
      IF(HELP23.NE.0.0) GOTO 31                                         1350
      IF(LERMSG) GOTO 39                                                1360
      IF(LFAR1(J)) GOTO 13                                              1370
      LFAR1(J)=.TRUE.                                                   1380
      FAR1AN(J)=SIGO(I)                                                 1390
      GOTO 13                                                           1400
   39 CALL FSWR02(2014,HELP4,SIGO(I))                                   1410
   32 CALL FSWR03(-1013,HELP1,HELP2,HELP3)                              1420
      GOTO 13                                                           1430
   31 FFAKT(I,J)=FSSNGL(HELP1/HELP23)                                   1440
      IF(.NOT.LERMSG.AND.LFAR1(J)) LFAR1A(J)=.TRUE.                     1450
      IF(HELP1.EQ.0.0) GOTO 44                                          1460
      IF(.NOT.LERMSG.AND.LFAR2(J)) LFAR2A(J)=.TRUE.                     1470
      GOTO 13                                                           1480
   44 IF(LERMSG) GOTO 40                                                1490
      IF(LFAR2(J)) GOTO 13                                              1500
      LFAR2(J)=.TRUE.                                                   1510
      FAR2AN(J)=SIGC(I)                                                 1520
      GOTO 13                                                           1530
   40 CALL FSWR02(2016,HELP4,SIGO(I))                                   1540
      GOTO 32                                                           1550
   12 CONTINUE                                                          1560
      IF(LERMSG) GOTO 35                                                1570
      DO 36 J=1,6                                                       1580
      HELP4=TF(J)                                                       1590
      IF(J.EQ.1.AND.ISPATE.NE.0) HELP4=TF(7)                            1600
      IF(LFAR1(J)) CALL FSWR03(2017,HELP4,FAR1AN(J),SIGO(MI))           1610
      IF(LFAR2(J)) CALL FSWR03(2018,HELP4,FAR2AN(J),SIGC(MI))           1620
   36 CONTINUE                                                          1630
C     AUSDRUCK UND AUSSCHREIBEN DER GRUPPENQUERSCHNITTE UND F-FAKTOREN. 1640
C     FUER IDUR=0 UND IGR=NANF 1. RECORD SCHREIBEN.                     1650
   35 IF(IDUR.LT.0) CALL FSWR03(3001,'FSTR','U4  ',3)                   1660
      IF(IDUR.GT.0.OR.IGR.NE.NANF) GOTO 3                               1670
      NN=0                                                              1680
      WRITE(JA) NN,STRK                                                 1690
      IF(TEST2) CALL FSWRC1(1005,JA)                                    1700
    3 CONTINUE                                                          1710
      NN=5                                                              1720
C     AUSGABE DER MITTLEREN QUERSCHNITTE.                               1730
      IGRINT=NE-IGR                                                     1740
      IF(IGRINT.LT.1) CALL FSWR03(3001,'FSTR','U4  ',4)                 1750
      WRITE(JA) NN,MAT,IGRINT,UGR,OGR                                   1760
      IF(ISPATE.EQ.1) GOTO 4                                            1770
      IF(ISPATE.NE.0) CALL FSWR03(3001,'FSTR','U5  ',4)                 1780
      NN=5                                                              1790
      WRITE(JA) NN,SIGA,SIGN,SIGNO1,SIGN1,SIGT1                         1800
      WRITE(NOUTP,1000) SIGA,SIGN,SIGNO1,SIGN1,SIGT1                    1810
 1000 FORMAT('0',22X,'SIGMA A',11X,'SIGMA N',10X,'SIGMA NC1',9X,        1820
     *'SIGMA N1',10X,'SIGMA T1'//16X,5E18.8)                            1830
      GOTO 5                                                            1840
    4 SG8C=SG8A-SG8F                                                    1850
      SIGC=SG8C                                                         1860
      NN=6                                                              1870
      WRITE(JA) NN,SIGC,SIGN,SIGF,SIGNO1,SIGN1,SIGT1                    1880
      WRITE(NOUTP,1001) SIGC,SIGN,SIGF,SIGNO1,SIGN1,SIGT1               1890
 1001 FORMAT('0',22X,'SIGMA C',11X,'SIGMA N',11X,'SIGMA F',10X,         1900
     *'SIGMA NO1',9X,'SIGMA N1',10X,'SIGMA T1'//16X,6E18.8)             1910
    5 CONTINUE                                                          1920
C     F-FAKTOREN AUSGEBEN.                                              1930
      IF(ISPATE.EQ.1) GOTO 6                                            1940
      IF(ISPATE.NE.0) CALL FSWR03(3001,'FSTR','U4  ',6)                 1950
      WRITE(NOUTP,1002)                                                 1960
 1002 FORMAT('0',5X,'SIGO',15X,'FA',16X,'FN',16X,'FNC1',14X,'FN1',15X,  1970
     *'FT1'/)                                                           1980
      LRJ=2                                                             1990
      GOTO 7                                                            2000
    6 WRITE(NOUTP,1003)                                                 2010
 1003 FORMAT('0',5X,'SIGO',15X,'FC',16X,'FN',16X,'FF',14X,'FNC1',14X,   2020
     *'FN1',15X,'FT1'/)                                                 2030
      LRJ=3                                                             2040
    7 CONTINUE                                                          2050
      NN=LRJ+4                                                          2060
      DO 8 I=1,MI                                                       2070
      WRITE(JA) NN,SIGO(I),(FFAKT(I,J),J=1,LRJ),(FFAKT(I,J),J=4,6)      2080
      WRITE(NOUTP,1004) SIGO(I),(FFAKT(I,J),J=1,LRJ),(FFAKT(I,J),J=4,6) 2090
 1004 FORMAT(F16.8,6E18.8)                                              2100
    8 CONTINUE                                                          2110
  333 RETURN                                                            2120
      END                                                               2130
```

```
      FUNCTION FSSNGL(A)                                                10
C     TRUNCATION OF THE REAL*8 NUMBER A TO THE REAL*4 VALUE FSSNGL.     20
C     IF NECESSARY ROUNDING UP IS DONE.                                 30
      REAL*8 A,AL                                                       40
      LOGICAL*1 L(8),LE(4)                                              50
      DIMENSION FL(2)                                                   60
      EQUIVALENCE (AL,FL(1),L(1)),(LE(1),E),(FL(2),I)                   70
      DATA 01/Z00000001/                                                80
      AL=A                                                              90
      FSSNGL=FL(1)                                                     100
      IF(I.GE.0) GOTO 333                                              110
      E=01                                                             120
      LE(1)=L(1)                                                       130
      FSSNGL=FSSNGL+E                                                  140
  333 RETURN                                                           150
      END                                                              160
```

```
      SUBROUTINE FSTRU5(A1,NA1,MA1,A2,NA2,MA2,MA2P,*)                   10
C     DER INHALT DES FELDES A1 WIRD IN DAS FELD A2 UMGESPEICHERT.       20
C     WENN DIE DIMENSION NICHT AUSREICHT, WIRD MA2P > 0 GESETZT         30
C     UND RETURN 1 GEMACHT.                                             40
C                                                                       50
      DIMENSION A1(MA1,4),A2(MA2,4)                                     60
      IF(NA1.GT.MA2) GOTO 773                                           70
      NA2=NA1                                                           80
      DO 1 I=1,NA2                                                      90
      DO 1 J=1,4                                                       100
    1 A2(I,J)=A1(I,J)                                                  110
  322 RETURN                                                           120
  773 MA2P=NA1-MA2                                                     130
      RETURN 1                                                         140
      END                                                              150
```

```
      SUBROUTINE FSQUER(TYP,UGR,OGR,NAB,MAB,AB,MABP,*,*)                10
C     VON DEM QUERSCHNITTSTYP TYP DES MATERIALS MAT WERDEN VON UGR BIS  20
C     OGR IN DEM FELD AB DIE ENTSPRECHENDEN GERADENSPEZIFIKATIONEN      30
C     ABGESPEICHERT.                                                    40
C     REICHT DIE FELDLAENGE NICHT AUS, SO WIRD MABP>0 GESETZT           50
C     UND RETURN 1 GEMACHT.                                             60
C     BEI FEHLERN IN DEN DATEN AUF KEDAK WIRD RETURN 2 GEMACHT.         70
C                                                                       80
      REAL*8 TYP,MAT,ARG3,BEST,TYPL,TYPSGT,TYPSGN,TYPSGA,TYPSGF         90
      LOGICAL*4 TEST1,TEST2,TEST3,LERMSG,FSTOLE,INSERT,FIRST,PRINT,    100
     *FELCON                                                           110
      DIMENSION AB(MAB,4),IARG2(4),ARG3(5),ETYPL(2),EMAT(2)             120
      EQUIVALENCE (ETYPL(1),TYPL),(EMAT(1),MAT)                         130
      DATA BEST/'BEST    '/,TYPSGT,TYPSGN,TYPSGA,TYPSGF/'SGT     ',     140
     **'SGN     ','SGA     ','SGF     '/                               150
      COMMON MAT,NR1(2),NO                                             160
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```
      COMMON/CFSTRU/ TEST1,TEST2,TEST3,LERMSG,GLSCH                    170
      TYPL=TYP                                                         180
      INSERT=.FALSE.                                                   190
      IF(UGR.GE.OGR.OR.MAB.LT.2) CALL FSWR03(3001,'FSQU','ER  ',1)     200
C     IGEL=ZAHL DER VON DER LIBRARY GELESENEN  PUNKTE.                 210
      IGEL=0                                                           220
C     IAKZ=ZAHL DER AKZEPTIERTEN PUNKTE. IAKZ<=IGEL.                   230
      IAKZ=0                                                           240
C     1. PUNKT DES QUERSCHNITTS HOLEN.                                 250
      IARG2(1)=3                                                       260
      ARG3(1)=MAT                                                      270
      ARG3(2)=BEST                                                     280
      ARG3(3)=TYP                                                      290
      IRC=0                                                            300
      CALL NDFLOC(IRC,IARG2,ARG3,ARG4,ARG5)                            310
      IF(IRC.NE.1) CALL FSWR03(3001,'FSQU','ER  ',2)                   320
      IF(IARG2(2).NE.1.OR.IARG2(3).NE.1.OR.IARG2(4).NE.0) CALL FSWR00(30 330
     *01)                                                              340
      ENERGA=ARG3(4)                                                   350
      QUERA=ARG3(5)                                                    360
      IGEL=IGEL+1                                                      370
      IF(TEST2) CALL FSWR07(1011,'FIRS',EMAT(1),EMAT(2),ETYPL(1),ETYPL(2 380
     *),ENERGA,QUERA)                                                  390
C     (1,) MIT DUMMY WERTEN FUELLEN.                                   400
      AB(1,1)=UGR                                                      410
      AB(1,2)=-999999.0                                                420
      AB(1,3)=-999999.0                                                430
      AB(1,4)=-999999.0                                                440
      NAB=1                                                            450
C     LAGE VON UGR UND OGR BEZUEGLICH DER VON DER LIBRARY GELESENEN    460
C     PUNKTE. (= BEDEUTET IMMER GLEICHHEIT IM SINNE VON TOLERANT.)     470
C     IFALL BEDEUTUNG                          AKTION                  480
C      10   1.G.D.P.(1.GELESENER DATENPUNKT)   WEITERE DATENPUNKTE     490
C           <=UGR. NOCH KEINE INFORMATION      EINLESEN.               500
C           UEBER OGR.                                                 510
C      11   WIE 10. ZUSAETZLICH L.G.D.P.       WARNUNG DRUCKEN. Q.S. VOM 520
C           (LETZTER GELESENER DATENPUNKT)     L.G.D.P. VON UGR BIS UGR 530
C           <=UGR.                             VERWENDEN. RETURN.      540
C      12   WIE 10. ZUSAETZLICH L.G.D.P.       NORMALFALL. SUBROUTINE  550
C           >=OGR.                             ABSCHLIESSEN. RETURN.   560
C      13   WIE 10. ZUSAETZLICH L.G.D.P.       WARNUNG DRUCKEN. Q.S. VOM 570
C           ZWISCHEN UGR UND OGR LIEGEND.      L.G.D.P. BIS OGR VERWENDEN 580
C                                              RETURN.                 590
C      20   1.G.D.P. >= OGR. NOCH KEINE        WARNUNG DRUCKEN. Q.S. VOM 600
C           INFORMATION UEBER OGR.             1.G.D.P. VON UGR BIS OGR 610
C                                              VERWENDEN. RETURN.      620
C      30   1.G.D.P. ZWISCHEN UGR UND OGR.     WEITERE DATENPUNKTE     630
C           SONST NOCH KEINE INFORMATION.      EINLESEN.               640
C      31   WIE 30. ZUSAETZLICH L.G.D.P.       FEHLER AUF LIBRARY.     650
C           <=UGR.                             FEHLERAUSDRUCK. RETURN 2. 660
C      32   WIE 30. ZUSAETZLICH L.G.D.P.       Q.S. VOM 1.G.D.P. VON UGR 670
C           >=OGR.                             BIS ZUR ENERGIE DES     680
C                                              1.G.D.P. VERWENDEN. DANN 690
C                                              NORMAL WEITER. RETURN.  700
C      33   WIE 30. ZUSAETZLICH L.G.D.P.       Q.S. VOM 1.G.D.P. UND   710
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C           ZWISCHEN UGR UND OGR LIEGEND.     L.G.D.P. IN DEM BEREICH      720
C                                             VERWENDEN, WO KEINE          730
C                                             DATEN VORHANDEN SIND.        740
C                                             SONST NORMAL. RETURN.        750
C     IFALL SETZEN.                                                        760
      IFALL=0                                                              770
      IF(ENERGA.LT.UGR.OR.FSTCLE(ENERGA,UGR,GLSCH)) GOTO 10                780
      IF(ENERGA.GT.OGR.OR.FSTOLE(ENERGA,OGR,GLSCH)) GOTO 20                790
C     IFALL=30                                                             800
   30 IFALL=30                                                             810
      GOTO 100                                                             820
   10 IFALL=10                                                             830
      GOTO 100                                                             840
   20 IFALL=20                                                             850
      IAKZ=IAKZ+1                                                          860
      IF(.NOT.TEST2) CALL FSWR07(1011,'FIRS',EMAT(1),EMAT(2),              870
     *ETYPL(1),ETYPL(2),ENERGA,QUERA)                                      880
      CALL FSWR04(2013,QUERA,' UGR',UGR,CGR)                               890
      NAB=NAB+1                                                            900
      IF(NAB.GT.MAB) CALL FSWR03(3001,'FSQU','ER  ',3)                     910
      AB(NAB,1)=OGR                                                        920
      AB(NAB,2)=0.0                                                        930
      AB(NAB,3)=QUERA                                                      940
      AB(NAB,4)=0.0                                                        950
      IF(AB(NAB,3).NE.0.0) AB(NAB,4)=1.0                                   960
      GOTO 330                                                             970
C     WEITERE DATENPUNKTE EINLESEN.                                        980
  100 QUERN=QUERA                                                          990
      ENERGN=ENERGA                                                       1000
      IF(IFALL.EQ.30) INSERT=.TRUE.                                       1010
  101 ENERGA=ENERGN                                                       1020
      QUERA=QUERN                                                         1030
      IRC=0                                                               1040
      CALL NDFNXT(IRC,IARG2,ARG3,ARG4,ARG5)                               1050
C     ENDE DER DATEN DES BETREFFENDEN TYPS ERREICHT?                      1060
      IF(IRC.EQ.1) GOTO 102                                               1070
      IF(FSTCLE(ENERGA,OGR,GLSCH)) GOTO 113                               1080
C     KEIN PUNKT DES BETREFFENDEN QUERSCHNITTS MEHR VORHANDEN.            1090
C     IGEL MUSS >= 2 SEIN.                                                1100
      IF(IGEL.LT.2) CALL FSWR05(3016,EMAT(1),EMAT(2),ETYPL(1),            1110
     *ETYPL(2),IGEL)                                                      1120
      IF(IGEL.LT.2) GOTO 773                                              1130
      IF(IFALL.EQ.10) GOTO 103                                            1140
      IF(IFALL.EQ.30) GOTO 104                                            1150
      CALL FSWR03(3001,'FSQU','ER  ',4)                                   1160
  103 CONTINUE                                                            1170
C     ( IFALL=10 ) . VERGLEICHE L.G.D.P. MIT UGR UND CGR.                 1180
      IF(ENERGA.LT.UGR.OR.FSTOLE(ENERGA,UGR,GLSCH)) GOTO 105              1190
      IF(ENERGA.GE.OGR.OR.FSTCLE(ENERGA,CGR,GLSCH)) CALL FSWR03(3001,     1200
     *'FSQU','ER  ',5)                                                    1210
C     IFALL=13                                                            1220
      IFALL=13                                                            1230
  116 CALL FSWR07(1011,' LAS',EMAT(1),EMAT(2),ETYPL(1),ETYPL(2),          1240
     *ENERGA,QUERA)                                                       1250
      CALL FSWR04(-2013,QUERN,'   E',ENERGA,CGR)                          1260
  106 NAB=NAB+1                                                           1270
      IF(NAB.GT.MAB) GOTO 330                                             1280
      AB(NAB,1)=OGR                                                       1290
      AB(NAB,2)=0.0                                                       1300
      AB(NAB,3)=QUERN                                                     1310
      AB(NAB,4)=0.0                                                       1320
      IF(AB(NAB,3).NE.0.0) AB(NAB,4)=1.0                                  1330
      GOTO 330                                                            1340
  105 CONTINUE                                                            1350
C     IFALL=11                                                            1360
      IFALL=11                                                            1370
      CALL FSWR07(1011,' LAS',EMAT(1),EMAT(2),ETYPL(1),ETYPL(2),          1380
     *ENERGN,QUERN)                                                       1390
      CALL FSWR04(-2013,QUERA,' UGR',UGR,OGR)                             1400
      GOTO 106                                                            1410
  104 CONTINUE                                                            1420
C     ( IFALL=30 ). VERGLEICHE L.G.D.P. MIT UGR UND CGR.                  1430
      IF(ENERGA.LT.UGR.OR.FSTOLE(ENERGA,UGR,GLSCH)) GOTO 107              1440
      IF(ENERGA.GT.CGR.OR.FSTCLE(ENERGA,CGR,GLSCH)) CALL FSWR03(3001,     1450
     *'FSQU','ER  ',6)                                                    1460
C     IFALL=33                                                            1470
      IFALL=33                                                            1480
      GOTO 116                                                            1490
C     IFALL=31                                                            1500
  107 IFALL=31                                                            1510
      CALL FSWR04(3017,EMAT(1),EMAT(2),ETYPL(1),ETYPL(2))                 1520
      GOTO 773                                                            1530
  102 CONTINUE                                                            1540
      ENERGN=ARG3(4)                                                      1550
      QUERN=ARG3(5)                                                       1560
      IGEL=IGEL+1                                                         1570
      IF(TEST3) CALL FSWRC2(1012,ENERGN,QUERN)                            1580
C     PRUEFUNG OB ENERGIEN ANSTEIGEN.                                     1590
      IF(ENERGN.GT.ENERGA) GOTO 108                                       1600
      CALL FSWR04(3017,EMAT(1),EMAT(2),ETYPL(1),ETYPL(2))                 1610
      GOTO 773                                                            1620
  108 CONTINUE                                                            1630
C     PUNKT EINFUEGEN?                                                    1640
      IF(INSERT) GOTO 109                                                 1650
C     ENERGN > UGR ?                                                      1660
      IF(ENERGN.LT.UGR.OR.FSTOLE(ENERGN,UGR,GLSCH)) GOTO 101              1670
      IF(ENERGA.LT.UGR.OR.FSTCLE(ENERGA,UGR,GLSCH)) GOTO 110              1680
      CALL FSWR04(3017,EMAT(1),EMAT(2),ETYPL(1),ETYPL(2))                 1690
      GOTO 773                                                            1700
  110 INSERT=.TRUE.                                                       1710
  109 IAKZ=IAKZ+1                                                         1720
C     GERADE BERECHNEN.                                                   1730
      NAB=NAB+1                                                           1740
      IF(NAB.GT.MAB) GOTO 111                                             1750
      AB(NAB,1)=ENERGN                                                    1760
      C=1.0/(ENERGN-ENERGA)                                               1770
      AB(NAB,2)=(QUERN-QUERA)*C                                           1780
      AB(NAB,3)=(QUERA*ENERGN-QUERN*ENERGA)*C                             1790
      AB(NAB,4)=1.0                                                       1800
      IEND=1                                                              1810
```

```
  114 IF(AB(NAB,2).NE.0.0.OR.AB(NAB,3).NE.0.0) GOTO 112                1820
      AB(NAB,4)=0.0                                                    1830
      GOTO 111                                                         1840
  112 Y1=QUERA                                                         1850
      IF(NAB.EQ.2) Y1=AB(2,2)*AB(1,1)+AB(2,3)                          1860
      Y2=QUERN                                                         1870
      IF(IEND.EQ.2) Y2=AB(NAB,2)*AB(NAB,1)+AB(NAB,3)                   1880
      IF(Y1*Y2.LT.0.0) AB(NAB,4)=-1.0                                  1890
  111 IF(IEND.EQ.2) GOTO 115                                           1900
C     ENERGN >= OGR ?                                                  1910
      IF(ENERGN.LT.OGR) GOTO 101                                       1920
  113 IF(NAB.GT.MAB) GOTO 115                                          1930
      AB(NAB,1)=OGR                                                    1940
      IEND=2                                                           1950
      GOTO 114                                                         1960
  115 IF(TEST3) WRITE(NO,1001) IGEL,IAKZ                               1970
 1001 FORMAT(' SUBROUTINE FSQUER. IGEL=',I6,'  IAKZ=',I6,'.')          1980
  330 IF(.NOT.TEST3) GOTO 332                                          1990
      DO 331 I=1,NAB                                                   2000
      WRITE(NO,1000) I,(AB(I,J),J=1,4)                                 2010
 1000 FORMAT(' AB: I=',I5,' E=',1PE13.6,' EV  A=',1PE13.6,' B=',       2020
     *1PE13.6,' AB(I,4)=',1PE12.4,'.')                                 2030
  331 CONTINUE                                                         2040
  332 CONTINUE                                                         2050
C     BEI NAB .GT. MAB KEINE PRUEFUNG DER QUERSCHNITTE AUF 0 ODER < 0. 2060
      IF(NAB.GT.MAB) GOTO 770                                          2070
C     FUER TYP=SGT,SGN,SGA,SGF TEST OB NEGATIV ODER =0.                2080
C     BEI SGT NEGATIV ODER GLEICH 0 WARNUNGSAUSDRUCK UND FEHLERSTOP.   2090
C     SONST NUR WARNUNGSAUSDRUCK.                                      2100
      IF(TYP.NE.TYPSGT.AND.TYP.NE.TYPSGN.AND.TYP.NE.TYPSGA.AND.        2110
     *TYP.NE.TYPSGF) GOTO 329                                          2120
      FIRST=.TRUE.                                                     2130
      PRINT=.FALSE.                                                    2140
      FELCON=.FALSE.                                                   2150
      DO 120 I=2,NAB                                                   2160
      IF(AB(I,4).GT.0.0) GOTO 121                                      2170
      PRINT=.TRUE.                                                     2180
      FELCON=.TRUE.                                                    2190
      IF(FIRST) GOTO 122                                               2200
  123 BE=AB(I,1)                                                       2210
      GOTO 120                                                         2220
  122 BA=AB(I-1,1)                                                     2230
      FIRST=.FALSE.                                                    2240
      GOTO 123                                                         2250
  121 IF(.NOT.PRINT) GOTO 120                                          2260
      PRINT=.FALSE.                                                    2270
      CALL FSWR06(2015,EMAT(1),EMAT(2),ETYPL(1),ETYPL(2),BA,BE)        2280
  120 CONTINUE                                                         2290
      IF(PRINT) CALL FSWR06(2015,EMAT(1),EMAT(2),ETYPL(1),ETYPL(2),BA,BE 2300
     *)                                                                2310
      IF(FELCON.AND.TYP.EQ.TYPSGT) GOTO 773                            2320
  329 IF(NAB.GT.MAB) GOTO 770                                          2330
  333 RETURN                                                           2340
  770 MABP=NAB-MAB                                                     2350
  777 RETURN 1                                                         2360
  773 RETURN 2                                                         2370
      END                                                              2380
```

```
      SUBROUTINE FSWR00(N)                                              10
C     DRUCKT MELDUNGEN, WARNUNGEN UND FEHLERMELDUNGEN.                  20
C     N=1      NULLSETZEN VON FELARR.                                   30
C     1000+1 <=  N  <= 1000+NMMAX    MELDUNGEN.                        40
C     2000+1 <=  N  <= 2000+NWMAX    WARNUNGEN.                        50
C     3000+1 <=  N  <= 3000+NEMAX    FEHLER.                           60
C                                                                       70
      INTEGER FELARR                                                    80
      DIMENSION FELARR(18,3)                                            90
      COMMON NRL(4),NO                                                 100
      COMMON/CFSTRF/ FELARR,NGMAX                                      110
  999 CONTINUE                                                         120
      NIN=N                                                            130
      NMMAX=15                                                         140
      NWMAX=18                                                         150
      NEMAX=17                                                         160
      NGMAX=MAXO(NMMAX,NWMAX,NEMAX)                                    170
C     VORSCHUB NUR, WENN N>0.                                          180
      IF(NIN.GT.0) WRITE(NO,1000)                                      190
 1000 FORMAT(' ')                                                      200
      NIN=IABS(NIN)                                                    210
C     TYP DER MELDUNG.                                                 220
      ITYP=0                                                           230
      IF(NIN.EQ.1) ITYP=4                                              240
      IF(NIN.GE.1001.AND.NIN.LE.(1000+NMMAX)) ITYP=1                   250
      IF(NIN.GE.2001.AND.NIN.LE.(2000+NWMAX)) ITYP=2                   260
      IF(NIN.GE.3001.AND.NIN.LE.(3000+NEMAX)) ITYP=3                   270
      IF(ITYP.EQ.0) GOTO 770                                           280
C     TYPVERTEILER.                                                    290
      GO TO(1,2,3,4),ITYP                                              300
                                                                       310
      GOTO 770                                                         320
    1 NI=NIN-1000                                                      330
C     M E L D U N G E N .   LABELS 1001, 1002, ...                     340
C                           FORMATSTATEMENTS 11001, 11002, ...         350
      FELARR(NI,1)=FELARR(NI,1)+1                                      360
      CALL FSWRS1(NI,IV1,IV2,IV3,IV4,IV5,IV6,IV7,IV8,IV9,&770)         370
                                                                       380
      GOTO 333                                                         390
    2 NI=NIN-2000                                                      400
C     W A R N U N G E N .   LABELS 2001, 2002, ...                     410
C                           FORMATSTATEMENTS 12001, 12002, ...         420
      FELARR(NI,2)=FELARR(NI,2)+1                                      430
      CALL FSWRS2(NI,IV1,IV2,IV3,IV4,IV5,IV6,IV7,IV8,IV9,&770)         440
      GOTO 333                                                         450
    3 NI=NIN-3000                                                      460
C     F E H L E R .   LABELS 3001, 3002, ...                           470
C                     FORMATSTATEMENTS 13001, 13002, ...               480
      FELARR(NI,3)=FELARR(NI,3)+1                                      490
      CALL FSWRS3(NI,IV1,IV2,IV3,IV4,IV5,IV6,IV7,IV8,IV9,&770,&773)    500
      GOTO 333                                                         510
```

```
C     NULLSETZEN VON FELARR.                                                    500
    4 DO 6 I=1,NGMAX                                                            510
      DO 6 J=1,3                                                                520
    6 FELARR(I,J)=0                                                             530
      GOTO 333                                                                  540
  333 RETURN                                                                    550
C     NICHT DEFINIERTE NACHRICHTENNUMMER.                                       560
  770 NULL=0                                                                    570
      WRITE(NO,3000) NULL                                                       580
 3000 FORMAT('0***   ERROR 3.',I2)                                             590
      WRITE(NO,771) N,NMMAX,NWMAX,NEMAX                                         600
  771 FORMAT('+',16X,'  PROGRAM OR MACHINE ERROR IN FSWRCO. N HAS THE VA        610
     *LUE',I12,'.'/                                                             620
     *' ',16X,'  BUT IT MUST BE IN ONE OF THE FOLLOWING INTERVALS:'/            630
     *' ',16X,'  1001 TO 1000+',I4/                                            640
     *' ',16X,'  2001 TO 2000+',I4/                                            650
     *' ',16X,'  3001 TO 3000+',I4)                                            660
  773 WRITE(NO,772)                                                             670
  772 FORMAT('0',120('*')/' ',45('*'),'   P R O G R A M   S T O P    ',        680
     *45('*')/' ',120('*'))                                                     690
  777 STOP                                                                      700
      ENTRY FSWRO1(N,IV1)                                                       710
      GOTO 999                                                                  720
      ENTRY FSWRO2(N,IV1,IV2)                                                   730
      GOTO 999                                                                  740
      ENTRY FSWRO3(N,IV1,IV2,IV3)                                               750
      GOTO 999                                                                  760
      ENTRY FSWRO4(N,IV1,IV2,IV3,IV4)                                           770
      GOTO 999                                                                  780
      ENTRY FSWRO5(N,IV1,IV2,IV3,IV4,IV5)                                       790
      GOTO 999                                                                  800
      ENTRY FSWRO6(N,IV1,IV2,IV3,IV4,IV5,IV6)                                   810
      GOTO 999                                                                  820
      ENTRY FSWRO7(N,IV1,IV2,IV3,IV4,IV5,IV6,IV7)                               830
      GOTO 999                                                                  840
      ENTRY FSWRO8(N,IV1,IV2,IV3,IV4,IV5,IV6,IV7,IV8)                           850
      GOTO 999                                                                  860
      ENTRY FSWRO9(N,IV1,IV2,IV3,IV4,IV5,IV6,IV7,IV8,IV9)                       870
      GOTO 999                                                                  880
      END                                                                       890
```

```
      SUBROUTINE FSWRS1(NI,IV1,IV2,IV3,IV4,IV5,IV6,IV7,IV8,IV9,*)               10
      COMMON NR1(4),NO                                                          20
C     M E L D U N G E N .   LABELS 1001, 1002, ...                              30
C                           FORMATSTATEMENTS 11001, 11002, ...                  40
      WRITE(NO,1000) NI                                                         50
 1000 FORMAT(' *** MESSAGE 3.',I2)                                              60
      GOTO (1001,1002,1003,1004,1005,1006,1007,1008,1009,1010,1011,1012,        70
     *1013,1014,1015                                                            80
     *),NI                                                                      90
      GOTO 770                                                                  100
 1001 WRITE(NO,11001) IV1,IV2                                                   110
11001 FORMAT('+',16X,'  PROGRAMM KENNZIFFER 3'/                                 120
     *       '+',16X,'  ______________________'/                                130
     *'0',16X,'  PROGRAMM ZUR BERECHNUNG VON RESONANZSELBSTABSCHIRMFAKTO        140
     *REN VON PUNKTWEISE GEGEBENEN'/                                            150
     *' ',16X,'  WIRKUNGSQUERSCHNITTEN FUER DAS MATERIAL ',2A4,'.'/)            160
      GOTO 333                                                                  170
 1002 WRITE(NO,11002) IV1                                                       180
11002 FORMAT('+',16X,'  PROGRAM 3 HAS ENDED CORRECTLY. KL HAS THE VALUE=        190
     *',I4,'.')                                                                 200
      GOTO 333                                                                  210
 1003 WRITE(NO,11003)                                                           220
11003 FORMAT('+',16X,'  AFTER CHANGING ARRAY DIMENSIONS PROGRAM WILL BE         230
     *CALLED ONCE MORE.')                                                       240
      GOTO 333                                                                  250
 1004 WRITE(NO,11004)                                                           260
11004 FORMAT('+',16X,'  PROGRAM-CONTROL-DATA HAVE BEEN CHECKED. NO ERROR       270
     *S FOUND.')                                                                280
      GOTO 333                                                                  290
 1005 IF(IV1.LT.10) WRITE(NO,11005) IV1                                         300
11005 FORMAT('+',16X,'  FIRST RECORD WRITTEN ON FT0',I1,'F001.')                310
      IF(IV1.GT.10) WRITE(NO,21005) IV1                                         320
21005 FORMAT('+',16X,'  FIRST RECORD WRITTEN ON FT',I2,'F001.')                 330
      GOTO 333                                                                  340
 1006 WRITE(NO,11006)                                                           350
11006 FORMAT('+',16X,'  ALL CROSS SECTION TYPES NEEDED FOR THE FOLLOWING       360
     * CALCULATIONS FOUND ON KEDAK.')                                           370
      GOTO 333                                                                  380
 1007 WRITE(NO,11007)                                                           390
11007 FORMAT('+',16X,'  INTEGRATION BOUNDARIES AND ASSOCIATED VALUES FOR       400
     * ONE GROUP HAVE BEEN DEFINED.')                                           410
      GOTO 333                                                                  420
 1008 WRITE(NO,11008)                                                           430
11008 FORMAT('+',16X,'  INTEGRATION OF THE FUNCTION(S)')                        440
      IF(IV1.LT.1.OR.IV1.GT.9) IV1=1                                            450
      GOTO (1,2,3,4,5,6,7,8,9),IV1                                              460
    1 WRITE(NO,12008)                                                           470
      GOTO 10                                                                   480
    2 WRITE(NO,13008)                                                           490
      GOTO 10                                                                   500
    3 WRITE(NO,14008)                                                           510
      GOTO 10                                                                   520
    4 WRITE(NO,15008)                                                           530
      GOTO 10                                                                   540
    5 WRITE(NO,16008)                                                           550
      GOTO 10                                                                   560
    6 WRITE(NO,17008)                                                           570
      GOTO 10                                                                   580
    7 WRITE(NO,18008)                                                           590
      GOTO 10                                                                   600
    8 WRITE(NO,19008)                                                           610
      GOTO 10                                                                   620
    9 WRITE(NO,20008)                                                           630
      GOTO 10                                                                   640
12008 FORMAT('+',51X,'F(E)')                                                    650
13008 FORMAT('+',51X,'    * F(E)')                                              660
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```
14008 FORMAT('+',51X,'SGN * MUEL * F(E)')                                  670
15008 FORMAT('+',51X,'1.0 / (SGT + SIGO) * F(E)')                          680
16008 FORMAT('+',51X,'1.0 / ((SGT + SIGO)**2) * F(E)')                     690
17008 FORMAT('+',51X,'    / (SGT + SIGO) * F(E)')                          700
18008 FORMAT('+',51X,'SGT / ((SGT + SIGO)**2) * F(E)')                     710
19008 FORMAT('+',51X,'SGN * MUEL / (SGT + SIGO) * F(E)')                   720
20008 FORMAT('+',51X,'SGN * MUEL / ((SGT + SIGO)**2) * F(E)')              730
   10 IF(IV1.NE.2.AND.IV1.NE.6) GOTO 11                                    740
      IF(IV2.EQ.1) WRITE(NO,21008)                                         750
      IF(IV2.EQ.2) WRITE(NO,22008)                                         760
      IF(IV2.EQ.3) WRITE(NO,23008)                                         770
      IF(IV2.EQ.4) WRITE(NO,24008)                                         780
21008 FORMAT('+',51X,'SGT')                                                790
22008 FORMAT('+',51X,'SGA')                                                800
23008 FORMAT('+',51X,'SGN')                                                810
24008 FORMAT('+',51X,'SGF')                                                820
   11 IF(IV1.GE.4) WRITE(NO,26008) IV3,IV4                                 830
26008 FORMAT(31X,'( FIRST SIGO=',1PE12.6,'  LAST SIGO=',1PE12.6,' )')      840
      GOTO 333                                                             850
 1009 WRITE(NO,11009) IV1,IV2,IV3,IV4,IV5,IV6,IV7,IV8,IV9                  860
11009 FORMAT('+',56X,'EXACT PORTION',13X,'INACCURATE PORTIONS'/             870
     *' ',60X,'YF(2)',16X,'YF(1)',12X,'YF(3)'/                             880
     *' ',16X,'  VALUE ',32X,1PE13.6,8X,1PE13.6,4X,1PE13.6/                890
     *' ',16X,'  VALUE IN % OF YF(1)+YF(2)+YF(3) ',10X,0PF6.2,15X,         900
     *0PF6.2,7X,0PF6.2/                                                    910
     *' ',16X,'  RELATIVE ERROR BETTER OR EQUAL THAN ',2X,1PE13.6,         920
     *8X,1PE13.6,4X,1PE13.6)                                               930
      GOTO 333                                                             940
 1010 WRITE(NO,11010) IV1,IV2,IV3,IV4,IV5,IV6                              950
11010 FORMAT('+',16X,'  ',A3,A4,' WEIGHTED INTEGRAL FROM=',1PE13.6,        960
     *' EV  TO=',1PE13.6,' EV  OF REACTION TYPE ',A3,' =',1PE13.6,'.')     970
      GOTO 333                                                             980
 1011 WRITE(NO,11011) IV1,IV2,IV3,IV4,IV5,IV6,IV7                          990
11011 FORMAT('+',16X,'  ',A4,'T POINT FOR MATERIAL ',2A4,' CROSS SECTION 1000
     * TYPE ',2A4,' HAS BEEN READ.'/' ',16X,'  E(1)=',1PE13.6,' EV  Q(1) 1010
     *=',1PE13.6,' BARN.')                                                1020
      GOTO 333                                                             1030
 1012 WRITE(NO,11012) IV1,IV2                                              1040
11012 FORMAT('+',16X,'  E=',1PE13.6,' EV  Q=',1PE13.6,' BARN.')            1050
      GOTO 333                                                             1060
 1013 WRITE(NO,11013) IV1,IV2,IV3                                          1070
11013 FORMAT('+',16X,'  TERM TO CALCULATE WAS:  ',                         1080
     *1PE13.6,'/(',1PE13.6,'*',1PE13.6,').')                              1090
      GOTO 333                                                             1100
 1014 WRITE(NO,11014) IV1,IV2,IV3,IV4,IV5,IV6                              1110
11014 FORMAT('+',16X,'  TERM TO CALCULATE WAS:'/                           1120
     *' ',16X,'  (',1PE13.6,'/',1PE13.6,'-',1PE13.6,'/',1PE13.6,          1130
     *') / (',1PE13.6,'-',1PE13.6,')')                                     1140
      GOTO 333                                                             1150
 1015 WRITE(NO,11015) IV1,IV2,IV3                                          1160
11015 FORMAT('+',16X,'  RESULT FROM=',1PE13.6,' EV  TO=',1PE13.6,          1170
     *' EV  IS=',1PE13.6,'.')                                              1180
      GOTO 333                                                             1190
  333 RETURN                                                               1200
  770 RETURN 1                                                             1210
      END                                                                  1220
```

```
      SUBROUTINE FSWRS2(NI,IV1,IV2,IV3,IV4,IV5,IV6,IV7,IV8,IV9,*)          10
      COMMON NR1(4),NO                                                     20
C     W A R N U N G E N .   LABELS 2001, 2002, ...                         30
C                           FORMATSTATEMENTS 12001, 12002, ...             40
      WRITE(NO,2000) NI                                                    50
 2000 FORMAT(' *** WARNING 3.',I2)                                         60
      GOTO (2001,2002,2003,2004,2005,2006,2007,2008,2009,2010,2011,2012,   70
     *2013,2014,2015,2016,2017,2018                                        80
     *),NI                                                                 90
      GOTO 770                                                             100
 2001 WRITE(NO,12001) IV1,IV2                                              110
12001 FORMAT('+',16X,'  FOR GROUP NUMBER',I4,' NO CALCULATIONS CAN BE DO   120
     *NE. IT IS THE GROUP WITH THE LOWER BOUNDARY IN THE'/                 130
     *' ',16X,'  THERMAL REGION. THE GROUP NUMBER FOR WHICH THE CALCULAT   140
     *IONS WILL START IS SET TO',I4,'.')                                   150
      GOTO 333                                                             160
 2002 WRITE(NO,12002) IV1,IV2,IV3                                          170
12002 FORMAT('+',16X,'  THE GROUP NUMBER',I4,' IS OUTSIDE THE GROUP STRU   180
     *CTURE DEFINED BY THE',I4,' GROUP BOUNDARIES.'/                       190
     *' ',16X,'  THE GROUP NUMBER FOR WHICH THE CALCULATIONS WILL START    200
     *IS SET TO',I4,'.')                                                   210
      GOTO 333                                                             220
 2003 WRITE(NO,12003) IV1,IV2                                              230
12003 FORMAT('+',16X,'  ADDITIONALLY THE GROUP NUMBER FOR WHICH THE CALC   240
     *ULATIONS SHOULD END IS SET TO',I4,','/                               250
     *' ',16X,'  BECAUSE IT HAS BEEN GREATER THAN',I4,'.')                 260
      GOTO 333                                                             270
 2004 WRITE(NO,12004)                                                      280
12004 FORMAT('+',16X,'  IN ROMBERG INTEGRATION DESIRED ACCURACY COULD NO   290
     *T BE REACHED BECAUSE OF ROUNDING ERRORS.'/                           300
     *' ',16X,'  APPROXIMATION TAKEN AND OTHER INFORMATION IS PRINTED IN   310
     * THE FOLLOWING.')                                                    320
      GOTO 333                                                             330
 2005 WRITE(NO,12005) IV1,IV2                                              340
12005 FORMAT('+',16X,'  FROM=',1PE13.6,                                    350
     *' EV  TO=',1PE13.6,' EV  HAS BEEN GIVEN THE RESULT ZERO BECAUSE')    360
      GOTO 333                                                             370
 2006 WRITE(NO,12006)                                                      380
12006 FORMAT('+',16X,'  THE POINTWISE GIVEN WEIGHTING SPECTRUM IS ZERO I   390
     *N THE GIVEN INTEGRATION RANGE.')                                     400
      GOTO 333                                                             410
 2007 WRITE(NO,12007)                                                      420
12007 FORMAT('+',16X,38X,' IS COMPLETELY ZERO IN THE GIVEN INTEGRATION R   430
     *ANGE.')                                                              440
   10 IF(IV1.EQ.3) WRITE(NO,13007)                                         450
      IF(IV1.EQ.1.AND.IV2.GT.3) WRITE(NO,14007)                            460
      IF(IV1.EQ.2.AND.IV2.GT.3) WRITE(NO,15007)                            470
      IF(IV1.EQ.1.AND.IV2.LE.3) WRITE(NO,16007)                            480
      IF(IV1.EQ.2.AND.IV2.LE.3) WRITE(NO,17007)                            490
13007 FORMAT('+',23X,'THE FUNCTION IN THE DENOMINATOR')                    500
14007 FORMAT('+',19X,'THE FIRST FUNCTION IN THE NUMERATOR')                510
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15007 FORMAT('+',18X,'THE SECCND FUNCTION IN THE NUMERATOR')
16CC7 FORMAT('+',36X,'THE FIRST FUNCTICN')
17007 FORMAT('+',35X,'THE SECCND FUNCTION')
      GCTO 333
 2008 WRITE(NO,12008)
12008 FORMAT('+',54X,' CHANGES THE SIGN IN THEGIVEN INTEGRATION RANGE.')
      GOTO 10
 2009 WRITE(NO,12009)
12009 FORMAT('+',16X,'  ADDITIONALLY'/' ',54X,' IS COMPLETELY ZERO IN TH
     * THE GIVEN INTEGRATION RANGE.')
      GCTO 10
 2010 WRITE(NO,12010)
12010 FORMAT('+',16X,'  ADDITIONALLY'/' ',54X,' CHANGES THESIGN IN THE G
     *IVEN INTEGRATION RANGE.')
      GOTO 10
 2011 WRITE(NO,12011) IV1
12011 FORMAT('+',16X,'  THE RESULT MAY BE INACCURATE. WISHED RELATIVE ER
     *ROR=',1PE13.6,'.')
      GCTO 333
 2012 WRITE(NO,12012)
12012 FORMAT('+',16X,'  THE AVERAGE GROUP CROSS SECTIONS FOR INFINITE DI
     *LUTION ARE SET TO ZERO BECAUSE'/' ',16X,'  THE INTEGRAL OF THE WEI
     *GHTING FUNCTION IS ZERO IN THE GIVEN INTEGRATION RANGE.')
      GCTO 333
 2013 WRITE(NO,12013) IV1,IV2,IV3,IV4
12013 FORMAT('+',16X,'  THIS CROSS-SECTION VALUE ( ',1PE13.6,
     *' BARN ) WILL BE TAKEN FROM',A4,'=',1PE13.6,' EV  TC OGR=',
     *1PE13.6,' EV.')
      GCTO 333
 2014 WRITE(NO,12014) IV1,IV2
12014 FORMAT('+',16X,'  THE SELF SHIELDING FACTOR ',A4,' ( SIGO=',
     *1PE13.6,' ) HAS BEEN SET TO 1.0,'/
     *' ',16X,'  BECAUSE IN CALCULATING THIS FACTOR A DIVISICN BY ZERO H
     *AD TO BE DONE.')
      GCTO 333
 2015 WRITE(NO,12015) IV1,IV2,IV3,IV4,IV5,IV6
12015 FORMAT('+',16X,'  FOR MATERIAL ',2A4,' THE CROSS SECTICN TYPE ',
     *2A4,' IS LESS OR EQUAL ZERO AT LEAST'/
     *' ',16X,'  IN SOME PARTS OF THE ENERGY RANGE ',1PE13.6,
     *' EV  UNTIL ',1PE13.6,' EV.')
      GCTO 333
 2016 WRITE(NO,12016) IV1,IV2
12016 FORMAT('+',16X,'  THE SELF SHIELDING FACTOR ',A4,' ( SIGO=',
     *1PE12.6,' ) HAS BEEN CALCULATED AS ZERC, BECAUSE')
      GCTO 333
 2017 WRITE(NO,12017) IV1,IV2,IV3
12017 FORMAT('+',16X,'  THE SELF SHIELDING FACTCR(S) ',A4,
     *' FROM SIGO=',1PE12.6,'  TO SIGO=',1PE12.6)
      WRITE(NO,13017)
13017 FORMAT(' ',16X,'  HAVE BEEN SET TO 1.0, BECAUSE IN CALCULATING THI
     *S FACTORS, DIVISION(S) BY ZERO HAD TO BE DONE.')
      GOTO 333
 2018 WRITE(NO,12017) IV1,IV2,IV3
      WRITE(NO,12018)
12018 FORMAT(' ',16X,'  HAVE BEEN CALCULATED AS ZERC.')
      GOTO 333
  333 RETURN
  770 RETURN 1
      END
```

```
      SUBRCUTINE FSWRS3(NI,IV1,IV2,IV3,IV4,IV5,IV6,IV7,IV8,IV9,*,*)
      COMMON NR1(4),NO
C     F E H L E R .   LABELS 3001, 3002, ...
C                     FORMATSTATEMENTS 13001, 13002, ...
      WRITE(NO,3000) NI
 3000 FORMAT(' ***   ERROR 3.',I2)
      GOTO (3001,3002,3003,3004,3005,3006,3007,3008,3009,3010,3011,3012,
     *3013,3014,3015,3016,3017
     *),NI
      GCTO 770
 3001 WRITE(NO,13001) IV1,IV2,IV3
13001 FORMAT('+',16X,'  PROGRAM- OR MACHINE-ERROR IN SUBRCUTINE ',
     *A4,A2,' TESTPCINT',I4,'.')
      GCTO 773
 3002 WRITE(NO,13002)
13002 FORMAT('+',16X,'  THE PROGRAM CONTROL DATA CR THE DATA GIVEN IN KE
     *DAK CR IN THE WEIGHTING SPECTRUM'/
     *' ',16X,'  WILL NCT ALLCW CALCULATION OF AVERAGE GROUP CROSS SECTI
     *CNS FOR INFINITE DILUTION AND OF'/
     *' ',16X,'  ENERGY RESONANCE SELF SHIELDING FACTCRS FROM ENERGY POI
     *NT WISE DATA IN THE RESCNANCE REGION.')
      GCTC 333
 3003 WRITE(NO,13003) IV1,IV2
13003 FORMAT('+',16X,'  THE NUMBER OF THE FIRST GROUP=',I4,
     *' FOR WHICH CALCULATICNS SHOULD BE DONE IS LESS'/
     *' ',16X,'  THAN THE NUMBER OF THE LAST GROUP=',I4,'.')
      GCTC 333
 3004 WRITE(NO,13004) IV1,IV2
13004 FORMAT('+',16X,'  IN THE CASE OF ONE AND ONLY ONE ENERGY SPECTRUM
     *ENBER(1) HAS THE VALUE ',1PE14.6,'.'/
     *' ',16X,'  BUT IT MUST BE EQUAL -1.0 OR GREATER OR EQUAL ',1PE14.6
     *,'.')
      GCTO 333
 3005 WRITE(NO,13005) IV1
13005 FORMAT('+',16X,'  ERRANOUES ENERGY GROUP BCUNDARIES IN GRCUP',
     *I5,'.')
      GOTO 333
 3006 WRITE(NO,13006) IV1,IV2,IV3
13006 FORMAT('+',16X,'  IN THE',I3,'. WEIGHTING SPECTRUM RANGE ABSOLUTE
     *VALUE OF ACTUELL NETYP=',I3/' ',16X,'  IS GREATER THAN THE MAXIMUM
     * POSSIBLE VALUE MNETYP=',I3,'.')
      GOTO 333
 3007 WRITE(NO,13007) IV1
13007 FORMAT('+',16X,' IN THE',I3,'. WEIGHTING SPECTRUM RANGE A POINTWIS
     *E SPECTRUM WAS WISHED.'/' ',16X,
     *'  NO SUCH SPECTRUM HAS BEEN MADE AVAILABLE TO THE PROGRAM.')
      GOTO 333
```

```
 3008 WRITE(NO,13008) IV1,IV2,IV3,IV4                                   480
13008 FORMAT('+',16X,'  NO DATA FOUND FOR MATERIAL ',2A4,' TYP ',2A4,'.'  490
     *)                                                                500
      GOTO 333                                                         510
 3009 WRITE(NO,13009) IV1,IV2, IV3, IV4, IV5,IV6                       520
13009 FORMAT('+',16X,'  THE VARIABLE ',A4,A2,' HAS THE VALUE ',I12,'.'/  530
     *' ',16X,'  BUT IT MUST BE ',A4,' ',A4,' ',I12,'.')               540
      GOTO 333                                                         550
 3010 WRITE(NO,13010) IV1,IV2, IV3, IV4, IV5,IV6                       560
13010 FORMAT('+',16X,'  THE VARIABLE ',A4,A2,' HAS THE VALUE ',1PE14.6,  570
     *'.'/' ',OP16X,'  BUT IT MUST BE ',OPA4,' ',A4,' ',1PE14.6,'.')   580
      GOTO 333                                                         590
 3011 WRITE(NO,13011) IV1,IV2,IV3, IV4, IV5, IV6,IV7                   600
13011 FORMAT('+',16X,'  THE ARRAY ELEMENT ',A4,A2,'(',I5,') HAS THE VALU  610
     *E ',I12,'.'/' ',16X,' BUT IT MUST BE ',A4,' ',A4,' ',I12,'.')    620
      GOTO 333                                                         630
 3012 WRITE(NO,13012) IV1,IV2,IV3, IV4, IV5, IV6,IV7                   640
13012 FORMAT('+',16X,'  THE ARRAY ELEMENT ',A4,A2,'(',I5,') HAS THE VALU  650
     *E ',1PE14.6,'.'/' ',OP16X,'  BUT IT MUST BE ',OPA4,' ',A4,' ',    660
     *1PE14.6,'.')                                                     670
      GOTO 333                                                         680
 3013 WRITE(NO,13013) IV1,IV2,IV3,IV4,IV5                              690
13013 FORMAT('+',16X,'  THE VARIABLE ',A4,A2,' HAS THE VALUE ',I12,'.'/  700
     *' ',16X,'  BUT IT MUST BE EQUAL ',I2,' OR EQUAL ',I2,'.')        710
      GOTO 333                                                         720
 3014 WRITE(NO,13014) IV1,IV2                                          730
13014 FORMAT('+',16X,'  THE POINTWISE WEIGHTING SPECTRUM IS NOT DEFINED  740
     *IN THE ENERGY RANGE ',1PE14.6,' EV  TO ',1PE14.6,' EV.')         750
      GOTO 333                                                         760
 3015 WRITE(NO,13015) IV1,IV2,IV3,IV4,IV5,IV6,IV7                      770
13015 FORMAT('+',16X,'  THE ',A4,A1,' ENERGY POINT OF THE POINTWISE WEIG  780
     *HTING SPECTRUM =',1PE14.6,' EV  IS ',A4,' THAN THE ',A4,A1/       790
     *' ',16X,'  BOUNDARY OF THE INTEGRATION RANGE =',1PE14.6,' EV.')   800
      GOTO 333                                                         810
 3016 WRITE(NO,13016) IV1,IV2,IV3,IV4,IV5                              820
13016 FORMAT('+',16X,'  FOR MATERIAL ',2A4,' CROSS SECTION TYPE ',      830
     *2A4,' ONLY ',I1,' POINT(S) HAVE BEEN FOUND ON THE LIBRARY.'/      840
     *' ',16X,'  ERRANEOUS LIBRARY ')                                  850
      GOTO 333                                                         860
 3017 WRITE(NO,13017)                                                  870
13017 FORMAT('+',16X,'  LIBRARY HAS BEEN FOUND ERRANEOUS. CHECK LIBRARY.  880
     *')                                                               890
      GOTO 333                                                         900
  333 RETURN                                                           910
  770 RETURN 1                                                         920
  773 RETURN 2                                                         930
      END                                                              940
```

```
      SUBROUTINE FSWRS9                                                 10
C     AUSDRUCK VON FELARR.                                              20
      LOGICAL*4 TEST1,TEST2,TEST3,LERMSG,PRINT                          30
      INTEGER FELARR                                                    40
      DIMENSION FELARR(18,3)                                            50
      COMMON NR1(4),NO                                                  60
      COMMON/CFSTRU/ TEST1,TEST2,TEST3,LERMSG                           70
      COMMON/CFSTRF/ FELARR,NGMAX                                       80
      DO 1 I=1,NGMAX                                                    90
      DO 1 J=2,3                                                       100
      IF(FELARR(I,J).EQ.0) GOTO 1                                      110
      GOTO 3                                                           120
    1 CONTINUE                                                         130
      WRITE(NO,1000)                                                   140
 1000 FORMAT('ONO WARNING- OR ERROR-MESSAGES PRODUCED IN MODULE FSTRUK.'  150
     *)                                                                160
  330 IF(.NOT.TEST1.AND..NOT.TEST2.AND..NOT.TEST3) GOTO 333             170
      WRITE(NO,1001)                                                   180
 1001 FORMAT('OTABLE OF MESSAGES PRODUCED OR PRINTED IN MODULE FSTRUK.'/  190
     *'OMESSAGE NUMBER  COUNT'/)                                       200
      DO 2 I=1,NGMAX                                                   210
      IF(FELARR(I,1).EQ.0) GOTO 2                                      220
      IP=I+1000                                                        230
      WRITE(NO,1002) IP,FELARR(I,1)                                    240
 1002 FORMAT(' ',5X,I4,7X,I4)                                          250
    2 CONTINUE                                                         260
  333 RETURN                                                           270
    3 PRINT=.TRUE.                                                     280
      DO 4 I=1,NGMAX                                                   290
      IF(FELARR(I,2).EQ.0) GOTO 4                                      300
      IF(.NOT.PRINT) GOTO 6                                            310
      WRITE(NO,1006)                                                   320
 1006 FORMAT(1H1)                                                      330
      CALL RAMANF(NO)                                                  340
      CALL A8FORM(NO,'WARNINGS')                                       350
      CALL A8FORM(NO,'PRODUCED')                                       360
      CALL RAMEND(NO)                                                  370
      WRITE(NO,1003)                                                   380
 1003 FORMAT('OTABLE OF WARNINGS PRINTED IN MODULE FSTRUK.'/           390
     *'OWARNING NUMBER  COUNT'/)                                       400
      PRINT=.FALSE.                                                    410
    6 IP=I+2000                                                        420
      WRITE(NO,1002) IP,FELARR(I,2)                                    430
    4 CONTINUE                                                         440
      PRINT=.TRUE.                                                     450
      DO 5 I=1,NGMAX                                                   460
      IF(FELARR(I,3).EQ.0) GOTO 5                                      470
      IF(.NOT.PRINT) GOTO 7                                            480
      WRITE(NO,1006)                                                   490
      CALL RAMANF(NO)                                                  500
      CALL A8FORM(NO,' ERRORS ')                                       510
      CALL A8FORM(NO,'PRODUCED')                                       520
      CALL RAMEND(NO)                                                  530
      WRITE(NO,1004)                                                   540
 1004 FORMAT('0',120('*')/' ',46('*'),'  ERRORS IN MODULE FSTRUK.  ',  550
     *46('*')/' ',120('*')/                                            560
     *'CTABLE OF ERRORS PRINTED IN MODULE FSTRUK.'/                     570
     *'OERROR NUMBER  COUNT.'/)                                        580
      PRINT=.FALSE.                                                    590
    7 IP=I+3000                                                        600
```

```
      WRITE(NO,1005) IP,FELARR(I,3)                                      610
 1005 FORMAT(' ',4X,I4,6X,I4)                                            620
    5 CONTINUE                                                           630
      GOTO 330                                                           640
      END                                                                650
```

```
      LOGICAL FUNCTION FSTOLE(A,B,GLSCH)                                  10
C     A TOLERANT ( AUSDRUCK NACH VORSCHLAG VON G. WILLERDING ) B          20
C       GENAU DANN WENN                                                   30
C     1)   A=B                                                           40
C        ODER                                                           50
C     2)   ABS((A-B)/AMAX1(ABS(A),ABS(B))) <= GLSCH                      60
C     WENN A TOLERANT B IST, HAT FSTOLE DEN WERT .TRUE. ANDERNFALLS      70
C     DEN WERT .FALSE.                                                  80
C     DIE RELATION IST SYMMETRISCH, D.H. A TOLERANT B GENAU DANN WENN    90
C     B TOLERANT A IST.                                                100
C                                                                      110
      IF(A.EQ.B) GOTO 2                                                120
      IF(ABS((A-B)/AMAX1(ABS(A),ABS(B))).LE.GLSCH) GOTO 2              130
    1 FSTOLE=.FALSE.                                                   140
      GOTO 333                                                         150
    2 FSTOLE=.TRUE.                                                    160
  333 RETURN                                                           170
      END                                                              180
```

```
      SUBROUTINE FSXINT(NXINT,MXINT,XINT,MXINTP,NV,V,ID1,ID2,*)           10
C     DIE WERTE V(J,1),J=1,NV , WELCHE DER BEDINGUNG                      20
C           XINT(1) <= V(J,1) <= XINT(NXINT)                              30
C     GENUEGEN, WERDEN IN XINT EINGEFUEGT.                                40
C     (DIE WERTE IN V MUESSEN GROESSER GLEICH 0.0 SEIN, SOWIE             50
C     UND EINE AUFSTEIGENDE REIHENFOLGE HABEN.)                           60
C     WERTE IN V, DIE NICHT BEI WERTEN IN XINT LIEGEN, WERDEN             70
C     NICHT UEBERNOMMEN.                                                  80
C     WIRD NXINT > MXINT SO WIRD MXINTP GESETZT UND RETURN 1 GEMACHT.     90
C     NXINT MUSS BEI EINEM FSXINT AUFRUF IMMER >= 2 SEIN. D.H. ES MUSS   100
C     VORHER EIN FSXIIN AUFRUF GEMACHT WORDEN SEIN.                      110
      LOGICAL*4 FSTOLE,TEST1,TEST2,TEST3,LERMSG                          120
      DIMENSION XINT(1),V(ID1,ID2)                                       130
      COMMON NR1(4),NO                                                   140
      COMMON/CFSTRU/ TEST1,TEST2,TEST3,LERMSG,GLSCH                      150
C                                                                        160
      IF(NXINT.GT.MXINT.OR.MXINT.LT.1.OR.NV.LT.1.OR.NXINT.LT.2.OR.       170
     *XINT(1).GE.XINT(NXINT)) CALL FSWR03(3001,'FSXI','NT  ',1)          180
C     I = LOOPINDEX IN XINT.                                             190
```

```
C     J = LOOPINDEX IN V.                                                200
      I=1                                                                210
      J=1                                                                220
C     TEST VON V(J,1).                                                   230
   10 IF(V(J,1).LT.0.0) CALL FSWR03(3001,'FSXI','NT  ',2)                240
      IF(J.LE.1) GOTO 2                                                  250
      IF(V(J,1).LT.V(J-1,1)) CALL FSWR03(3001,'FSXI','NT  ',3)           260
    2 CONTINUE                                                           270
C     VERGLEICHE V(J,1) MIT XINT(I)                                      280
      IF(FSTOLE(V(J,1),XINT(I),GLSCH)) GOTO 11                           290
      IF(V(J,1).GT.XINT(I)) GOTO 12                                      300
C     V(J,1) IST KLEINER ALS XINT(I). WENN I GROESSER ALS 1, WERT        310
C            EINFUEGEN UND J HOCHZAEHLEN.                                320
C            FUER I=1 NUR J HOCHZAEHLEN.                                 330
   13 IF(I.LE.1) GOTO 23                                                 340
      NXINT=NXINT+1                                                      350
      IF(NXINT.GT.MXINT) GOTO 88                                         360
      I=I+1                                                              370
      DO 3 II=I,NXINT                                                    380
    3 XINT(NXINT+I-II)=XINT(NXINT+I-II-1)                                390
      XINT(I-1)=V(J,1)                                                   400
   23 J=J+1                                                              410
      IF(J.LE.NV) GOTO 10                                                420
C     ALLE WERTE EINGEFUEGT. RETURN.                                     430
  330 IF(TEST2) WRITE(NO,1000) NXINT,(XINT(II),II=1,NXINT)               440
 1000 FORMAT('0INTEGRATIONSINTERVALS: NXINT=',I6,'.'/                    450
     *(' ',1P5E14.6,6X))                                                 460
  333 RETURN                                                             470
C     FELD XINT ZU KLEIN.                                                480
   88 MXINTP=NV-J+1                                                      490
  888 RETURN 1                                                           500
   11 CONTINUE                                                           510
C     V(J,1) GLEICH XINT(I). J HOCHZAEHLEN.                              520
      GOTO 23                                                            530
   12 CONTINUE                                                           540
C     V(J,1) GROESSER ALS XINT(I). I HOCHZAEHLEN.                        550
      I=I+1                                                              560
C     WENN I > NXINT WIRD, SIND ALLE WERTE <= XINT(NXINT) EINGEFUEGT.    570
C                        R E T U R N .                                   580
      IF(I.LE.NXINT) GOTO 10                                             590
      GOTO 330                                                           600
      ENTRY FSXIIN(NXINT,MXINT,XINT,UGR,OGR)                             610
C     INITIALISIERUNGSENTRY. DAS FELD XINT WIRD GLEICH -1.0 GESETZT.     620
C     XINT(1) WIRD GLEICH UGR UND XINT(2) WIRD GLEICH OGR GESETZT.       630
C     UGR MUSS KLEINER ALS OGR SEIN.                                     640
C     NXINT GIBT AN, WIE WEIT DAS FELD GEFUELLT IST. ES WIRD GLEICH 2    650
C     GESETZT.                                                           660
      IF(UGR.GE.OGR.OR.FSTOLE(UGR,OGR,GLSCH).OR.MXINT.LT.3)              670
     *CALL FSWR03(3001,'FSXI','NT  ',4)                                  680
      XINT(1)=UGR                                                        690
      XINT(2)=OGR                                                        700
      NXINT=2                                                            710
      DO 1 II=3,MXINT                                                    720
    1 XINT(II)=-1.0                                                      730
      GOTO 330                                                           740
      END                                                                750
```

```
      SUBROUTINE FSGRAL(RESULT,NXINT,XINT,NABWF,ABWF,MABWF,                  10
     *                  NABQ1,ABQ1,MABQ1,NABQ2,ABQ2,MABQ2,NABQ3,ABQ3,MABQ3,  20
     *                  KMROM,AUXROM,KMROMP,EPSROM,DRINWA,                   30
     *                  IFAR,LFAR,LFARA,FARIN,FARAN,IFUNAR,*,*)              40
C     INTEGRATION EINER FUNKTION ENTSPRECHEND ITYP.                          50
C     ITYP   INTEGRAL VON                                                    60
C       1    PHI                                                           70
C       2    F1 * PHI                                                      80
C       3    F1*F2 * PHI                                                   90
C       4    1/F3 * PHI                                                   100
C       5    1/F3**2 * PHI                                                110
C       6    F1/F3 * PHI                                                  120
C       7    F1/F3**2 * PHI                                               130
C       8    F1*F2/F3 * PHI                                               140
C       9    F1*F2/F3**2 * PHI                                            150
C     PHI IST DURCH ABWF BZW. FORMELMAESSIG ODER ALS FUNKTION - JE NACH    160
C     WERT VON NFTYP - GEGEBEN.                                            170
C     F1, F2 UND F3 SIND DURCH ABQ1, ABQ2 BZW. ABQ3 GEGEBEN.               180
C     DURCHFUEHRUNG DER INTEGRATION IN DEN INTERVALLEN                     190
C     XINT(I-1) ... XINT(I)  MIT I=2,NXINT.                                200
C     RETURN 1 WIRD GEMACHT, WENN KMROM VERGROESSERT WERDEN MUSS.          210
C     DANN IST KMROMP GROESSER ALS 0.                                      220
C     RETURN 2 WIRD GEMACHT, WENN SGT <= 0 FESTGESTELLT WIRD.              230
C                                                                          240
      EXTERNAL DPHI,FSNU01,FSNU02,FSNU03,FSNU04,FSNU05,FSNU06,FSNU07,      250
     *FSNU08,FSNU09,FSAN02,FSAN03,FSAN04,FSAN05,FSAN06,FSAN07,            260
     *FSAN08,FSAN09                                                       270
      LOGICAL*4 TEST1,TEST2,TEST3,SPRUC,FSGRAL,FSTOLE,DRUCK,DRUCKL,        280
     *          SPRU3,LERMSG,LFAR(2,3),LFARA(2,3)                          290
      REAL*8 RESULT,Y,FSNU01,FSNU02,FSNU03,FSNU04,FSNU05,FSNU06,FSNU07,    300
     *FSNU08,FSNU09,FSAN02,FSAN03,FSAN04,FSAN05,FSAN06,FSAN07,FSAN08,     310
     *FSAN09                                                              320
      DIMENSION XINT(1),ABWF(MABWF,4),ABQ1(MABQ1,4),ABQ2(MABQ2,4),        330
     *          ABQ3(MABQ3,4),AUXROM(1),YF(3),YFP(3),FARIN(2,3,2),         340
     *          FARAN(2,3),IFUNAR(2,3),YFEPS(3)                            350
      COMMON NR1(4),NC                                                    360
      COMMON/CFSTRU/ TEST1,TEST2,TEST3,LERMSG,GLSCH,MNFTYP,NFTYP,ITYP,    370
     *               ITYPFU,NR2(3),       AW,BW,A1,B1,A2,B2,A3,B3,BSIGO,  380
     *               XIA,XIE,L,Y,NDIMP,DRUCKL                            390
C     FEHLERABFRAGEN.                                                     400
      IF(ITYP.LT.1.OR.ITYP.GT.9.OR.NXINT.LT.2) CALL FSWR03(3001,          410
     *'FSGR','AL  ',1)                                                    420
C     STEUERGROESSEN FUER INTEGRALBERECHNUNG IM TESTFALL DRUCKEN.         430
      IF(TEST3) WRITE(NC,100) NFTYP,XINT(1),NXINT,XINT(NXINT)             440
  100 FORMAT('0SUBROUTINE FSGRAL.  NFTYP=',I3,                            450
     *'  XINT(1)=',1PE13.6,'  NXINT=',0PI6,'  XINT(NXINT)=',              460
     *1PE13.6,'.')                                                        470
      IF(TEST3) CALL FSWR04(1008,ITYP,ITYPFU,BSIGO,BSIGO)                 480
C     RESULT GLEICH NULL SETZEN.                                          490
      RESULT=0.0                                                          500
C     POINTER FUER PUNKTWEISE FUNKTIONEN SETZEN.                          510
      IABWF=2                                                             520
      IABQ1=2                                                             530
      IABQ2=2                                                             540
      IABQ3=2                                                             550
C     SETZEN VON ANFANGSWERTEN FUER A UND B.                              560
      AW=ABWF(IABWF,2)                                                    570
      BW=ABWF(IABWF,3)                                                    580
      A1=ABQ1(IABQ1,2)                                                    590
      B1=ABQ1(IABQ1,3)                                                    600
      A2=ABQ2(IABQ2,2)                                                    610
      B2=ABQ2(IABQ2,3)                                                    620
      A3=ABQ3(IABQ3,2)                                                    630
      B3=ABQ3(IABQ3,3)                                                    640
C     ANFANGSWERTE FUER FEHLERDRUCKSTEUERUNG BEI FSROMB FEHLERN.          650
      DRUCKL=.FALSE.                                                      660
      DRUCK=.FALSE.                                                       670
C     ANFANGSWERTE FUER MIKROINTEGRALWERT UND YF UND YFEPS.               680
      Y=0.0                                                               690
      DO 53 I=1,3                                                         700
      YF(I)=0.0                                                           710
   53 YFEPS(I)=0.0                                                        720
C     FEHLERTEST                                                          730
      IF(IABS(NFTYP).GT.MNFTYP) CALL FSWR03(3001,'FSGR','AL  ',2)         740
C     BEI NUMERISCHER INTEGRATION FSROMB INITIALISIEREN.                  750
      IF(NFTYP.LE.0) CALL FSROMI(EPSROM,KMROM,DRINWA,YF,YFEPS,AUXROM)     760
C     SETZEN VON IGRIAR.                                                  770
      GOTO (1000,2000,3000,4000,5000,6000,7000,8000,9000),ITYP            780
      CALL FSWR03(3001,'FSGR','AL  ',3)                                   790
 1000 CONTINUE                                                            800
      IF(NFTYP.EQ.0.OR.NFTYP.LE.-2) GOTO 1901                             810
      IF(NFTYP.EQ.1) GOTO 1910                                            820
      IF(NFTYP.EQ.2) GOTO 1920                                            830
      IF(NFTYP.EQ.-1) GOTO 1902                                           840
      CALL FSWR03(3001,'FSGR','AL  ',4)                                   850
 1901 ASSIGN 1001 TO IGRIAR                                               860
      GOTO 9                                                              870
 1902 ASSIGN 1002 TO IGRIAR                                               880
      GOTO 9                                                              890
 1910 ASSIGN 1010 TO IGRIAR                                               900
      GOTO 9                                                              910
 1920 ASSIGN 1020 TO IGRIAR                                               920
      GOTO 9                                                              930
 2000 CONTINUE                                                            940
      IF(NFTYP.EQ.0.OR.NFTYP.LE.-2) GOTO 2901                             950
      IF(NFTYP.EQ.1) GOTO 2910                                            960
      IF(NFTYP.EQ.2) GOTO 2920                                            970
      IF(NFTYP.EQ.-1) GOTO 2902                                           980
      CALL FSWR03(3001,'FSGR','AL  ',5)                                   990
 2901 ASSIGN 2001 TO IGRIAR                                              1000
      GOTO 9                                                             1010
 2902 ASSIGN 2002 TO IGRIAR                                              1020
      GOTO 9                                                             1030
 2910 ASSIGN 2010 TO IGRIAR                                              1040
      GOTO 9                                                             1050
 2920 ASSIGN 2020 TO IGRIAR                                              1060
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      GOTO 9                                                            1070
3000  CONTINUE                                                          1080
      IF(NFTYP.EQ.0.OR.NFTYP.LE.-2) GOTO 3901                           1090
      IF(NFTYP.EQ.1) GOTO 3910                                          1100
      IF(NFTYP.EQ.2) GOTO 3920                                          1110
      IF(NFTYP.EQ.-1) GOTO 3902                                         1120
      CALL FSWR03(3001,'FSGR','AL  ',6)                                 1130
3901  ASSIGN 3001 TO IGRIAR                                             1140
      GOTO 9                                                            1150
3902  ASSIGN 3002 TO IGRIAR                                             1160
      GOTO 9                                                            1170
3910  ASSIGN 3010 TO IGRIAR                                             1180
      GOTO 9                                                            1190
3920  ASSIGN 3020 TO IGRIAR                                             1200
      GOTO 9                                                            1210
4000  CONTINUE                                                          1220
      IF(NFTYP.EQ.0.OR.NFTYP.LE.-2) GOTO 4901                           1230
      IF(NFTYP.EQ.1) GOTO 4910                                          1240
      IF(NFTYP.EQ.2) GOTO 4920                                          1250
      IF(NFTYP.EQ.-1) GOTO 4902                                         1260
      CALL FSWR03(3001,'FSGR','AL  ',7)                                 1270
4901  ASSIGN 4001 TO IGRIAR                                             1280
      GOTO 9                                                            1290
4902  ASSIGN 4002 TO IGRIAR                                             1300
      GOTO 9                                                            1310
4910  ASSIGN 4010 TO IGRIAR                                             1320
      GOTO 9                                                            1330
4920  ASSIGN 4020 TO IGRIAR                                             1340
      GOTO 9                                                            1350
5000  CONTINUE                                                          1360
      IF(NFTYP.EQ.0.OR.NFTYP.LE.-2) GOTO 5901                           1370
      IF(NFTYP.EQ.1) GOTO 5910                                          1380
      IF(NFTYP.EQ.2) GOTO 5920                                          1390
      IF(NFTYP.EQ.-1) GOTO 5902                                         1400
      CALL FSWR03(3001,'FSGR','AL  ',8)                                 1410
5901  ASSIGN 5001 TO IGRIAR                                             1420
      GOTO 9                                                            1430
5902  ASSIGN 5002 TO IGRIAR                                             1440
      GOTO 9                                                            1450
5910  ASSIGN 5010 TO IGRIAR                                             1460
      GOTO 9                                                            1470
5920  ASSIGN 5020 TO IGRIAR                                             1480
      GOTO 9                                                            1490
6000  CONTINUE                                                          1500
      IF(NFTYP.EQ.0.OR.NFTYP.LE.-2) GOTO 6901                           1510
      IF(NFTYP.EQ.1) GOTO 6910                                          1520
      IF(NFTYP.EQ.2) GOTO 6920                                          1530
      IF(NFTYP.EQ.-1) GOTO 6902                                         1540
      CALL FSWR03(3001,'FSGR','AL  ',9)                                 1550
6901  ASSIGN 6001 TO IGRIAR                                             1560
      GOTO 9                                                            1570
6902  ASSIGN 6002 TO IGRIAR                                             1580
      GOTO 9                                                            1590
6910  ASSIGN 6010 TO IGRIAR                                             1600
      GOTO 9                                                            1610

6920  ASSIGN 6020 TO IGRIAR                                             1620
      GOTO 9                                                            1630
7000  CONTINUE                                                          1640
      IF(NFTYP.EQ.0.OR.NFTYP.LE.-2) GOTO 7901                           1650
      IF(NFTYP.EQ.1) GOTO 7910                                          1660
      IF(NFTYP.EQ.2) GOTO 7920                                          1670
      IF(NFTYP.EQ.-1) GOTO 7902                                         1680
      CALL FSWR03(3001,'FSGR','AL  ',10)                                1690
7901  ASSIGN 7001 TO IGRIAR                                             1700
      GOTO 9                                                            1710
7902  ASSIGN 7002 TO IGRIAR                                             1720
      GOTO 9                                                            1730
7910  ASSIGN 7010 TO IGRIAR                                             1740
      GOTO 9                                                            1750
7920  ASSIGN 7020 TO IGRIAR                                             1760
      GOTO 9                                                            1770
8000  CONTINUE                                                          1780
      IF(NFTYP.EQ.0.OR.NFTYP.LE.-2) GOTO 8901                           1790
      IF(NFTYP.EQ.1) GOTO 8910                                          1800
      IF(NFTYP.EQ.2) GOTO 8920                                          1810
      IF(NFTYP.EQ.-1) GOTO 8902                                         1820
      CALL FSWR03(3001,'FSGR','AL  ',11)                                1830
8901  ASSIGN 8001 TO IGRIAR                                             1840
      GOTO 9                                                            1850
8902  ASSIGN 8002 TO IGRIAR                                             1860
      GOTO 9                                                            1870
8910  ASSIGN 8010 TO IGRIAR                                             1880
      GOTO 9                                                            1890
8920  ASSIGN 8020 TO IGRIAR                                             1900
      GOTO 9                                                            1910
9000  CONTINUE                                                          1920
      IF(NFTYP.EQ.0.OR.NFTYP.LE.-2) GOTO 9901                           1930
      IF(NFTYP.EQ.1) GOTO 9910                                          1940
      IF(NFTYP.EQ.2) GOTO 9920                                          1950
      IF(NFTYP.EQ.-1) GOTO 9902                                         1960
      CALL FSWR03(3001,'FSGR','AL  ',12)                                1970
9901  ASSIGN 9001 TO IGRIAR                                             1980
      GOTO 9                                                            1990
9902  ASSIGN 9002 TO IGRIAR                                             2000
      GOTO 9                                                            2010
9910  ASSIGN 9010 TO IGRIAR                                             2020
      GOTO 9                                                            2030
9920  ASSIGN 9020 TO IGRIAR                                             2040
      GOTO 9                                                            2050
C     LOOP UEBER ALLE INTERVALLE.                                       2060
    9 XIE=XINT(1)                                                       2070
      I=1                                                               2080
    2 I=I+1                                                             2090
      IF(I.GT.NXINT) GOTO 3                                             2100
      XIA=XIE                                                           2110
      XIE=XINT(I)                                                       2120
    8 SFRUO=.FALSE.                                                     2130
      XIEE=-1.0E+10                                                     2140
      IF(XIA.GE.XIE) CALL FSWR03(3001,'FSGR','AL  ',13)                 2150
C     PUNKTWEISE WICHTUNGSFUNKTION ?                                    2160
```

```
      IF(IABS(NFTYP).NE.1) GOTO 4                                       2170
C     EVENTUELL POINTER FUER ABWF HOCHZAEHLEN.                          2180
      IF(XIE.LE.ABWF(IABWF,1)) GOTO 52                                  2190
      IABWF=IABWF+1                                                     2200
      IF(IABWF.GT.NABWF) CALL FSWR03(3001,'FSGR','AL  ',14)             2210
      AW=ABWF(IABWF,2)                                                  2220
      BW=ABWF(IABWF,3)                                                  2230
   52 IF(FSGRA1(ABWF,IABWF,MABWF,XIA,XIE)) CALL FSWR03(3001,            2240
     *'FSGR','AL  ',15)                                                 2250
C     WICHTUNGSFUNKTION = 0 ?                                           2260
      IF(ABWF(IABWF,4).NE.0.0) GOTO 4                                   2270
C     SPRUNGBEDINGUNG SETZEN. XIEE AUF ABWF(IABWF,1) SETZEN. WARNUNG    2280
C     DRUCKEN. I HOCHZAEHLEN.                                           2290
      IF(.NOT.FSTOLE(ABWF(IABWF-1,1),XIA,GLSCH)) CALL FSWR03(3001,      2300
     *'FSGR','AL  ',16)                                                 2310
      SPRU0=.TRUE.                                                      2320
      XIEE=ABWF(IABWF,1)                                                2330
      CALL FSWR03(2005,ITYP,XIA,XIEE)                                   2340
      CALL FSWR00(-2006)                                                2350
    4 CONTINUE                                                          2360
C     PRUEFUNG DER "QUERSCHNITTSGRADEN" ENTSPRECHEND ITYP.              2370
      IF(ITYP.EQ.1) GOTO 5                                              2380
      IF(ITYP.EQ.2) GOTO 10                                             2390
      IF(ITYP.EQ.3) GOTO 20                                             2400
      IF(ITYP.GE.4.AND.ITYP.LE.9) GOTO 30                               2410
      CALL FSWR03(3001,'FSGR','AL  ',17)                                2420
   30 CONTINUE                                                          2430
C     FUNKTION F3.                                                      2440
      CALL FSGRA2(3,ABQ3,IABQ3,MABQ3,NABQ3,XIA,XIE,XIEE,SPRU0,SPRU3,    2450
     *IFAR,LFAR,LFARA,FARIN,FARAN,IFUNAR,.TRUE.)                        2460
      IF(SPRU3) GOTO 777                                                2470
      IF(ITYP.EQ.6.OR.ITYP.EQ.7) GOTO 10                                2480
      IF(ITYP.EQ.4.OR.ITYP.EQ.5) GOTO 5                                 2490
   20 CONTINUE                                                          2500
C     FUNKTION F2.                                                      2510
      CALL FSGRA2(2,ABQ2,IABQ2,MABQ2,NABQ2,XIA,XIE,XIEE,SPRU0,SPRU3,    2520
     *IFAR,LFAR,LFARA,FARIN,FARAN,IFUNAR,.FALSE.)                       2530
   10 CONTINUE                                                          2540
C     FUNKTION F1.                                                      2550
      CALL FSGRA2(1,ABQ1,IABQ1,MABQ1,NABQ1,XIA,XIE,XIEE,SPRU0,SPRU3,    2560
     *IFAR,LFAR,LFARA,FARIN,FARAN,IFUNAR,.TRUE.)                        2570
    5 CONTINUE                                                          2580
C     WENN KEIN FEHLER, MIT INTEGRALBERECHNUNG BEGINNEN.                2590
C     ANDERNFALLS I UND ENTSPRECHENDE IAB.. HOCHZAEHLEN UND ZUM         2600
C     SCHLEIFENENDE SPRINGEN.                                           2610
      IF(.NOT.SPRU0) GOTO 6                                             2620
C     I HOCHZAEHLEN.                                                    2630
    7 I=I+1                                                             2640
      IF(I.GT.NXINT) GOTO 3                                             2650
      IF(XINT(I).LT.XIEE.OR.FSTOLE(XINT(I),XIEE,GLSCH)) GOTO 7          2660
      XIA=XINT(I-1)                                                     2670
      XIE=XINT(I)                                                       2680
C     IAB HOCHZAEHLEN                                                   2690
      IF(ITYP.EQ.1) GOTO 41                                             2700
      IF(ITYP.EQ.2) GOTO 11                                             2710
      IF(ITYP.EQ.3) GOTO 21                                             2720
      IF(ITYP.GE.4.AND.ITYP.LE.9) GOTO 31                               2730
      CALL FSWR03(3001,'FSGR','AL  ',18)                                2740
   31 CONTINUE                                                          2750
C     IABQ3 HOCHZAEHLEN.                                                2760
      CALL FSGRA3(ABQ3,IABQ3,MABQ3,NABQ3,XIA,XIE)                       2770
      A3=ABQ3(IABQ3,2)                                                  2780
      B3=ABQ3(IABQ3,3)                                                  2790
      IF(ITYP.EQ.6.OR.ITYP.EQ.7) GOTO 11                                2800
      IF(ITYP.EQ.4.OR.ITYP.EQ.5) GOTO 41                                2810
   21 CONTINUE                                                          2820
C     IABQ2 HOCHZAEHLEN                                                 2830
      CALL FSGRA3(ABQ2,IABQ2,MABQ2,NABQ2,XIA,XIE)                       2840
      A2=ABQ2(IABQ2,2)                                                  2850
      B2=ABQ2(IABQ2,3)                                                  2860
   11 CONTINUE                                                          2870
C     IABQ1 HOCHZAEHLEN                                                 2880
      CALL FSGRA3(ABQ1,IABQ1,MABQ1,NABQ1,XIA,XIE)                       2890
      A1=ABQ1(IABQ1,2)                                                  2900
      B1=ABQ1(IABQ1,3)                                                  2910
   41 CONTINUE                                                          2920
      IF(IABS(NFTYP).NE.1) GOTO 8                                       2930
C     IABWF HOCHZAEHLEN.                                                2940
      CALL FSGRA3(ABWF,IABWF,MABWF,NABWF,XIA,XIE)                       2950
      AW=ABWF(IABWF,2)                                                  2960
      BW=ABWF(IABWF,3)                                                  2970
      GOTO 8                                                            2980
    6 CONTINUE                                                          2990
C     I N T E G R A T I O N .                                           3000
C     VERTEILER FUER DIE VERSCHIEDENEN INTEGRALE UND INTEGRATIONSARTEN. 3010
      GOTO IGRIAR,(1001,1002,1010,1020,2001,2002,2010,2020,             3020
     *3001,3002,3010,3020,4001,4002,4010,4020,5001,5002,5010,5020,      3030
     *6001,6002,6010,6020,7001,7002,7010,7020,8001,8002,8010,8020,      3040
     *9001,9002,9010,9020)                                              3050
C     ITYP=1. INTEGRAL VON PHI.                                         3060
 1001 CALL FSROMB(DPHI,&445)                                            3070
      GOTO 1                                                            3080
 1002 CALL FSROMB(FSNU01,&445)                                          3090
      GOTO 1                                                            3100
 1010 L=11                                                              3110
      GOTO 60                                                           3120
 1020 L=12                                                              3130
      GOTO 60                                                           3140
C     ITYP=2. INTEGRAL VON F1 * PHI.                                    3150
 2001 CALL FSROMB(FSAN02,&445)                                          3160
      GOTO 1                                                            3170
 2002 CALL FSROMB(FSNU02,&445)                                          3180
      GOTO 1                                                            3190
 2010 L=21                                                              3200
      GOTO 60                                                           3210
 2020 L=22                                                              3220
      GOTO 60                                                           3230
C     ITYP=3. INTEGRAL VON F1*F2 * PHI.                                 3240
 3001 CALL FSROMB(FSAN03,&445)                                          3250
      GOTO 1                                                            3260
```

```
 3002 CALL FSROMB(FSNU03,&445)
      GOTO 1
 3010 L=31
      GOTO 60
 3020 L=32
      GOTO 60
C     ITYP=4. INTEGRAL VON 1/F3 * PHI.
 4001 CALL FSROMB(FSAN04,&445)
      GOTO 1
 4002 CALL FSROMB(FSNU04,&445)
      GOTO 1
 4010 L=41
      GOTO 60
 4020 L=42
      GOTO 60
C     ITYP=5. INTEGRAL VON 1/F3**2 * PHI.
 5001 CALL FSROMB(FSAN05,&445)
      GOTO 1
 5002 CALL FSROMB(FSNU05,&445)
      GOTO 1
 5010 L=51
      GOTO 60
 5020 L=52
      GOTO 60
C     ITYP=6. INTEGRAL VON F1/F3 * PHI.
 6001 CALL FSROMB(FSAN06,&445)
      GOTO 1
 6002 CALL FSROMB(FSNU06,&445)
      GOTO 1
 6010 L=61
      GOTO 60
 6020 L=62
      GOTO 60
C     ITYP=7. INTEGRAL VON F1/F3**2 * PHI.
 7001 CALL FSROMB(FSAN07,&445)
      GOTO 1
 7002 CALL FSROMB(FSNU07,&445)
      GOTO 1
 7010 L=71
      GOTO 60
 7020 L=72
      GOTO 60
C     ITYP=8. INTEGRAL VON F1*F2/F3 * PHI.
 8001 CALL FSROMB(FSAN08,&445)
      GOTO 1
 8002 CALL FSROMB(FSNU08,&445)
      GOTO 1
 8010 L=81
      GOTO 60
 8020 L=82
      GOTO 60
C     ITYP=9. INTEGRAL VON F1*F2/F3**2 * PHI.
 9001 CALL FSROMB(FSAN09,&445)
      GOTO 1
 9002 CALL FSROMB(FSNU09,&445)
      GOTO 1
 9010 L=91
      GOTO 60
 9020 L=92
      GOTO 60
C     LOOP ENDE FUER LOOP UEBER ALLE INTERVALLE
    1 IF(DRUCKL) DRUCK=.TRUE.
      RESULT=RESULT*Y
      GOTO 2
    3 RESUL4=RESULT
C     FEHLERTEST.
      IF(NFTYP.GT.0) GOTO 50
C     FALLS DRUCK=.TRUE. ODER NFTYP<=0 UND ANTEIL VON YF(1) BZW. YF(3)
C     AM ERGEBNIS RESULT MEHR ALS 1% AUSMACHEN: WARNUNGSAUSDRUCK.
      IF(RESULT.EQ.0.0) GOTO 50
      IF(ABS(YF(1)/RESUL4).GE.1.0E-1.OR.ABS(YF(3)/RESULL4).GE.1.0E-2)
     *DRUCK=.TRUE.
   50 IF(.NOT.TEST3.AND..NOT.DRUCK) GOTO 333
      CALL FSWR04(1008,ITYP,ITYPFU,BSIG0,BSIG0)
      CALL FSWR03(-1015,XINT(1),XINT(NXINT),RESULT)
      IF(DRUCK) CALL FSWR01(-2011,EPSROM)
      IF((NFTYP.GT.0).OR.(.NOT.TEST3.AND..NOT.DRUCK)) GOTO 333
      YFP(1)=0.0
      YFP(2)=0.0
      YFP(3)=0.0
      IF(RESULT.EQ.0) GOTO 51
      YFP(1)=ABS(YF(1)/RESUL4)*100.0
      YFP(2)=ABS(YF(2)/RESUL4)*100.0
      YFP(3)=ABS(YF(3)/RESUL4)*100.0
   51 CALL FSWR09(-1009,YF(2),YF(1),YF(3),YFP(2),YFP(1),YFP(3),
     *YFEPS(2),YFEPS(1),YFEPS(3))
  333 RETURN
  445 KMROMP=NDIMP
      RETURN 1
  777 RETURN 2
   60 CALL FSEXIN
      IF(TEST2) WRITE(NO,101) ITYP,ITYPFU,BSIG0,XIA,XIE,Y
  101 FORMAT(' ANALYT  ITYP=',I2,'  ITYPFU=',I2,'  SIG0=',1PE13.6,
     *'  XL=',1PE13.6,'  XH=',1PE13.6,'  Y=',1PE13.6)
      GOTO 1
      END
```

```
      REAL FUNCTION FSNU01*8(X)                                          10
      REAL*8 X                                                           20
      COMMON/CFSTRU/ NR1(12),AW,BW                                       30
      FSNU01=DBLE(AW)*X+DBLE(BW)                                         40
      RETURN                                                             50
      END                                                                60
```

```
      REAL FUNCTION FSNU02*8(X)                                         10
      REAL*8 X                                                          20
      COMMON/CFSTRU/ NR1(12),AW,BW,A1,B1                                30
      FSNU02=(DBLE(AW)*X+DBLE(BW))*(DBLE(A1)*X+DBLE(B1))                40
      RETURN                                                            50
      END                                                               60
```

```
      REAL FUNCTION FSNU03*8(X)                                         10
      REAL*8 X                                                          20
      COMMON/CFSTRU/ NR1(12),AW,BW,A1,B1,A2,B2                          30
      FSNU03=(DBLE(AW)*X+DBLE(BW))*(DBLE(A1)*X+DBLE(B1))*(DBLE(A2)*X+DBL 40
     *E(B2))                                                            50
      RETURN                                                            60
      END                                                               70
```

```
      REAL FUNCTION FSNU04*8(X)                                         10
      REAL*8 X                                                          20
      COMMON/CFSTRU/ NR1(12),AW,BW,NR2(4),A3,B3,BSIGO                   30
      FSNU04=(DBLE(AW)*X+DBLE(BW))/(DBLE(A3)*X+DBLE(B3)+DBLE(BSIGO))    40
      RETURN                                                            50
      END                                                               60
```

```
      REAL FUNCTION FSNU05*8(X)                                         10
      REAL*8 X                                                          20
      COMMON/CFSTRU/ NR1(12),AW,BW,NR2(4),A3,B3,BSIGO                   30
      FSNU05=(DBLE(AW)*X+DBLE(BW))/((DBLE(A3)*X+DBLE(B3)+DBLE(BSIGO))**2 40
     *)                                                                 50
      RETURN                                                            60
      END                                                               70
```

```
      REAL FUNCTION FSNU06*8(X)                                         10
      REAL*8 X                                                          20
      COMMON/CFSTRU/ NR1(12),AW,BW,A1,B1,NR2(2),A3,B3,BSIGO             30
      FSNU06=(DBLE(AW)*X+DBLE(BW))*(DBLE(A1)*X+DBLE(B1))/               40
     *(DBLE(A3)*X+DBLE(B3)+DBLE(BSIGO))                                 50
      RETURN                                                            60
      END                                                               70
```

```
      REAL FUNCTION FSNU07*8(X)                                         10
      REAL*8 X                                                          20
      COMMON/CFSTRU/ NR1(12),AW,BW,A1,B1,NR2(2),A3,B3,BSIGO             30
      FSNU07=(DBLE(AW)*X+DBLE(BW))*(DBLE(A1)*X+DBLE(B1))/               40
     *((DBLE(A3)*X+DBLE(B3)+DBLE(BSIGO))**2)                            50
      RETURN                                                            60
      END                                                               70
```

```
      REAL FUNCTION FSNU08*8(X)                                         10
      REAL*8 X                                                          20
      COMMON/CFSTRU/ NR1(12),AW,BW,A1,B1,A2,B2,A3,B3,BSIGO              30
      FSNU08=(DBLE(AW)*X+DBLE(BW))*(DBLE(A1)*X+DBLE(B1))*(DBLE(A2)*X+   40
     *DBLE(B2))/(DBLE(A3)*X+DBLE(B3)+DBLE(BSIGO))                       50
      RETURN                                                            60
      END                                                               70
```

```
      REAL FUNCTION FSNU09*8(X)                                         10
      REAL*8 X                                                          20
      COMMON/CFSTRU/ NR1(12),AW,BW,A1,B1,A2,B2,A3,B3,BSIGO              30
      FSNU09=(DBLE(AW)*X+DBLE(BW))*(DBLE(A1)*X+DBLE(B1))*(DBLE(A2)*X+   40
     *DBLE(B2))/((DBLE(A3)*X+DBLE(B3)+DBLE(BSIGO))**2)                  50
      RETURN                                                            60
      END                                                               70
```

```
      REAL FUNCTION FSAN02*8(X)                                         10
      REAL*8 X,DPHI                                                     20
      COMMON/CFSTRU/ NR1(14),A1,B1                                      30
      FSAN02=DPHI(X)*(DBLE(A1)*X+DBLE(B1))                              40
      RETURN                                                            50
      END                                                               60
```

```
      REAL FUNCTION FSAN03*8(X)                                         10
      REAL*8 X,DPHI                                                     20
      COMMON/CFSTRU/ NR1(14),A1,B1,A2,B2                                30
      FSAN03=DPHI(X)*(DBLE(A1)*X+DBLE(B1))*(DBLE(A2)*X+DBLE(B2))        40
      RETURN                                                            50
      END                                                               60
```

```
      REAL FUNCTION FSANO4*8(X)                                         10
      REAL*8 X,DPHI                                                     20
      COMMON/CFSTRU/ NR1(18),A3,B3,BSIGO                                30
      FSANO4=DPHI(X)/(DBLE(A3)*X+DBLE(B3)+DBLE(BSIGO))                  40
      RETURN                                                            50
      END                                                               60
```

```
      REAL FUNCTION FSANO5*8(X)                                         10
      REAL*8 X,DPHI                                                     20
      COMMON/CFSTRU/ NR1(18),A3,B3,BSIGO                                30
      FSANO5=DPHI(X)/((DBLE(A3)*X+DBLE(B3)+DBLE(BSIGO))**2)             40
      RETURN                                                            50
      END                                                               60
```

```
      REAL FUNCTION FSANO6*8(X)                                         10
      REAL*8 X,DPHI                                                     20
      COMMON/CFSTRU/ NR1(14),A1,B1,NR2(2),A3,B3,BSIGO                   30
      FSANO6=DPHI(X)*(DBLE(A1)*X+DBLE(B1))/(DBLE(A3)*X+DBLE(B3)+DBLE(BSI 40
     *GO))                                                              50
      RETURN                                                            60
      END                                                               70
```

```
      REAL FUNCTION FSANO7*8(X)                                         10
      REAL*8 X,DPHI                                                     20
      COMMON/CFSTRU/ NR1(14),A1,B1,NR2(2),A3,B3,BSIGO                   30
      FSANO7=DPHI(X)*(DBLE(A1)*X+DBLE(B1))/((DBLE(A3)*X+DBLE(B3)+DBLE(BS 40
     *IGO))**2)                                                         50
      RETURN                                                            60
      END                                                               70
```

```
      REAL FUNCTION FSANO8*8(X)                                         10
      REAL*8 X,DPHI                                                     20
      COMMON/CFSTRU/ NR1(14),A1,B1,A2,B2,A3,B3,BSIGO                    30
      FSANO8=DPHI(X)*(DBLE(A1)*X+DBLE(B1))*(DBLE(A2)*X+DBLE(B2))/       40
     *(DBLE(A3)*X+DBLE(B3)+DBLE(BSIGO))                                 50
      RETURN                                                            60
      END                                                               70
```

```
      REAL FUNCTION FSANO9*8(X)                                         10
      REAL*8 X,DPHI                                                     20
      COMMON/CFSTRU/ NR1(14),A1,B1,A2,B2,A3,B3,BSIGO                    30
      FSANO9=DPHI(X)*(DBLE(A1)*X+DBLE(B1))*(DBLE(A2)*X+DBLE(B2))/       40
     *((DBLE(A3)*X+DBLE(B3)+DBLE(BSIGO))**2)                            50
      RETURN                                                            60
      END                                                               70
```

```
      SUBROUTINE FSEXIN                                                 10
C     EXPLIZITE ANALYTISCHE INTEGRATION.                                20
      REAL*8 YR8,HO,H1,H2,H3,RO,R1,Z1,Z2,Z3,Z4,Z5,Z6,Z7,FSLOMQ,CQ,FF,    30
     *       DA1,DA2,DB1,DB2,DAW,DBW,DXIA,DXIE,DD,Y,ZL,Q                40
      COMMON/CFSTRU/ NR1(11),CONST,AW,BW,A1,B1,A2,B2,A3,B3,BSIGO,       50
     *XIA,XIE,L,Y                                                       60
      DA1=DBLE(A1)                                                      70
      DB1=DBLE(B1)                                                      80
      DA2=DBLE(A2)                                                      90
      DB2=DBLE(B2)                                                     100
      DAW=DBLE(AW)                                                     110
      DBW=DBLE(BW)                                                     120
      DXIA=DBLE(XIA)                                                   130
      DXIE=DBLE(XIE)                                                   140
      DD=DXIE-DXIA                                                     150
      LSPR=L/10                                                        160
      LSPR=2*LSPR+(L-LSPR*10-2)                                        170
      GOTO (11,12,21,22,31,32,41,42,51,52,61,62,71,72,81,82,91,92),LSPR 180
      ITP=1                                                            190
      GOTO 770                                                         200
C     INTEGRAL VON F=(AW*X+BW)                                         210
   11 N=0                                                              220
      IUNNUL=1                                                         230
      H1=DAW                                                           240
      HO=DBW                                                           250
      GOTO 1                                                           260
C     INTEGRAL VON F=CONST/X                                           270
   12 N=0                                                              280
      IUNNUL=0                                                         290
      HO=1.0D+0                                                        300
      GOTO 2                                                           310
C     INTEGRAL VON F=(AW*X+BW)*(A1*X+B1)                               320
   21 N=0                                                              330
      IUNNUL=2                                                         340
      H2=DAW*DA1                                                       350
      H1=DAW*DB1+DBW*DA1                                               360
      HO=DBW*DB1                                                       370
      GOTO 1                                                           380
C     INTEGRAL VON F=CONST/X * (A1*X+B1)                               390
   22 N=0                                                              400
      IUNNUL=1                                                         410
      H1=DA1                                                           420
      HO=DB1                                                           430
      GOTO 2                                                           440
```

```
C      INTEGRAL VON F=(AW*X+BW)*(A1*X+B1)*(A2*X+B2)                      450
   31 N=0                                                               460
      IUNNUL=3                                                          470
      Z1=DA1*DA2                                                        480
      Z2=DA1*DB2+DB1*DA2                                                490
      Z3=DB1*DB2                                                        500
      H3=DAW*Z1                                                         510
      H2=DAW*Z2+DBW*Z1                                                  520
      H1=DAW*Z3+DBW*Z2                                                  530
      HC=DBW*Z3                                                         540
      GOTO 1                                                            550
C      INTEGRAL VON  F=CONST/X * (A1*X+B1)*(A2*X+B2)                    560
   32 N=0                                                               570
      IUNNUL=2                                                          580
      H2=DA1*DA2                                                        590
      H1=DA1*DB2+DB1*DA2                                                600
      HC=DB1*DB2                                                        610
      GOTO 2                                                            620
C      INTEGRAL VON F=(AW*X+BW)/(A3*X+B3+BSIGC)                         630
   41 N=1                                                               640
      IUNNUL=1                                                          650
      H1=DAW                                                            660
      HC=DBW                                                            670
      GOTO 1                                                            680
C      INTEGRAL VON F=CONST/X * 1.0/(A3*X+B3+BSIGO)                     690
   42 N=1                                                               700
      IUNNUL=0                                                          710
      HC=1.0D+0                                                         720
      GOTO 2                                                            730
C      INTEGRAL VON F=(AW*X+BW)/((A3*X+B3+BSIGO)**2)                    740
   51 N=2                                                               750
      IUNNUL=1                                                          760
      H1=DAW                                                            770
      H0=DBW                                                            780
      GOTO 1                                                            790
C      INTEGRAL VON F=CONST/X * 1.0/((A3*X+B3+BSIGO)**2)                800
   52 N=2                                                               810
      IUNNUL=0                                                          820
      H0=1.0D+0                                                         830
      GOTO 2                                                            840
C      INTEGRAL VON F=(AW*X+BW)*(A1*X+B1)/(A3*X+B3+BSIGC)               850
   61 N=1                                                               860
      IUNNUL=2                                                          870
      H2=DAW*DA1                                                        880
      H1=DAW*DB1+DBW*DA1                                                890
      H0=DBW*DB1                                                        900
      GOTO 1                                                            910
C      INTEGRAL VON F=CONST/X * (A1*X+B1)/(A3*X+B3+BSIGO)               920
   62 N=1                                                               930
      IUNNUL=1                                                          940
      H1=DA1                                                            950
      HC=DB1                                                            960
      GOTO 2                                                            970
C      INTEGRAL VON F=(AW*X+BW)*(A1*X+B1)/((A3*X+B3+BSIGO)**2)          980
   71 N=2                                                               990
      IUNNUL=2                                                         1000
      H2=DAW*DA1                                                       1010
      H1=DAW*DB1+DBW*DA1                                               1020
      H0=DBW*DB1                                                       1030
      GOTO 1                                                           1040
C      INTEGRAL VON F=CONST/X * (A1*X+B1)/((A3*X+B3+BSIGO)**2)          1050
   72 N=2                                                              1060
      IUNNUL=1                                                         1070
      H1=DA1                                                           1080
      H0=DB1                                                           1090
      GOTO 2                                                           1100
C      INTEGRAL VON F=(AW*X+BW)*(A1*X+B1)*(A2*X+B2)/(A3*X+B3+BSIGO)     1110
   81 N=1                                                              1120
      IUNNUL=3                                                         1130
      Z1=DA1*DA2                                                       1140
      Z2=DA1*DB2+DB1*DA2                                               1150
      Z3=DB1*DB2                                                       1160
      H3=DAW*Z1                                                        1170
      H2=DAW*Z2+DBW*Z1                                                 1180
      H1=DAW*Z3+DBW*Z2                                                 1190
      HC=DBW*Z3                                                        1200
      GOTO 1                                                           1210
C      INTEGRAL VON F=CONST/X * (A1*X+B1)*(A2*X+B2)/(A3*X+B3+BSIGO)     1220
   82 N=1                                                              1230
      IUNNUL=2                                                         1240
      H2=DA1*DA2                                                       1250
      H1=DA1*DB2+DB1*DA2                                               1260
      HC=DB1*DB2                                                       1270
      GOTO 2                                                           1280
C      INTEGRAL VON F=(AW*X+BW)*(A1*X+B1)*(A2*X+B2)/((A3*X+B3+BSIGO)**2) 1290
   91 N=2                                                              1300
      IUNNUL=3                                                         1310
      Z1=DA1*DA2                                                       1320
      Z2=DA1*DB2+DB1*DA2                                               1330
      Z3=DB1*DB2                                                       1340
      H3=DAW*Z1                                                        1350
      H2=DAW*Z2+DBW*Z1                                                 1360
      H1=DAW*Z3+DBW*Z2                                                 1370
      HC=DBW*Z3                                                        1380
      GOTO 1                                                           1390
C      INTEGRAL VON F=CONST/X * (A1*X+B1)*(A2*X+B2)/((A3*X+B3+BSIGO)**2) 1400
   92 N=2                                                              1410
      IUNNUL=2                                                         1420
      H2=DA1*DA2                                                       1430
      H1=DA1*DB2+DB1*DA2                                               1440
      HC=DB1*DB2                                                       1450
      GOTO 2                                                           1460
C*********************************************************************** 1470
C*********************************************************************** 1480
C INTEGRATION VON F1=(H3*X**3+H2*X**2+H1*X+HC)/(R1*X+RC)**N   N=0,1,2    1490
C*********************************************************************** 1500
C*********************************************************************** 1510
    1 YR8=0.0D+0                                                        1520
      IF(N.EQ.0) GOTO 1055                                             1530
      R1=DBLE(A3)                                                      1540
```

```
      RO=DBLE(B3)+DBLE(BSIGO)                                          1550
      IF(N.EQ.1) GOTO 1155                                             1560
      IF(N.EQ.2) GOTO 1255                                             1570
      ITP=2                                                            1580
  770 CALL FSWR03(3001,'FSEX','IN  ',ITP)                              1590
  333 Y=YR8                                                            1600
      RETURN                                                           1610
 1055 CONTINUE                                                         1620
C     N=0  R1 UND RO OHNE BEDEUTUNG.                                   1630
C     F1=H3*X**3+H2*X**2+H1*X+HO                                       1640
C     INTEGRAL VON F1 = 0.25*H3*X**4+0.33333333*H2*X**3+               1650
C                       0.5*H1*X**2+HO*X                               1660
      ITP=3                                                            1670
      GOTO (10551,10552,10553),IUNNUL                                  1680
      GOTO 770                                                         1690
10553 YR8=YR8+0.25D+0*H3*(DXIE**2+DXIA**2)*(DXIE+DXIA)*DD              1700
10552 YR8=YR8+0.33333333333333333*H2*DD*(3.0D+0*DXIA**2+DD*(3.0D+0*DXIA 1710
     **DD))                                                            1720
10551 YR8=YR8+(0.5D+0*H1*(DXIE+DXIA)+HO)*DD                            1730
      IF(N.EQ.1) YR8=YR8/RO                                            1740
      IF(N.EQ.2) YR8=YR8/(RO**2)                                       1750
      GOTO 333                                                         1760
 1155 CONTINUE                                                         1770
C     N=1                                                              1780
C     TEST VON R1 UND RO.                                              1790
      IF(R1.EQ.0.0) GOTO 1151                                          1800
      IF(RO.EQ.0.0) GOTO 1190                                          1810
 1199 CONTINUE                                                         1820
C     N=1  R1 UND RO UNGLEICH NULL.                                    1830
C     F1=(H3*X**3+H2*X**2+H1*X+HO)/(R1*X+RO)                           1840
C     INTEGRAL VON F1 = H3/(R1**4)*(0.33333333*(R1*X+RO)**3            1850
C         -1.5*RO*(R1*X+RO)**2+3.0*RO**2*(R1*X+RO)-RO**3*ALOG(R1*X+RO)) 1860
C     +H2/(R1**3)*(0.5*(R1*X+RO)**2-2.0*RO*(R1*X+RO)                   1870
C         +RO**2*ALOG(R1*X+RO))                                        1880
C     +H1/(R1**2)*(R1*X-RO*ALOG(R1*X+RO))                              1890
C     +HO/R1*ALOG(R1*X+RO)                                             1900
      ITP=4                                                            1910
      FF=R1/RO                                                         1920
      Q=FF*DD/(1.0D+0+FF*DXIA)                                         1930
      ZL=FSLOMQ(DXIE,DXIA,FF)                                          1940
      Z5=ZL-0.5*Q*Q                                                    1950
      Z1=Z5+Q                                                          1960
      GOTO (11991,11992,11993),IUNNUL                                  1970
      GOTO 770                                                         1980
11993 YR8=YR8+H3/(R1**4)*(R1**3*DD*(DXIA*DXIA+DXIA*DD+                 1990
     *0.33333333333333333D+0*DD*DD-DXIA/(1.0D+0+FF*DXIA)*(DXIA+0.5D+0* 2000
     *DD*(2.0D+0+FF*DXIA)/(1.0D+0+FF*DXIA)))-RO**3*ZL)                 2010
11992 YR8=YR8+H2/R1**3*(R1*R1*DD*(0.5D+0*DD+FF*DXIA*DXIA/(             2020
     *1.0D+0+FF*DXIA))+RO*RO*Z5)                                       2030
11991 YR8=YR8+H1/(R1**2)*(R1*DD*FF*DXIA/(1.0D+0+FF*DXIA)-RO*Z5)        2040
     *       +HO/R1*Z1                                                 2050
      GOTO 333                                                         2060
 1151 CONTINUE                                                         2070
C     N=1  R1=0.0                                                      2080
      ITP=5                                                            2090
      IF(RO.EQ.0.0) GOTO 770                                           2100
C     N=1  R1=0.0  RO UNGLEICH NULL.                                   2110
C     FUNKTION UND INTEGRAL WIE 1055 VERSEHEN MIT FAKTOR 1/RO.         2120
      GOTO 1055                                                        2130
 1190 CONTINUE                                                         2140
C     N=1  R1 UNGLEICH NULL  RO=0.0                                    2150
C     F1=1/R1*(H3*X**2+H2*X+H1+HO/X)                                   2160
C     INTEGRAL VON F1 = 1/R1*(0.33333333*H3*X**3+0.5*H2*X**2           2170
C                            +H1*X+HO*ALOG(X))                         2180
      ITP=6                                                            2190
      GOTO (11901,11902,11903),IUNNUL                                  2200
      GOTO 770                                                         2210
11903 YR8=YR8+0.33333333333333333*H3*DD*(3.0D+0*DXIA**2+DD*(3.0D+0*DXIA 2220
     **DD))                                                            2230
11902 YR8=YR8+0.5D+0*H2*DD*(DXIE+DXIA)                                 2240
11901 YR8=YR8+H1*DD + HO*ALOG(DXIE/DXIA)                               2250
      YR8=YR8/R1                                                       2260
      GOTO 333                                                         2270
 1255 CONTINUE                                                         2280
C     N=2                                                              2290
C     TEST VON R1 UND RO.                                              2300
      IF(R1.EQ.0.0) GOTO 1251                                          2310
      IF(RO.EQ.0.0) GOTO 1290                                          2320
 1299 CONTINUE                                                         2330
C     N=2  R1 UND RO UNGLEICH NULL.                                    2340
C     F1=(H3*X**3+H2*X**2+H1*X+HO)/((R1*X+RO)**2)                      2350
C     INTEGRAL VON F1 = H3/(R1**4)*(0.5*(R1*X+RO)**2-3.0*RO*(R1*X+RO)  2360
C        +3.0*RO**2*ALOG(R1*X+RO)+(RO**3)/(R1*X+RO))                   2370
C     +H2/(R1**3)*((R1*X+RO)-2.0*RO*ALOG(R1*X+RO)-(RO**2)/(R1*X+RO))   2380
C     +H1/(R1**2)*(RO/(R1*X+RO)+ALOG(R1*X+RO))                         2390
C        -HO/R1*1.0/(R1*X+RO)                                          2400
      ITP=7                                                            2410
      FF=R1/RO                                                         2420
      Q=FF*DD/(1.0D+0+FF*DXIA)                                         2430
      DQ=1.0D+0/((1.0D+0+FF*DXIE)*(1.0D+0+FF*DXIA))                    2440
      Z4=-FF*DD*DQ                                                     2450
      ZL=FSLOMQ(DXIE,DXIA,FF)                                          2460
      Z5=ZL-0.5*Q*Q                                                    2470
      Z1=Z5+Q                                                          2480
      Z7=Z5+FF*FF*DD*DXIE*DQ                                           2490
      GOTO (12991,12992,12993),IUNNUL                                  2500
      GOTO 770                                                         2510
12993 YR8=YR8+H3/(R1**4)*(R1*R1*DD*(0.5D+0*DQ+(DQ+FF*DXIA*(FF*DXIE*DXIA 2520
     *      -DD))*DQ)+3.0D+0*RO*RO*Z5)                                 2530
12992 YR8=YR8+H2/(R1**3)*RO*(FF*FF*DD*DXIA/(1.0D+0+FF*DXIA)-Z5-Z7)     2540
12991 YR8=YR8+(1.0D+0/R1)*(H1/R1*Z7 - HO*Z4/RO)                        2550
      GOTO 333                                                         2560
 1251 CONTINUE                                                         2570
C     N=2  R1=0.0                                                      2580
      ITP=8                                                            2590
      IF(RO.EQ.0.0) GOTO 770                                           2600
C     N=2  R1=0.0  RO UNGLEICH NULL.                                   2610
C     FUNKTION UND INTEGRAL WIE 1055 MIT FAKTOR 1.0/(RO**2).           2620
      GOTO 1055                                                        2630
 1290 CONTINUE                                                         2640
```

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C      N=2  R1 UNGLEICH NULL  R0=0.0                                          2650
C      F1=1.0/R1**2*(H3*X+H2+H1/X+HC/X**2)                                    2660
C      INTEGRAL VON F1 = 1.0/R1**2*(0.5*H3*X**2+H2*X+H1*ALOG(X)-H0/X)        2670
       ITP=9                                                                  2680
       GOTO (12901,12902,12903),IUNNUL                                        2690
       GOTO 770                                                               2700
12903  YR8=YR8+0.5*H3*(DXIE+DXIA)*DD                                          2710
12902  YR8=YR8+H2*DD                                                          2720
12901  YR8=YR8+H1*DLOG(DXIE/DXIA)-HC*(1.0/DXIE-1.0/DXIA)                      2730
       YR8=YR8/R1**2                                                          2740
       GOTO 333                                                               2750
C*************************************************************************  2760
C*************************************************************************  2770
C  INTEGRATION VON F2=CONST*(H2*X**2+H1*X+HC)/(X*(R1*X+RC)**N)  N=0,1,2       2780
C*************************************************************************  2790
C*************************************************************************  2800
    2  YR8=0.0D+0                                                           2810
       IUNSP=IUNNUL+1                                                         2820
       IF(N.EQ.0) GOTO 2055                                                   2830
       R1=DBLE(A3)                                                            2840
       R0=DBLE(B3)+DBLE(BSIGO)                                                2850
       IF(N.EQ.1) GOTO 2155                                                   2860
       IF(N.EQ.2) GOTO 2255                                                   2870
       ITP=10                                                                 2880
       GOTO 770                                                               2890
 2055  CONTINUE                                                               2900
C      N=0  R1 UND R0 OHNE BEDEUTUNG.                                         2910
C      F2=CONST*(H2*X+H1+H0/X)                                                2920
C      INTEGRAL VON F2 = CONST*(0.5*H2*X**2+H1*X+HC*ALOG(X))                  2930
       ITP=11                                                                 2940
       GOTO (20550,20551,20552),IUNSP                                         2950
       GOTO 770                                                               2960
20552  YR8=YR8+0.5*H2*(DXIE**2-DXIA**2)                                       2970
20551  YR8=YR8+H1*DC                                                          2980
20550  YR8=YR8+H0*DLOG(DXIE/DXIA)                                             2990
       IF(N.EQ.1) YR8=YR8/R0                                                  3000
       IF(N.EQ.2) YR8=YR8/(R0**2)                                             3010
 2000  YR8=CONST*YR8                                                          3020
       GOTO 333                                                               3030
 2155  CONTINUE                                                               3040
C      N=1                                                                    3050
C      TEST VON R1 UND R0.                                                    3060
       IF(R1.EQ.0.0) GOTO 2151                                                3070
       IF(R0.EQ.0.0) GOTO 2190                                                3080
 2195  CONTINUE                                                               3090
C      N=1  R1 UND R0 UNGLEICH 0.0                                            3100
C      F2=(H2*X**2+H1*X+H0)/(X*(R1*X+R0))                                     3110
C      INTEGRAL VON F2 = H2/R1**2*(R1*X-R0*ALOG(R1*X+RC))                     3120
C         +H1/R1*ALOG(R1*X+R0)                                                3130
C         -H0/R0*(ALOG(R1*X+RC)-ALOG(X))                                      3140
       ITP=12                                                                 3150
       FF=R1/R0                                                               3160
       Q=FF*DD/(1.0D+0+FF*DXIA)                                               3170
       Z1=FSLOMQ(DXIE,DXIA,FF)-0.5*Q*Q+Q                                      3180
       GOTO (21990,21991,21992),IUNSP                                         3190
       GOTO 770                                                               3200
21992  YR8=YR8+H2/(R1**2)*(R1*DD-R0*Z1)                                       3210
21991  YR8=YR8+H1/R1*Z1                                                       3220
21990  YR8=YR8-H0/R0*(Z1-DLOG(DXIE/DXIA))                                     3230
       GOTO 2000                                                              3240
 2151  CONTINUE                                                               3250
C      N=1  R1=0.0                                                            3260
       ITP=13                                                                 3270
       IF(R0.EQ.0.0) GOTO 770                                                 3280
C      N=1  R1=0.0   R0 UNGLEICH 0.0                                          3290
C      FUNKTION UND INTEGRAL WIE 2055 MIT FAKTOR 1/R0                         3300
       GOTO 2055                                                              3310
 2190  CONTINUE                                                               3320
C      N=1  R1 UNGLEICH 0.0  R0=0.0                                           3330
C      F2=1/R1*(H2+H1/X+H0/X**2)                                              3340
C      INTEGRAL VON F2 = 1/R1*(H2*X+H1*ALOG(X)-H0/X)                          3350
       ITP=14                                                                 3360
       GOTO (21900,21901,21902),IUNSP                                         3370
       GOTO 770                                                               3380
21902  YR8=YR8+H2*DD                                                          3390
21901  YR8=YR8+H1*DLOG(DXIE/DXIA)                                             3400
21900  YR8=YR8-H0*(1.0/DXIE-1.0/DXIA)                                         3410
       YR8=YR8/R1                                                             3420
       GOTO 2000                                                              3430
 2255  CONTINUE                                                               3440
C      N=2                                                                    3450
C      TEST VON R1 UND R0.                                                    3460
       IF(R1.EQ.0.0) GOTO 2251                                                3470
       IF(R0.EQ.0.0) GOTO 2290                                                3480
 2299  CONTINUE                                                               3490
C      N=2  R1 UND R0 UNGLEICH 0.0                                            3500
C      F2=(H1*X**2+H1*X+H0)/(X*(R1*X+R0)**2)                                  3510
C      INTEGRAL VON F2 = H2/(R1**2)*(R0/(R1*X+R0)+ALOG(R1*X+R0)               3520
C         -H1/R1*1.0/(R1*X+R0)                                                3530
C         -H0/(R0**2)*(ALOG(R1*X+RC)-ALOG(X)+R1*X/(R1*X+R0))                  3540
       ITP=15                                                                 3550
       FF=R1/R0                                                               3560
       Q=FF*DD/(1.0D+0+FF*DXIA)                                               3570
       DQ=1.0D+0/((1.0D+0+FF*DXIE)*(1.0D+0+FF*DXIA))                          3580
       ZL=FSLOMG(DXIE,DXIA,FF)                                                3590
       Z5=ZL-0.5*Q*Q                                                          3600
       Z1=Z5+Q                                                                3610
       Z4=-FF*DD*DQ                                                           3620
       Z7=Z5+FF*FF*DD*DXIE*DQ                                                 3630
       GOTO (22990,22991,22992),IUNSP                                         3640
       GOTO 770                                                               3650
22992  YR8=YR8+H2/(R1**2)*Z7                                                  3660
22991  YR8=YR8-H1/R1*Z4/R0                                                    3670
22990  YR8=YR8-H0/(R0**2)*(Z1-DLOG(DXIE/DXIA)+R1*(DXIE/(                     3680
     *R1*DXIE+R0)-DXIA/(R1*DXIA+R0)))                                         3690
       GOTO 2000                                                              3700
 2251  CONTINUE                                                               3710
C      N=2  R1=0.0                                                            3720
       ITP=16                                                                 3730
       IF(R0.EQ.0.0) GOTO 770                                                 3740
```

```
C      N=2  R1=0.0  R0 UNGLEICH 0.0                                    3750
C      FUNKTION UND INTEGRAL WIE 2055 MIT FAKTOR 1.0/(R0**2)           3760
       GOTO 2055                                                       3770
 2290 CONTINUE                                                         3780
C      N=2  R1 UNGLEICH 0.0  R0=0.0                                    3790
C      F2=1.0/(R1**2)*(H2/X+H1/X**2+H0/X**3)                           3800
C      INTEGRAL VON F2 = 1.0/(R1**2)*(H2*ALOG(X)-H1/X-0.5*H0/X**2)     3810
       ITP=17                                                          3820
       GOTO (22900,22901,22902),IUNSP                                  3830
       GOTO 770                                                        3840
22902 YR8=YR8+H2*DLOG(DXIE/DXIA)                                       3850
22901 YR8=YR8-H1*(1.0/DXIE-1.0/DXIA)                                   3860
22900 YR8=YR8-0.5*H0*(1.0/(DXIE**2)-1.0/(DXIA**2))                     3870
      YR8=YR8/(R1**2)                                                  3880
      GOTO 2000                                                        3890
      END                                                              3900
```

```
      REAL FUNCTION FSLOMQ*8(XIE,XIA,F)                                10
C     ES IST  Q = F*(XIE-XIA)/(1+F*XIA)                                20
C     DANN GILT                                                        30
C     LOG((1+F*XIE)/(1+F*XIA)) = LOG(1+Q)                              40
C     FSLOMQ BERECHNET LOG(1+Q)-Q+0.5*Q**2                             50
C     ES MUSS GELTEN: XIE,XIA > 0 ; XIE>XIA ;                          60
      REAL*8 XIE,XIA,F,DLOGM,FEL1,FEHLER,FELREL,FDLOGM,FELEND,Q        70
      COMMON NR1(4),N0                                                 80
      IF(XIE.LE.0.0D+0.OR.XIA.LE.0.0D+0.OR.XIE.LE.XIA)                 90
     *CALL FSWR03(3001,'FSLO','MQ  ',1)                               100
      NMAX=20                                                         110
      Q=1.0D+0/(1.0D+0+F*XIA)                                         120
      DLOGM=DLOG((1.0D+0+F*XIE)*Q)                                    130
      Q=F*(XIE-XIA)*Q                                                 140
      DLOGM=DLOGM-Q*(1.0D+0-0.5D+0*Q)                                 150
      IF(DABS(DLOGM).GT.1.0E-4.OR.DABS(Q).GE.1.0D+0) GOTO 330         160
      FELEND=DFLOAT(NMAX+1)*DLOG10(DABS(Q))-DLOG10(DFLOAT(NMAX+1))-   170
     *DLOG10(DABS(DLOGM))                                             180
      IF(Q.LT.0.0) FELEND=FELEND-DFLOAT(NMAX+1)*DLOG10(1.0D+0+Q)      190
      IF(FELEND.GT.-15.0D+0) GOTO 330                                 200
      FSLOMQ=0.0D+0                                                   210
    3 N=3                                                             220
      FEL1=0.3333333333333333*Q**3                                    230

    1 FSLOMQ=FSLOMQ+FEL1                                              240
      FEL1=(-1)**N*Q**(N+1)/(N+1)                                     250
      IF(Q.GE.0.0) FEHLER=FEL1                                        260
      IF(Q.LT.0.0) FEHLER=FEL1/((1.0D+0+Q)**(N+1))                    270
      FELREL=DABS(FEHLER/FSLOMQ)                                      280
      IF(FELREL.LE.1.0E-15) GOTO 333                                  290
      N=N+1                                                           300
      IF(N.LE.NMAX) GOTO 1                                            310
      WRITE(N0,1000) XIE,XIA,F,DLOGM,FELEND,FSLOMQ,FEHLER,FELREL,N,NMAX 320
 1000 FORMAT(' ',1P6E15.7/' ',1P2E15.7,0P2I12)                        330
      CALL FSWR03(3001,'FSLO','MQ  ',2)                               340
  330 FSLOMQ=DLOGM                                                    350
```

```
  333 CONTINUE                                                        360
      RETURN                                                          370
      END                                                             380
```

```
      LOGICAL FUNCTION FSGRA1(AB,IAB,MAB,XIA,XIE)                      10
      LOGICAL*4 FSTOLE                                                 20
      DIMENSION AB(MAB,4)                                              30
      COMMON/CFSTRU/ NR1(4),GLSCH                                      40
      FSGRA1=.FALSE.                                                   50
      IF((AB(IAB-1,1).GT.XIA.AND..NOT.FSTOLE(AB(IAB-1,1),XIA,GLSCH)).OR.  60
     *  (AB(IAB,1).LT.XIE.AND..NOT.FSTOLE(AB(IAB,1),XIE,GLSCH)))       70
     *FSGRA1=.TRUE.                                                    80
      RETURN                                                           90
      END                                                             100
```

```
      SUBROUTINE FSGRA2(IFUN,AB,IAB,MAB,NAB,XIA,XIE,XIEE,SPRU0,SPRU3,  10
     *IFAR,LFAR,LFARA,FARIN,FARAN,IFUNAR,NUDUR)                        20
      LOGICAL*4 SPRU0,FSGRA1,FSTOLE,NUDUR,SPRU3,LERMSG,LFAR(2,3),      30
     *LFARA(2,3)                                                       40
      DIMENSION AB(MAB,4),FARIN(2,3,2),FARAN(2,3),IFUNAR(2,3)          50
      COMMON/CFSTRU/ NR1(3),LERMSG,GLSCH,NR2(2),ITYP,ITYPFU,NR3(5),    60
     *A1,B1,A2,B2,A3,B3,BSIG0                                          70
      SPRU3=.FALSE.                                                    80
      IF(XIE.LT.AB(IAB,1).OR.FSTOLE(XIE,AB(IAB,1),GLSCH)) GOTO 5       90
      IAB=IAB+1                                                       100
      IF(IAB.GT.NAB) CALL FSWR03(3001,'FSGR','A2  ',1)                110
      IF(IFUN.LE.0.OR.IFUN.GT.3) CALL FSWR03(3001,'FSGR','A2  ',2)    120
      GOTO (11,12,13),IFUN                                            130
   11 A1=AB(IAB,2)                                                    140
      B1=AB(IAB,3)                                                    150
      GOTO 5                                                          160
   12 A2=AB(IAB,2)                                                    170
      B2=AB(IAB,3)                                                    180
      GOTO 5                                                          190
   13 A3=AB(IAB,2)                                                    200
      B3=AB(IAB,3)                                                    210
      GOTO 5                                                          220
    5 IF(FSGRA1(AB,IAB,MAB,XIA,XIE)) CALL FSWR03(3001,'FSGR','A2  ',3) 230
      IF(SPRU0) GOTO 1                                                240
C     F=0?                                                            250
      IF(AB(IAB,4).NE.0.0) GOTO 2                                     260
      IPRINT=1                                                        270
    3 IF(.NOT.FSTOLE(AB(IAB-1,1),XIA,GLSCH)) CALL FSWR03(3001,        280
     *'FSGR','A2  ',4)                                                290
      SPRU0=.TRUE.                                                    300
      SPRU3=.TRUE.                                                    310
      XIEE=AMAX1(XIEE,AB(IAB,1))                                      320
      IF(LERMSG.OR.ITYP.LE.3) GOTO 14                                 330
      IF(LFAR(IPRINT,IFAR)) GOTO 15                                   340
```

```
      LFAR(IPRINT,IFAR)=.TRUE.                                          350
      FARIN(IPRINT,IFAR,1)=XIA                                          360
      FARIN(IPRINT,IFAR,2)=XIEE                                         370
      FARAN(IPRINT,IFAR)=BSIGO                                          380
      IFUNAR(IPRINT,IFAR)=IFUN                                          390
      GOTO 333                                                          400
   15 IF(FARIN(IPRINT,IFAR,1).NE.XIA.AND.FARIN(IPRINT,IFAR,2).NE.XIEE   410
     *.AND.IFUNAR(IPRINT,IFAR).NE.IFUN) CALL FSWR03(3001,'FSGR','A2  ',  420
     *5)                                                                430
      GOTO 333                                                          440
   14 CALL FSWR04(1008,ITYP,ITYPFU,BSIGO,BSIGO)                         450
      CALL FSWR02(-2005,XIA,XIEE)                                       460
      IF(IPRINT.EQ.1) CALL FSWR02(-2007,IFUN,ITYP)                      470
      IF(IPRINT.EQ.2) CALL FSWR02(-2008,IFUN,ITYP)                      480
      GOTO 333                                                          490
C     F NULLDURCHGANG?                                                  500
    2 IF(.NOT.NUDUR) GOTO 331                                           510
      IF(AB(IAB,4).GE.0.0) GOTO 332                                     520
      IFRINT=2                                                          530
      GOTO 3                                                            540
    1 CONTINUE                                                          550
      IF(.NOT.LERMSG) GOTO 333                                          560
C     ZUSAETZLICHE TEST BEI SCHON VORHANDENEM FEHLER IM INTERVALL XIA    570
C     BIS XIEE.                                                         580
      J=IAB                                                             590
    4 IF(J.GT.NAB.OR.AB(J-1,1).GE.XIEE.OR.FSTOLE(AB(J-1,1),XIEE,GLSCH))  600
     * GOTO 333                                                         610
      IF(NUDUR.AND.AB(J,4).LT.0.0) CALL FSWR02(-2010,IFUN,ITYP)         620
      IF(AB(J,4).EQ.0.0) CALL FSWR02(-2009,IFUN,ITYP)                   630
      J=J+1                                                             640
      GOTO 4                                                            650
  331 IF(LERMSG.OR.ITYP.LE.3) GOTO 333                                  660
      IF(LFAR(1,IFAR)) LFARA(1,IFAR)=.TRUE.                             670
  332 IF(LERMSG.OR.ITYP.LE.3) GOTO 333                                  680
      IF(LFAR(2,IFAR)) LFARA(2,IFAR)=.TRUE.                             690
      GOTO 333                                                          700
  333 RETURN                                                            710
      END                                                               720
```

```
      SUBROUTINE FSGRA3(AB,IAB,MAB,NAB,XIA,XIE)                          10
      DIMENSION AB(MAB,4)                                                20
      LOGICAL*4 FSTOLE,FSGRAL                                            30
      COMMON/CFSTRU/ NR1(4),GLSCH                                        40
    2 IF(XIE.LE.AB(IAB,1)) GOTO 1                                        50
      IAB=IAB+1                                                          60
      IF(IAB.GT.NAB) CALL FSWR03(3001,'FSGR','A3  ',1)                   70
      GOTO 2                                                             80
    1 IF(IAB.GT.NAB.OR.FSGRA1(AB,IAB,MAB,XIA,XIE)) CALL FSWR03(3001,     90
     *'FSGR','A3  ',2)                                                  100
  333 RETURN                                                            110
      END                                                               120
```

```
      SUBROUTINE FSROMB(FCT,*)                                           10
C     BERECHNET MIT HILFE DER ROMBERG METHODE DAS INTEGRAL VON FCT(X)     20
C     VON XL BIS XH.                                                     30
C     B E S C H R E I B U N G   D E R   P A R A M E T E R .              40
C     XL        UNTERE INTEGRATIONSGRENZE.                               50
C     XH        OBERE INTEGRATIONSGRENZE.                                60
C     EPS       OBERE GRENZE FUER BETRAG DES RELATIVEN FEHLERS.          70
C     NDIM      DIMENSION DES HILFFELDES AUX.                            80
C               NDIM-1=MAXIMAL MOEGLICHE ZAHL DER HALBIERUNGEN           90
C                      DES INTERVALLS XL...XH.                          100
C     NDIMP     ZUSAETZLICH BENOETIGTE WORTE IN AUX.                     110
C     ORINWA    SCHRANKE FUER FEHLERAUSDRUCK. BESCHREIBUNG SIEHE FSTRUK. 120
C     DRUCK     LOGISCHE VARIABLE. .FALSE. : KEIN TEST- ODER FEHLER-     130
C                                            AUSDRUCK IST ERFOLGT.      140
C                                  .TRUE.  : TEST- ODER FEHLER-AUSDRUCK  150
C                                            IST ERFOLGT.               160
C     FCT       NAME DER ZU INTEGRIERENDEN FUNKTION.                     170
C     Y         ERGEBNIS DER BERECHNUNG. ( APPROXIMATION FUER DAS        180
C                                          INTEGRAL. )                  190
C     YF        FELD, ZU DEM Y ADDIERT WIRD. AUSWAHL DES ELEMENTES       200
C               ERFOLGT NACH FOLGENDEM SCHEMA:                           210
C               YF(1) ZAHL DER HALBIERUNGEN WAR KLEINER ALS 3.           220
C                     (NDIMAK<=4). RELATIVER FEHLER WURDE ERREICHT       230
C                     ODER UNTERSCHRITTEN.                               240
C               YF(2) ZAHL DER HALBIERUNGEN WAR >= 3 (NDIMAK>=4).        250
C                     RELATIVER FEHLER WURDE ERREICHT ODER UNTER=         260
C                     SCHRITTEN.                                         270
C                     ODER:                                              280
C                     BEI NDIMAK=4 TRATEN RUNDUNGSFEHLER AUF. ES WIRD DER 290
C                     WERT VON NDIMAK=3 GENOMMEN, FALLS DAS ZUGEHOERIGE  300
C                     DELREL SCHON KLEINER ODER GLEICH DEM GEWUENSCHTEN  310
C                      RELATIVEN FEHLER WAR.                             320
C               YF(3) ZAHL DER HALBIERUNGEN WAR >= 3 (NDIMAK>=4).        330
C                     RELATIVER FEHLER WURDE WEGEN RUNDUNGSFEHLER        340
C                     N I C H T   ERREICHT. (U.U. FEHLERAUSDRUCK.        350
C                                            SIEHE ORINWA.)              360
C     AUX       HILFSFELD DER DIMENSION NDIM.                            370
C     RETURN 1  WIRD EPS NICHT INNERHALB VON NDIM-1 HALBIERUNGEN         380
C               ERREICHT, SO WIRD NDIMP=1 GESETZT UND RETURN 1 GEMACHT.  390
C                                                                        400
      LOGICAL*4 TEST1,TEST2,TEST3,LERMSG,DRUCK,INTKLE                    410
      REAL*8 SM,AUX,H,Q,HH,X,P,HD,FCT,Y                                  420
      DIMENSION AUX(1),YF(3),YFEPS(3)                                    430
      COMMON NR1(4),NC                                                   440
      COMMON/CFSTRU/ TEST1,TEST2,TEST3,LERMSG,GLSCH,NR2(2),ITYP,ITYPFU,  450
     *NR3(11),BSIGO,XL,XH,NR4(1),Y,NDIMP,DRUCK                          460
C     FEHLERABFRAGE.                                                     470
      IF(XL.GT.XH.OR.NDIM.LT.4) CALL FSWR03(3001,'FSRC','MB  ',1)        480
C     VORBEREITUNGEN FUER DEN ROMBERG-LOOP.                              490
      AUX(1)=0.5*(FCT(DBLE(XL))+FCT(DBLE(XH)))                          500
      H=XH-XL                                                           510
      NDIMAK=1                                                          520
      IADD=0                                                            530
      IF(H.EQ.0.0) GOTO 12                                              540
      INTKLE=.FALSE.                                                    550
```

```
      IF(ABS((XH-XL)/XH).LE.10.0*GLSCH) INTKLE=.TRUE.                    560
    2 HH=H                                                              570
      DELT2=0.0                                                         580
      P=1.0                                                             590
      JJ=1                                                              600
      IF(TEST3) WRITE(NO,1001)                                          610
 1001 FORMAT(' ROMBERG. PRINTOUT OF ARRAY AUX.')                        620
      IF(TEST3) WRITE(NO,1002) AUX(1)                                   630
      IZ=0                                                              640
      DO 7 I=2,NDIM                                                     650
      NDIMAK=I                                                          660
      Y=AUX(1)                                                          670
      DELT1=DELT2                                                       680
      HD=HH                                                             690
      HH=0.5*HH                                                         700
      P=0.5*P                                                           710
      X=XL+HH                                                           720
      SM=0.0D+0                                                         730
      DO 3 J=1,JJ                                                       740
      SM=SM+FCT(X)                                                      750
    3 X=X+HD                                                            760
      AUX(I)=0.5*AUX(I-1)+P*SM                                          770
C     R O M B E R G   EXTRAPOLATION.                                    780
      Q=1.0                                                             790
      JI=I-1                                                            800
      DO 4 J=1,JI                                                       810
      II=I-J                                                            820
      Q=Q+Q                                                             830
      Q=Q+Q                                                             840
    4 AUX(II)=AUX(II+1)+(AUX(II+1)-AUX(II))/(Q-1.0)                     850
C     TESTAUSDRUCK.                                                     860
      IF(TEST3) WRITE(NO,1002) (AUX(J),J=1,NDIMAK)                      870
 1002 FORMAT(' ',1P6D21.12)                                             880
C     ENDE DER ROMBERG EXTRAPOLATION.                                   890
      DELT2=DABS(Y-AUX(1))                                              900
      IF(TEST3) WRITE(NO,1003) DELT2                                    910
 1003 FORMAT(' DELT2=',1PE13.6)                                         920
C     BEI GROSSEN INTERVALLEN NOCH KEINE FEHLERABFRAGE IN DEN ERSTEN    930
C     ZWEI HALBIERUNGEN.                                                940
      IF(I.LT.4.AND..NOT.INTKLE) GOTO 7                                 950
C     RELATIVER FEHLER KLEINER GLEICH EPS?                              960
      IF(DELT2.EQ.0.0) GOTO 13                                          970
      DELREL=DELT2/DMAX1(DABS(Y),DABS(AUX(1)))                          980
      IF(TEST3) WRITE(NO,1004) DELREL                                   990
 1004 FORMAT(' DELREL=',1PE13.6)                                       1000
      IF(DELREL.LE.EPS) GOTO 12                                        1010
      IF(I.LT.4) GOTO 7                                                1020
      IF(DELT2.GE.DELT1) GOTO 11                                       1030
    7 JJ=JJ+JJ                                                        1040
      NDIMP=I                                                          1050
      RETURN 1                                                         1060
   11 IZ=IZ+1                                                          1070
      IF(IZ.LE.1) GOTO 7                                               1080
      IADD=3                                                           1090
      DELREL=-1.0                                                      1100
      IF(Y.NE.0.0) DELREL=DELT1/DABS(Y)                                1110
      Y=H*Y                                                            1120
      IF(DELREL.GT.EPS) GOTO 200                                       1130
      IADD=2                                                           1140
      GOTO 201                                                         1150
   13 DELREL=0.0                                                       1160
   12 Y=H*AUX(1)                                                       1170
  200 IF(IADD.NE.0) GOTO 201                                           1180
      IF(NDIMAK.LT.4) IADD=1                                           1190
      IF(NDIMAK.GE.4) IADD=2                                           1200
  201 YF(IADD)=YF(IADD)+Y                                              1210
      YEEPS(IADD)=AMAX1(YEEPS(IADD),DELREL)                            1220
C                                                                      1230
      DRUCK=.FALSE.                                                    1240
      IF(DELREL.GT.DRINWA*EPS.OR.DELREL.EQ.-1.0) DRUCK=.TRUE.          1250
      IF(DRUCK) CALL ESWRCO(2004)                                      1260
      IF(TEST2.OR.DRUCK) WRITE(NO,1000) ITYP,ITYPEU,BSIGO,XL,XH,Y,EPS, 1270
     *DELREL,DELT1,DELT2,IADD,NDIMAK,(AUX(J),J=1,NDIMAK)               1280
 1000 FORMAT(' ROMBERG  ITYP=',I2,'  ITYPEU=',I2,'  SIGO=',1PE13.6,    1290
     *'  XL=',1PE13.6,'  XH=',1PE13.6,'  Y=',1PE13.6/                  1300
     *' ',8X,'  EPS=',1PE13.6,'  DELREL=',1PE13.6,'  DELT1=',1PE13.6,  1310
     *'  DELT2=',1PE13.6,'  IADD=',0PI1,4X,'AUX(I),I=1,',I3,':'/       1320
     *(' ',8X,1P5E18.6))                                               1330
  333 RETURN                                                           1340
      ENTRY ESROMI(EPS,NDIM,DRINWA,YF,YEEPS,AUX)                       1350
      GOTO 333                                                         1360
      END                                                              1370
```

```
      BLOCK DATA                                                         10
      COMMON/CESDUR/ IDUR                                                20
      DATA IDUR/0/                                                       30
      END                                                                40
```

```
      SUBROUTINE SUND (MM,ENG,NEE,REFE,EFE,ITYP,ITNAM,SGO,DUE,XINTE,     10
     1ZINT,XNEN,STREU,LDIM,LDIMP,SE,FSE)                                 20
      REAL*8 MAT,ITNAM,FEST,NFEST,NN,MMM                                 30
      DIMENSION ENG(MM),REFE(NEE),EFE(NEE),ITNAM(ITYP),NN(11),FEST(5),   40
     1NFEST(5),SGO(MM),NSATZ(4),SE(LDIM),FSE(LDIM),DUE(MM),XINTE(MM),    50
     2ZINT(MM),XNEN(MM),STREU(MM),E(4),F(4),FLUSS(2),SF(2)               60
      COMMON MAT,ISTRUK,ISPA,NOUTP,JA,NANF,NEND,KL                       70
      EQUIVALENCE (FEST(1),NFEST(1))                                     80
      WRITE (NOUTP,1)                                                    90
    1 FORMAT(1H0/1H0/' PROGRAMM KENNZIFFER 4'/' PROGRAMM ZUR BERECHNUNG  100
     1VON GRUPPENWIRKUNGSQUERSCHNITTEN BEI UNENDLICHER VERDUENNUNG'/)    110
      CALL FSPIE                                                         120
      IIS=ISPA                                                           130
      REFHL=0.01                                                         140
      LDIF=0                                                             150
      LDIMP=0                                                            160
```

```
      NEFE=NFE                                                          170
      IF(NFE.EQ.1)  NEFE=0                                              180
      NGR=MM-NANF                                                       190
      NEN=MM+1-NENC                                                     200
      CALL DOPW (8HBEST     ,NFEST(2))                                  210
      CALL DOPW (8HSGA      ,NN(1))                                     220
      CALL DOPW (8HSGF      ,NN(2))                                     230
      CALL DOPW (8HSGN      ,NN(3))                                     240
      CALL DOPW (8HMUEL     ,NN(4))                                     250
      CALL DOPW (8HNUE      ,NN(5))                                     260
      CALL DOPW (8HSGC      ,NN(6))                                     270
      CALL DOPW (8HSTR      ,NN(7))                                     280
      CALL DOPW (8HALPHA    ,NN(8))                                     290
      CALL DOPW (8HETA      ,NN(9))                                     300
      CALL DOPW (8HSGG      ,NN(10))                                    310
      CALL DOPW (8HH  01    ,NN(11))                                    320
      CALL DOPW (8HSGKE     ,MMM)                                       330
      INR=0                                                             340
      NFEST(1)=MAT                                                      350
      NFEST(3)=NN(2)                                                    360
      NSATZ(1)=3                                                        370
      CALL NDFLOC (NSUCH1,NSATZ,FEST,NUDAT,NC)                          380
      IF(NSUCH1) 1000,1000,1001                                         390
 1000 ISPA=0                                                            400
      GO TO 1002                                                        410
 1001 ISPA=1                                                            420
 1002 IF(ISPA.EQ.IIS)  GO TO 1003                                       430
 1003 IF(ISPA.EQ.0)  GO TO 2                                            440
      LL=0                                                              450
      DO 3 I=1,ITYP                                                     460
      IF(ITNAM(I).EQ.NN(1)) GO TO 4                                     470
      IF(ITNAM(I).NE.NN(2)) GO TO 3                                     480
    4 LL=LL+1                                                           490
      IF(LL.EQ.2)  GO TO 5                                              500
    3 CONTINUE                                                          510
    8 WRITE (NOUTP,6) MAT                                               520
    6 FORMAT(1HO/' ***WARNING 4. 1 : THE GROUP CROSS SECTION SGC CANNOT 530
     1BE CALCULATED FOR ',A9/19X,'BECAUSE THE REACTION TYPES SGA AND SGF 540
     2 ARE NOT SPECIFIED IN THE INPUT')                                 550
      GO TO 5                                                           560
C                                                                       570
    2 DO 7 I=1,ITYP                                                     580
      IF(ITNAM(I).EQ.NN(1))  GO TO 5                                    590
    7 CONTINUE                                                          600
      GO TO 8                                                           610
C                                                                       620
    5 IGRUP=NEN-1                                                       630
      DO 9 I=NGR,IGRUP                                                  640
    9 SGC(I)=0.                                                         650
      JJJ=1                                                             660
C                                                                       670
C                                                                       680
      DO 10 JJ=1,ITYP                                                   690
      LETA=0                                                            700
      LALF=0                                                            710
      IF(ITNAM(JJ).EQ.NN(5))  GO TO 124                                 720
      IF(ITNAM(JJ).EQ.NN(9))  GO TO 124                                 730
      IF(ITNAM(JJ).NE.NN(9))  GO TO 11                                  740
C                                                                       750
  124 IF(ISPA.NE.0)  GO TO 12                                           760
      WRITE (NOUTP,13) MAT,ITNAM(JJ)                                    770
   13 FORMAT(1HO/' ***WARNING 4. 2 : THE GROUP CROSS SECTION FOR ',2A9,  780
     1' CANNOT BE CALCULATED,'/ 18X,'BECAUSE THE VALUES OF SGF ARE ZERO' 790
     1)                                                                 800
      DO 170 M=NGR,IGRUP                                                810
  170 XINTE(M)=0.                                                       820
      K=NGR                                                             830
      GO TO 200                                                         840
   12 IF(ITNAM(JJ).NE.NN(5))  GO TO 14                                  850
   81 NFEST(3)=NN(2)                                                    860
      GO TO 15                                                          870
   14 NFEST(3)=NN(10)                                                   880
      GO TO 15                                                          890
C                                                                       900
   11 IF(ITNAM(JJ).NE.NN(4))  GO TO 32                                  910
      NFEST(3)=NN(3)                                                    920
C                                                                       930
   15 CALL NDFLOC (NSUCH1,NSATZ,FEST,NUDAT,NC)                          940
      MOD=0                                                             950
      JB=1                                                              960
      IF(NSUCH1)16,16,17                                                970
   16 WRITE (NOUTP,18) (NFEST(I),I=1,3),ITNAM(JJ)                       980
   18 FORMAT(1HO/' ***WARNING 4. 3 : DATA FOR ',3A9,' COULD NOT BE FOUND 990
     1 IN THE KEDAK LIBRARY '/19X,'THIS TYPE IS USED TO CALCULATE THE GR 1000
     2OUP CROSS SECTION ',A9)                                           1010
      SE(1)=ENG(NGR)                                                    1020
      FSE(1)=0.                                                         1030
      SE(2)=ENG(NEN)                                                    1040
      FSE(2)=0.                                                         1050
      GO TO 31                                                          1060
   17 SE(1)=FEST(4)                                                     1070
      FSE(1)=FEST(5)                                                    1080
      IF(SE(1)-ENG(NGR))47,47,20                                        1090
   20 WRITE (NOUTP,21) ENG(NGR),(NFEST(I),I=1,3),SE(1)                  1100
   21 FORMAT(1HO/' ***WARNING 4. 4 : THE LOWER ENERGY GROUP BOUNDARY ',  1110
     1E16.8,'EV IS NOT IN THE AVAILABLE ENERGY RANGE ON KEDAK FOR '/19X, 1120
     23A9,' THE LOWER ENERGY GROUP BOUNDARY HAS BEEN MODYFIED TO ',     1130
     3E16.8,'EV')                                                       1140
   47 M=2                                                               1150
   26 CALL NDFNXT(NSUCH1,NSATZ,FEST,NUDAT,NC)                           1160
      IF(NSUCH1)22,22,23                                                1170
   23 IF(FEST(4)-ENG(NGR))24,24,25                                      1180
   24 SE(1)=FEST(4)                                                     1190
      FSE(1)=FEST(5)                                                    1200
      GO TO 26                                                          1210
   25 IF(JB.EQ.2)  GO TO 902                                            1220
      IF(FEST(5).EQ.0.AND.FSE(1).EQ.0.AND.ITNAM(JJ).EQ.NN(5))  GO TO 900 1230
      IF(FEST(5).EQ.0.AND.FSE(1).EQ.0.AND.ITNAM(JJ).EQ.NN(4))  GO TO 24  1240
      IF(FEST(5).EQ.0.AND.FSE(1).EQ.0.AND.LETA.EQ.1)  GO TO 24          1250
      GO TO 175                                                         1260
  900 FEST(5)=1.E20                                                     1270
      MOD=1                                                             1280
```

```
      WRITE (NOUTP,901)  SE(1),FEST(4)                                  1290
  901 FORMAT(1HO/' ***MESSAGE 4. 8 : FOR THE CALCULATION OF NUE  SGF IS  1300
     1MODIFIED FROM 0. TO 1.E20'/19X,'AT THE ENERGYPOINTS',E16.8,' AND', 1310
     2E16.8)                                                            1320
      GO TO 902                                                         1330
  175 JB=2                                                              1340
  902 IF(FEST(4)-ENG(NEN))27,28,28                                      1350
   27 SE(M)=FEST(4)                                                     1360
      FSE(M)=FEST(5)                                                    1370
      M=M+1                                                             1380
      IF(M-LDIM)26,26,29                                                1390
   29 M=1                                                               1400
      LDIF=LDIF+1                                                       1410
      GO TO 26                                                          1420
   22 M=M-1                                                             1430
      GO TO 30                                                          1440
   28 SE(M)=FEST(4)                                                     1450
      FSE(M)=FEST(5)                                                    1460
      IF(MOD.EQ.1.AND.ITNAM(JJ).EQ.NN(5))  FSE(1)=1.E20                 1470
   30 DO 180 I=1,M                                                      1480
      IF(FSE(I).GE.0)  GO TO 180                                        1490
  172 WRITE (NOUTP,171) FEST(1),FEST(3),SE(I),FSE(I)                    1500
  171 FORMAT(/2A10,' ENERGY',E16.8,' CROSS SECTION ON KEDAK NEGATIVE',  1510
     1E16.8)                                                            1520
  180 CONTINUE                                                          1530
      IF(LDIF.EQ.0)  GO TO 31                                           1540
      LDIMP=(LDIF-1)*LDIM+M+1                                           1550
      WRITE (NOUTP,400) ITNAM(JJ)                                       1560
  400 FORMAT(1HO/' ***MESSAGE 4. 2 : STORAGE NOT SUFFICIENT TO CALCULATE 1570
     1 ',A9)                                                            1580
      RETURN                                                            1590
C                                                                       1600
   31 IS=1                                                              1610
      GO TO 34                                                          1620
   32 IS=0                                                              1630
   34 DO 33 I=NGR,IGRUP                                                 1640
      ZINT(I)=0.                                                        1650
      XNEN(I)=0.                                                        1660
   33 DUE(I)=0.                                                         1670
      I=NGR                                                             1680
      K=NGR                                                             1690
C                                                                       1700
      IF(ITNAM(JJ).EQ.NN(4))  GO TO 125                                 1710
      IF(ITNAM(JJ).NE.NN(5))  GO TO 35                                  1720
  125 NFEST(3)=ITNAM(JJ)                                                1730
  476 E(3)=AMAX1(ENG(I),SF(1))                                          1740
   42 IF(E(3).LT.ENG(I+1))  GO TO 76                                    1750
      I=I+1                                                             1760
      IF(I.GT.IGRUP)  GO TO 10                                          1770
      GO TO 42                                                          1780
   76 CALL NDFLOC (NSUCH1,NSATZ,FEST,NUDAT,NC)                          1790
      IF(NSUCH1) 36,36,37                                               1800
   36 WRITE (NOUTP,38) (NFEST(J),J=1,3)                                 1810
   38 FORMAT(1HO/' ***WARNING 4. 5 : DATA FOR ',3A9,' COULD NOT BE FOUND 1820
     1 IN THE KEDAK LIBRARY')                                           1830
      GO TO 300                                                         1840
```

```
   37 IF(FEST(4)-E(3)  )  39,39,40                                      1850
   40 WRITE (NOUTP,21) ENG(I),(NFEST(J),J=1,3),FEST(4)                  1860
      IF(FEST(4)-ENG(I +1))39,304,304                                   1870
   39 E(1)=FEST(4)                                                      1880
      F(1)=FEST(5)                                                      1890
      IF(FEST(3).EQ.NN(4))  GO TO 173                                   1900
      IF(F(1).GE.0)  GO TO 173                                          1910
      WRITE (NOUTP,171) FEST(1),FEST(3),E(1),F(1)                       1920
  173 CALL NDFNXT (NSUCH1,NSATZ,FEST,NUDAT,NC)                          1930
      IF(NSUCH1)43,43,44                                                1940
   43 WRITE (NOUTP,45) (FEST(J),J=1,3)                                  1950
   45 FORMAT (1HO/' ***WARNING 4. 6 : DATA FOR ',3A9,' ARE NOT AVAILABLE 1960
     1 ON KEDAK IN THE DESIRED ENERGY GROUPS')                          1970
      GO TO 10                                                          1980
   44 IF(FEST(4)-E(3)  )39,39,46                                        1990
   46 IF (F(1).EQ.0.AND.FEST(5).EQ.0)  GO TO 39                         2000
      E(2)=FEST(4)                                                      2010
      F(2)=FEST(5)                                                      2020
      IF(FEST(3).EQ.NN(4))  GO TO 174                                   2030
      IF(F(2).GE.0)  GO TO 174                                          2040
      WRITE (NOUTP,171) FEST(1),FEST(3),E(2),F(2)                       2050
C                                                                       2060
  174 E(3)=AMAX1(ENG(I ),E(1),SE(1))                                    2070
  921 IF(E(3).LT.ENG(I+1))  GO TO 925                                   2080
      I=I+1                                                             2090
      IF(I.LE.IGRUP)  GO TO 921                                         2100
      WRITE (NOUTP,477) MAT,ITNAM(JJ),NFEST(3)                          2110
  477 FORMAT(' ***WARNING 4. 8 :',A9,' TYPE ',A9,' CANNOT BE CALCULATED, 2120
     1 BECAUSE ',A9,' IS NOT'/19X,'AVAILABLE ON KEDAK IN THE DESIRED ENE 2130
     2RGY RANGE')                                                       2140
      GO TO 10                                                          2150
  925 MARK=0                                                            2160
      WRITE(NOUTP,48)E(3)                                               2170
   48 FORMAT(1HO/' ***MESSAGE 4. 1 : BEGIN OF THE INTEGRATION AT',E16.8, 2180
     1' EV')                                                            2190
      K=I                                                               2200
      II=1                                                              2210
      SF(1)=FSE(1)                                                      2220
      F(3)=F(1)                                                         2230
      IF(E(3).EQ.SE(1))  GO TO 49                                       2240
      L=0                                                               2250
      IF(E(3).EQ.E(1))  GO TO 50                                        2260
      L=1                                                               2270
   50 DO 60 II=1,M                                                      2280
      IF(SE(II)-E(3))60,260,61                                          2290
  260 IF(ITNAM(JJ).NE.NN(5))  GO TO 903                                 2300
      IF(MOD.EQ.0)  GO TO 903                                           2310
      CALL GRUP (I,II,M,ENG,SE,FSE,SF(1),MOD)                          2320
  903 SF(1)=FSE(II)                                                     2330
      GO TO 261                                                         2340
   60 CONTINUE                                                          2350
   61 II=II-1                                                           2360
      IF(ITNAM(JJ).NE.NN(5))  GO TO 907                                 2370
      IF(MOD.EQ.0)  GO TO 907                                           2380
      CALL GRUP (I,II,M,ENG,SE,FSE,SF(1),MOD)                          2390
  907 SF(1)=FSE(II)+(FSE(II+1)-FSE(II))/(SE(II+1)-SE(II))*(E(3)-SE(II)) 2400
```

```
  261 IF(L.EQ.0)  GO TO 51                                                  2410
   49 F(3)=F(1)+(F(2)-F(1))/(E(2)-E(1))*(E(3)-E(1))                         2420
C                                                                          2430
   51 IF(NFE.EQ.1)  GO TO 56                                               2440
      DO 53 NI=1,NFE                                                       2450
      IF(REFE(NI)-E(3))53,54,55                                            2460
   53 CONTINUE                                                             2470
   54 FLUSS(1)=EFE(NI)                                                     2480
      NI=NI+1                                                              2490
      GO TO 56                                                             2500
   55 FLUSS(1)=EFE(NI-1)+(EFE(NI)-EFE(NI-1))/(REFE(NI)-REFE(NI-1))*(E(3)   2510
     1-REFE(NI-1))                                                         2520
C                                                                          2530
   56 II=II+1                                                              2540
   67 KW=0                                                                 2550
C                                                                          2560
      IF(NFE.EQ.1)  GO TO 57                                               2570
      E(4)=AMINI(ENG(I+1),E(2),SE(II),REFE(NI))                            2580
      IF(ITNAM(JJ).NE.NN(5))  GO TO 911                                    2590
      IF(MOD.EQ.0)  GO TO 911                                              2600
      IF(MARK.EQ.0)  GO TO 911                                             2610
      MARK=0                                                               2620
      CALL GRUP (I,II,M,ENG,SE,FSE,SF(1),MOD)                              2630
  911 IF(E(4).EQ.ENG(I+1))  GO TO 58                                       2640
      IF(E(4).EQ.E(2))  GO TO 59                                           2650
      IF(E(4).EQ.SE(II)) GO TO 62                                          2660
      FLUSS(2)=EFE(NI)                                                     2670
      NI=NI+1                                                              2680
   63 CALL FL (FSE(II-1),FSE(II),SE(II-1),SE(II),E(4),SF(2))               2690
  164 CALL FL(F(1),F(2),E(1),E(2),E(4),F(4))                               2700
      GO TO 66                                                             2710
   58 IF(E(4).NE.E(2).AND.E(4).NE.SE(II).AND.E(4).NE.REFE(NI))  GO TO      2720
     1157                                                                  2730
      IW=0                                                                 2740
      IK=0                                                                 2750
      IF=0                                                                 2760
      IF(E(4).EQ.E(2))  GO TO 158                                          2770
  162 IF(E(4).EQ.SE(II))  GO TO 159                                        2780
  163 IF(E(4).EQ.REFE(NI))  GO TO 160                                      2790
      GO TO 165                                                            2800
  158 F(4)=F(2)                                                            2810
      E(1)=E(2)                                                            2820
      F(1)=F(2)                                                            2830
      CALL NDFNXT(NSUCH1,NSATZ,FEST,NUDAT,NC)                              2840
      IF(NSUCH1.LE.0)  GO TO 161                                           2850
      E(2)=FEST(4)                                                         2860
      F(2)=FEST(5)                                                         2870
      IW=1                                                                 2880
      IF(FEST(3).EQ.NN(4))  GO TO 162                                      2890
      IF(F(2).GE.0)  GO TO 162                                             2900
      WRITE (NOUTP,171) FEST(1),FEST(3),E(2),F(2)                          2910
      GO TO 162                                                            2920
  159 SF(2)=FSE(II)                                                        2930
      II=II+1                                                              2940
      IK=1                                                                 2950
      GO TO 163                                                            2960
  160 FLUSS(2)=EFE(NI)                                                     2970
      NI=NI+1                                                              2980
      IF=1                                                                 2990
  165 IF(IF.EQ.0)  GO TO 166                                               3000
  167 IF(IK.EQ.1.AND.IW.EQ.0)  GO TO 164                                   3010
      IF(IK.EQ.1.AND.IW.EQ.1)  GO TO 66                                    3020
      IF(IK.EQ.0.AND.IW.EQ.0)  GO TO 63                                    3030
      CALL FL (FSE(II-1),FSE(II),SE(II-1),SE(II),E(4),SF(2))               3040
      GO TO 66                                                             3050
  166 CALL FL (EFE(NI-1),EFE(NI),REFE(NI-1),REFE(NI),E(4),FLUSS(2))        3060
      GO TO 167                                                            3070
  157 CALL FL(EFE(NI-1),EFE(NI),REFE(NI-1),REFE(NI),E(4),FLUSS(2))         3080
      GO TO 63                                                             3090
   59 F(4)=F(2)                                                            3100
      E(1)=E(2)                                                            3110
      F(1)=F(2)                                                            3120
      CALL NDFNXT(NSUCH1,NSATZ,FEST,NUDAT,NC)                              3130
      IF(NSUCH1.GT.0)  GO TO 65                                            3140
  161 WRITE(NOUTP,68) (FEST(J),J=1,3),E(2)                                 3150
   68 FORMAT(1HO/' ***WARNING 4. 7 : FOR',3A9,' NO DATA ARE AVAILABLE AF   3160
     1TER',E16.8,' EV')                                                    3170
      KW=1                                                                 3180
      GO TO 73                                                             3190
   65 E(2)=FEST(4)                                                         3200
      F(2)=FEST(5)                                                         3210
      IF(FEST(3).EQ.NN(4))  GO TO 176                                      3220
      IF(F(2).GE.0)  GO TO 176                                             3230
      WRITE (NOUTP,171) FEST(1),FEST(3),E(2),F(2)                          3240
  176 IF(E(4).NE.SE(II).AND.E(4).NE.REFE(NI))  GO TO 152                   3250
      IW=0                                                                 3260
      IF(E(4).EQ.SE(II))  GO TO 153                                        3270
  155 IF(E(4).EQ.REFE(NI))  GO TO 154                                      3280
  153 SF(2)=FSE(II)                                                        3290
      II=II+1                                                              3300
      LW=1                                                                 3310
      IF(E(4).NE.REFE(NI))  GO TO 156                                      3320
  154 FLUSS(2)=EFE(NI)                                                     3330
      NI=NI+1                                                              3340
      IF(LW.EQ.1)  GO TO 66                                                3350
      CALL FL (FSE(II-1),FSE(II),SE(II-1),SE(II),E(4),SF(2))               3360
      GO TO 66                                                             3370
  152 CALL FL (FSE(II-1),FSE(II),SE(II-1),SE(II),E(4),SF(2))               3380
  156 CALL FL(EFE(NI-1),EFE(NI),REFE(NI-1),REFE(NI),E(4),FLUSS(2))         3390
      GO TO 66                                                             3400
   62 SF(2)=FSE(II)                                                        3410
      II=II+1                                                              3420
      IF(E(4).NE.REFE(NI))  GO TO 150                                      3430
      FLUSS(2)=EFE(NI)                                                     3440
      NI=NI+1                                                              3450
      GO TO 151                                                            3460
  150 CALL FL(EFE(NI-1),EFE(NI),REFE(NI-1),REFE(NI),E(4),FLUSS(2))         3470
  151 CALL FL(F(1),F(2),E(1),E(2),E(4),F(4))                               3480
   66 IF(LALF.EQ.1)  GO TO 77                                              3490
      ZINT(I)=ZINT(I)+(F(3)*SF(1)*FLUSS(1)+F(4)*SF(2)*FLUSS(2))*0.5*(      3500
```

```
     1E(4)-E(3))                                                                3510
       XNEN(I)=XNEN(I)+(SF(1)*FLUSS(1)+SF(2)*FLUSS(2))*0.5*(E(4)-E(3))          3520
    79 E(3)=E(4)                                                                3530
       FLUSS(1)=FLUSS(2)                                                        3540
       F(3)=F(4)                                                                3550
       SF(1)=SF(2)                                                              3560
       IF(E(4).NE.ENG(I+1))  GO TO 67                                           3570
    73 XINTE(I)=ZINT(I)/XNEN(I)                                                 3580
       I=I+1                                                                    3590
       MARK=1                                                                   3600
       E(3)=E(4)                                                                3610
       F(3)=F(4)                                                                3620
       IF(E(4).EQ.SE(II))  II=II+1                                              3630
       IF(E(4).NE.E(2))  GO TO 115                                              3640
       E(1)=E(2)                                                                3650
       F(1)=F(2)                                                                3660
       CALL NDFNXT(NSUCH1,NSATZ,FEST,NUDAT,NC)                                  3670
       IF(NSUCH1.GT.0)  GO TO 64                                                3680
   264 WRITE (NOUTP,68) (FEST(J),J=1,3),E(2)                                    3690
       GO TO 200                                                                3700
    64 E(2)=FEST(4)                                                             3710
       F(2)=FEST(5)                                                             3720
       IF(FEST(3).EQ.NN(4))  GO TO 115                                          3730
       IF(F(2).GE.0)  GO TO 115                                                 3740
       WRITE (NOUTP,171) FEST(1),FEST(3),E(2),F(2)                              3750
   115 IF(KW.EQ.1)  GO TO 200                                                   3760
       IF(I.GT.IGRUP)  GO TO 200                                                3770
       GO TO 67                                                                 3780
C                                                                               3790
    57 E(4)=AMIN1(ENG(I+1),E(2),SE(II))                                         3800
       IF(ITNAM(JJ).NE.NN(5))  GO TO 912                                        3810
       IF(MOD.EQ.0)  GO TO 912                                                  3820
       IF(MARK.EQ.0)  GO TO 912                                                 3830
       MARK=0                                                                   3840
       CALL GRUP (II,II,M,ENG,SE,FSE,SF(1),MOD)                                3850
   912 IF((E(4)-E(3))/E(3).GE.1.E-3)  GO TO 143                                 3860
       IF(E(4).EQ.E(3))  GO TO 114                                              3870
       FLUSS(1)=PHI(E(3))                                                       3880
       FLUSS(2)=PHI(E(4))                                                       3890
       CALL FL (FSE(II-1),FSE(II),SE(II-1),SE(II),E(4),SF(2))                   3900
       CALL FL (F(1),F(2),E(1),E(2),E(4),F(4))                                  3910
       IF(LALF.EQ.1)  GO TO 144                                                 3920
       Z2=(F(3)*SF(1)*FLUSS(1)+F(4)*SF(2)*FLUSS(2))*0.5*(E(4)-E(3))             3930
       X2=(SF(1)*FLUSS(1)+SF(2)*FLUSS(2))*0.5*(E(4)-E(3))                       3940
       GO TO 145                                                                3950
   144 Z2=(SF(1)*FLUSS(1)+SF(2)*FLUSS(2))*0.5*(E(4)-E(3))                       3960
       X2=(F(3)*FLUSS(1)+F(4)*FLUSS(2))*0.5*(E(4)-E(3))                         3970
   145 F(3)=F(4)                                                                3980
       SF(1)=SF(2)                                                              3990
       FLUSS(1)=FLUSS(2)                                                        4000
       GO TO 112                                                                4010
   143 L=1                                                                      4020
       MN=3                                                                     4030
       S=SF(1)                                                                  4040
       FF=F(3)                                                                  4050
    70 Z2=0.                                                                    4060
       X2=0.                                                                    4070
       EE33=E(3)                                                                4080
       FLUSS(1)=PHI(EE33)                                                       4090
       SF(1)=S                                                                  4100
       F(3)=FF                                                                  4110
       LL=1                                                                     4120
    69 EE44=E(3)+(E(4)-E(3))/FLOAT(MN)*FLOAT(LL)                                4130
   121 CALL FL(FSE(II-1),FSE(II),SE(II-1),SE(II),EE44,SF(2))                    4140
       CALL FL(F(1),F(2),E(1),E(2),EE44,F(4))                                   4150
       FLUSS(2)=PHI(EE44)                                                       4160
       IF(LALF.EQ.1)  GO TO 77                                                  4170
       Z2=Z2+(F(3)*SF(1)*FLUSS(1)+F(4)*SF(2)*FLUSS(2))*0.5*(EE44-EE33)          4180
       X2=X2+(SF(1)*FLUSS(1)+SF(2)*FLUSS(2))*0.5*(EE44-EE33)                    4190
    80 LL=LL+1                                                                  4200
       EE33=EE44                                                                4210
       F(3)=F(4)                                                                4220
       SF(1)=SF(2)                                                              4230
       FLUSS(1)=FLUSS(2)                                                        4240
       IF(LL.LT.MN)    GO  TO  69                                               4250
       IF(LL.GT.MN)  GO TO (71,72),L                                            4260
       EE44=E(4)                                                                4270
       GO TO 121                                                                4280
    71 Z1=Z2                                                                    4290
       X1=X2                                                                    4300
       MN=MN*2                                                                  4310
       L=2                                                                      4320
       GO TO 70                                                                 4330
    72 IF(Z1.EQ.0..OR.X1.EQ.0.)  GO TO 111                                      4340
       IF((Z1-Z2)/Z1.GT.RFEHL. OR.(X1-X2)/X1.GT.RFEHL)  GO TO 71                4350
       GO TO 112                                                                4360
   111 IF(Z1.EQ.0..AND.X1.EQ.0.)  GO TO 114                                     4370
       IF(Z1.EQ.0.)  GO TO 113                                                  4380
       IF((Z1-Z2)/Z1.GT.RFEHL)  GO TO 71                                        4390
       GO TO 112                                                                4400
   113 IF((X1-X2)/X1.GT.RFEHL)  GO TO 71                                        4410
   112 ZINT(I)=ZINT(I)+Z2                                                       4420
       XNEN(I)=XNEN(I)+X2                                                       4430
   114 IF(E(4).EQ.ENG(I+1))  GO TO 73                                           4440
       E(3)=E(4)                                                                4450
       F(3)=F(4)                                                                4460
       IF(E(4).EQ.E(2))  GO TO 74                                               4470
       II=II+1                                                                  4480
       GO TO 57                                                                 4490
    74 E(1)=E(2)                                                                4500
       F(1)=F(2)                                                                4510
       CALL NDFNXT(NSUCH1,NSATZ,FEST,NUDAT,NC)                                  4520
       IF(NSUCH1.LE.0)  GO TO 73                                                4530
       E(2)=FEST(4)                                                             4540
       F(2)=FEST(5)                                                             4550
       IF(FEST(3).EQ.NN(4))  GO TO 177                                          4560
       IF(F(2).GE.0)  GO TO 177                                                 4570
       WRITE (NOUTP,171) FEST(1),FEST(3),E(2),F(2)                              4580
   177 IF(E(1).EQ.SE(II))  II=II+1                                              4590
       GO TO 57                                                                 4600
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C                                                                               4610
   35 IF(ITNAM(JJ).EQ.NN(8))  GO TO 123                                         4620
      IF(ITNAM(JJ).NE.NN(9))  GO TO 75                                          4630
  123 IF(LETA.EQ.0) GO TO 82                                                    4640
      NFEST(3)=NN(5)                                                            4650
      GO TO 476                                                                 4660
   82 NFEST(3)=NN(2)                                                            4670
      LALF=1                                                                    4680
      GO TO 476                                                                 4690
   77 IF(NFE.EQ.1) GO TO 78                                                     4700
      ZINT(I)=ZINT(I)+(SF(1)*FLUSS(1)+SF(2)*FLUSS(2))*0.5*(E(4)-E(3))           4710
      XNEN(I)=XNEN(I)+(F(3)*FLUSS(1)+F(4)*FLUSS(2))*0.5*(E(4)-E(3))             4720
      GO TO 79                                                                  4730
   78 Z2=Z2+(SF(1)*FLUSS(1)+SF(2)*FLUSS(2))*0.5*(EE44-EE33)                     4740
      X2=X2+(F(3)*FLUSS(1)+F(4)*FLUSS(2))*0.5*(EE44-EE33)                       4750
      GO TO 80                                                                  4760
C                                                                               4770
   75 NFEST(3)=ITNAM(JJ)                                                        4780
      CALL NDFLOC (NSUCH1,NSATZ,FEST,NUDAT,NC)                                  4790
      IF(NSUCH1)36,36,83                                                        4800
   83 IF(FEST(4)-ENG(I))84,84,85                                                4810
   85 WRITE (NOUTP,21) ENG(I),(NFEST(J),J=1,3),FEST(4)                          4820
   87 IF(FEST(4)-ENG(I+1))84,86,86                                              4830
   86 XINTE(I)=0.                                                               4840
      I=I+1                                                                     4850
      IF(I-IGRUP)87,87,303                                                      4860
   84 E(1)=FEST(4)                                                              4870
      F(1)=FEST(5)                                                              4880
      IF(FEST(3).EQ.NN(4))  GO TO 181                                           4890
      IF(F(1).GE.0)  GO TO 181                                                  4900
      WRITE (NOUTP,171) FEST(1),FEST(3),E(1),F(1)                               4910
  181 CALL NDFNXT(NSUCH1,NSATZ,FEST,NUDAT,NC)                                   4920
      IF(NSUCH1)43,43,88                                                        4930
   88 IF(FEST(4)-ENG(I))84,84,89                                                4940
   89 E(2)=FEST(4)                                                              4950
      F(2)=FEST(5)                                                              4960
      IF(FEST(3).EQ.NN(4))  GO TO 178                                           4970
      IF(F(2).GE.0)  GO TO 178                                                  4980
      WRITE (NOUTP,171) FEST(1),FEST(3),E(2),F(2)                               4990
  178 E(3)=AMAX1(ENG(I),E(1))                                                   5000
      WRITE (NOUTP,48)E(3)                                                      5010
   91 IF(E(3).LT.ENG(I+1))  GO TO 90                                            5020
      I=I+1                                                                     5030
      IF(I.GT.IGRUP)  GO TO 10                                                  5040
      GO TO 91                                                                  5050
   90 K=I                                                                       5060
      F(3)=F(1)+(F(2)-F(1))/(E(2)-E(1))*(E(3)-E(1))                             5070
C                                                                               5080
      IF(NFE.EQ.1) GO TO 96                                                     5090
      DO 93 NI=1,NFE                                                            5100
      IF(REFE(NI)-E(3))93,94,95                                                 5110
   93 CONTINUE                                                                  5120
   94 FLUSS(1)=EFE(NI)                                                          5130
      NI=NI+1                                                                   5140
      GO TO 96                                                                  5150
   95 FLUSS(1)=EFE(NI-1)+(EFE(NI)-EFE(NI-1))/(REFE(NI)-REFE(NI-1))*(E(3)        5160
     1-REFE(NI-1))                                                              5170
C                                                                               5180
   96 KW=0                                                                      5190
      IF(NFE.EQ.1) GO TO 105                                                    5200
      E(4)=AMIN1(ENG(I+1),E(2),REFE(NI))                                        5210
      IF(E(4).EQ.ENG(I+1)) GO TO 97                                             5220
      IF(E(4).EQ.E(2)) GO TO 98                                                 5230
      FLUSS(2)=EFE(NI)                                                          5240
      NI=NI+1                                                                   5250
  100 CALL FL (F(1),F(2),E(1),E(2),E(4),F(4))                                   5260
      GO TO 99                                                                  5270
   97 IF(E(4).NE.E(2).AND.E(4).NE.REFE(NI))  GO TO 131                          5280
      IW=0                                                                      5290
      IK=0                                                                      5300
      IF(E(4).EQ.E(2))  GO TO 132                                               5310
  136 IF(E(4).EQ.REFE(NI))  GO TO 133                                           5320
      GO TO 140                                                                 5330
  132 F(4)=F(2)                                                                 5340
      E(1)=E(2)                                                                 5350
      F(1)=F(2)                                                                 5360
      IW=1                                                                      5370
      CALL NDFNXT(NSUCH1,NSATZ,FEST,NUDAT,NC)                                   5380
      IF(NSUCH1.LE.0)  GO TO 135                                                5390
      E(2)=FEST(4)                                                              5400
      F(2)=FEST(5)                                                              5410
      IF(FEST(3).EQ.NN(4))  GO TO 136                                           5420
      IF(F(2).GE.0)  GO TO 136                                                  5430
      WRITE (NOUTP,171) FEST(1),FEST(3),E(2),F(2)                               5440
      GO TO 136                                                                 5450
  133 FLUSS(2)=EFE(NI)                                                          5460
      NI=NI+1                                                                   5470
      IK=1                                                                      5480
  140 IF(IW.EQ.1.AND.IK.EQ.1)  GO TO 99                                         5490
      IF(IW.EQ.1.AND.IK.EQ.0)  GO TO 137                                        5500
      GO TO 100                                                                 5510
  137 CALL FL (EFE(NI-1),EFE(NI),REFE(NI-1),REFE(NI),E(4),FLUSS(2))             5520
      GO TO 99                                                                  5530
  131 CALL FL (EFE(NI-1),EFE(NI),REFE(NI-1),REFE(NI),E(4),FLUSS(2))             5540
      GO TO 100                                                                 5550
   98 F(4)=F(2)                                                                 5560
      E(1)=E(2)                                                                 5570
      F(1)=F(2)                                                                 5580
      CALL NDFNXT(NSUCH1,NSATZ,FEST,NUDAT,NC)                                   5590
      IF(NSUCH1.GT.0)  GO TO 102                                                5600
  135 WRITE (NOUTP,68) (FEST(J),J=1,3),E(2)                                     5610
      KW=1                                                                      5620
      GO TO 103                                                                 5630
  102 E(2)=FEST(4)                                                              5640
      F(2)=FEST(5)                                                              5650
      IF(FEST(3).EQ.NN(4))  GO TO 179                                           5660
      IF(F(2).GE.0)  GO TO 179                                                  5670
      WRITE (NOUTP,171) FEST(1),FEST(3),E(2),F(2)                               5680
  179 IF(E(4).EQ.REFE(NI))  GO TO 130                                           5690
      CALL FL(EFE(NI-1),EFE(NI),REFE(NI-1),REFE(NI),E(4),FLUSS(2))              5700
      GO TO 99                                                                  5710
```

```
130 FLUSS(2)=EFE(NI)                                                    5720
    NI=NI+1                                                             5730
 99 ZINT(I)=ZINT(I)+(F(3)*FLUSS(1)+F(4)*FLUSS(2))*0.5*(E(4)-E(3))       5740
    XNEN(I)=XNEN(I)+(FLUSS(1)+FLUSS(2))*0.5*(E(4)-E(3))                 5750
    IF(MAT.NE.NN(11))  GO TO 104                                        5760
    IF(ITNAM(JJ).NE.NN(3))  GO TO 104                                   5770
    EN=ALOG(E(4)/E(3))                                                  5780
    SF1=F(3)*FLUSS(1)                                                   5790
    SF3=F(4)*FLUSS(2)                                                   5800
    DUE(I)=DUE(I)+SF1*EN+SF3-SF1-(SF3-SF1)/(E(4)-E(3))*E(3)*EN          5810
104 E(3)=E(4)                                                           5820
    FLUSS(1)=FLUSS(2)                                                   5830
    F(3)=F(4)                                                           5840
    IF(E(4).NE.ENG(I+1)) GO TO 96                                       5850
103 XINTE(I)=ZINT(I)/XNEN(I)                                            5860
    IF(MAT.EQ.NN(11).AND.ITNAM(JJ).EQ.NN(3))  STREU(I)=DUE(I)/XNEN(I)   5870
    I=I+1                                                               5880
    E(3)=E(4)                                                           5890
    F(3)=F(4)                                                           5900
    IF(E(4).NE.E(2))  GO TO 120                                         5910
    E(1)=E(2)                                                           5920
    F(1)=F(2)                                                           5930
    CALL NDFNXT(NSUCH1,NSATZ,FEST,NUDAT,NC)                             5940
    IF(NSUCH1.GT.0)  GO TO 101                                          5950
265 WRITE (NOUTP,68) (FEST(J),J=1,3),E(2)                               5960
    GO TO 200                                                           5970
101 E(2)=FEST(4)                                                        5980
    F(2)=FEST(5)                                                        5990
    IF(FEST(3).EQ.NN(4))  GO TO 120                                     6000
    IF(F(2).GE.0)  GO TO 120                                            6010
    WRITE (NOUTP,171) FEST(1),FEST(3),E(2),F(2)                         6020
120 IF(KW.EQ.1) GO TO 200                                               6030
    IF(I.GT.IGRUP) GO TO 200                                            6040
    GO TO 96                                                            6050
C                                                                       6060
105 E(4)=AMIN1(ENG(I+1),E(2))                                           6070
    IF((E(4)-E(3))/E(3).GE.1.E-3)  GO TO 141                            6080
    FLUSS(1)=PHI(E(3))                                                  6090
    FLUSS(2)=PHI(E(4))                                                  6100
    CALL FL (F(1),F(2),E(1),E(2),E(4),F(4))                             6110
    Z2=(F(3)*FLUSS(1)+F(4)*FLUSS(2))*0.5*(E(4)-E(3))                    6120
    X2=(FLUSS(1)+FLUSS(2))*0.5*(E(4)-E(3))                              6130
    IF(MAT.NE.NN(11))  GO TO 142                                        6140
    IF(ITNAM(JJ).NE.NN(3))  GO TO 142                                   6150
    EN=ALOG(E(4)/E(3))                                                  6160
    SF1=F(3)*FLUSS(1)                                                   6170
    SF3=F(4)*FLUSS(2)                                                   6180
    Z3=SF1*EN+SF3-SF1-(SF3-SF1)/(E(4)-E(3))*E(3)*EN                     6190
142 FLUSS(1)=FLUSS(2)                                                   6200
    F(3)=F(4)                                                           6210
    GO TO 117                                                           6220
141 L=1                                                                 6230
    MN=3                                                                6240
    FF=F(3)                                                             6250
110 Z2=0.                                                               6260
    Z3=0.                                                               6270
    X2=0.                                                               6280
    EE33=E(3)                                                           6290
    FLUSS(1)=PHI(EE33)                                                  6300
    F(3)=FF                                                             6310
    LL=1                                                                6320
107 EE44=E(3)+(E(4)-E(3))/FLOAT(MN)*FLOAT(LL)                           6330
122 CALL FL (F(1),F(2),E(1),E(2),EE44,F(4))                             6340
    FLUSS(2)=PHI(EE44)                                                  6350
    Z2=Z2+(F(3)*FLUSS(1)+F(4)*FLUSS(2))*0.5*(EE44-EE33)                 6360
    X2=X2+(FLUSS(1)+FLUSS(2))*0.5*(EE44-EE33)                           6370
C                                                                       6380
    IF(MAT.NE.NN(11))  GO TO 106                                        6390
    IF(ITNAM(JJ).NE.NN(3))  GO TO 106                                   6400
    EN=ALOG(EE44/EE33)                                                  6410
    SF1=F(3)*FLUSS(1)                                                   6420
    SF3=F(4)*FLUSS(2)                                                   6430
    Z3=Z3+SF1*EN+SF3-SF1-(SF3-SF1)/(EE44-EE33)*EE33*EN                  6440
C                                                                       6450
106 LL=LL+1                                                             6460
    EE33=EE44                                                           6470
    F(3)=F(4)                                                           6480
    FLUSS(1)=FLUSS(2)                                                   6490
    IF(LL.LT.MN) GO TO 107                                              6500
    IF(LL.GT.MN)  GO TO (108,109),L                                     6510
    EE44=E(4)                                                           6520
    GO TO 122                                                           6530
108 Z1=Z2                                                               6540
    X1=X2                                                               6550
    MN=MN*2                                                             6560
    L=2                                                                 6570
    GO TO 110                                                           6580
109 IF(Z1.EQ.0..OR.X1.EQ.0.)  GO TO 116                                 6590
    IF((Z1-Z2)/Z1.GT.RFEHL.OR.(X1-X2)/X1.GT.RFEHL) GO TO 108            6600
    GO TO 117                                                           6610
116 IF(Z1.EQ.0..AND.X1.EQ.0.)  GO TO 118                                6620
    IF(Z1.EQ.0.)  GO TO 119                                             6630
    IF((Z1-Z2)/Z1.GT.RFEHL)  GO TO 108                                  6640
    GO TO 117                                                           6650
119 IF((X1-X2)/X1.GT.RFEHL)  GO TO 108                                  6660
117 ZINT(I)=ZINT(I)+Z2                                                  6670
    XNEN(I)=XNEN(I)+X2                                                  6680
118 IF(MAT.EQ.NN(11).AND.ITNAM(JJ).EQ.NN(3)) DUE(I)=DUE(I)+Z3           6690
    IF(E(4).EQ.ENG(I+1)) GO TO 103                                      6700
    E(3)=E(4)                                                           6710
    F(3)=F(4)                                                           6720
    E(1)=E(2)                                                           6730
    F(1)=F(2)                                                           6740
    CALL NDFNXT(NSUCH1,NSATZ,FEST,NUDAT,NC)                             6750
    IF(NSUCH1.LE.0) GOTO 103                                            6760
    E(2)=FEST(4)                                                        6770
    F(2)=FEST(5)                                                        6780
    IF(FEST(3).EQ.NN(4))  GO TO 105                                     6790
    IF(F(2).GE.0)  GO TO 105                                            6800
    WRITE (NOUTP,171) FEST(1),FEST(3),E(2),F(2)                         6810
```

```
      GO TO 105
C
C     AUSDRUCKEN DER ERGEBNISSE
C
  200 IF(ITNAM(JJ).NE.NN(9))  GO TO 211
      IF(LETA.EQ.1) GO TO 213
      DO 212 N=K,IGRUP
  212 STREU(N)=XINTE(N)
      LETA=1
      LALF=0
      GO TO 81
  213 DO 214 N=K,IGRUP
  214 XINTE(N)=XINTE(N)/(1.+STREU(N))
  211 IF(JJJ.EQ.2) GO TO 201
      N=0
      WRITE (JA) N,MMM
      JJJ=2
  201 NNN=NEN-1
      N=2
      WRITE (JA) N,K,NNN
      IST=MM-K
      NI=MM-NNN
      WRITE (NOUTP,202) MAT,ITNAM(JJ),IST,NI
  202 FORMAT(1HO,2A9,3X,'GRUPPE',I3,' BIS',I3)
      N=4
      WRITE (JA) N,MAT,ITNAM(JJ)
      N=NEN-K
      WRITE (JA) N,(XINTE(LL),LL=K,IGRUP)
      WRITE (NOUTP,203) (XINTE(LL),LL=K,IGRUP)
  203 FORMAT(1H ,7E16.8/(1X,7E16.8))
      IF(ITNAM(JJ).EQ.NN(1)) GO TO 204
      IF(ITNAM(JJ).EQ.NN(2)) GO TO 205
      GO TO 206
  204 DO 207 N=K,IGRUP
  207 SGC(N)=SGC(N)+XINTE(N)
      IF(INR.EQ.1) GO TO 210
      INR=1
      GO TO 10
  205 DO 209 N=K,IGRUP
  209 SGC(N)=SGC(N)-XINTE(N)
      IF(INR.EQ.1) GO TO 210
      INR=1
      GO TO 10
  210 N=2
      WRITE (JA) N,K,NNN
      N=4
      WRITE (JA) N,MAT,NN(6)
      N=NEN-K
      WRITE (JA)N,(SGC(LL),LL=K,IGRUP)
      WRITE (NOUTP,202) MAT,NN(6),IST,NI
      WRITE (NOUTP,203) (SGC(LL),LL=K,IGRUP)
      GO TO 10
  206 IF(MAT.NE.NN(11)) GO TO 10
      IF(ITNAM(JJ).NE.NN(3)) GO TO 10
      N=2
      WRITE (JA) N,K,NNN
      N=4
      WRITE (JA) N,MAT,NN(7)
      N=NEN-K
      WRITE (JA) N,(STREU(LL),LL=K,IGRUP)
      WRITE (NOUTP,202) MAT,NN(7),IST,NI
      WRITE (NOUTP,203) (STREU(LL),LL=K,IGRUP)
      GO TO 10
C
  300 IF(I-IGRUP)301,301,303
  301 DO 302 N=I,IGRUP
  302 XINTE(N)=0.
      GO TO 303
  304 XINTE(I)=0.
      I=I+1
      IF(I-IGRUP)37,37,303
  303 NNN=NEN-1
      IF(MM-K.LT.MM-NNN) GO TO 10
      GO TO 200
   10 CONTINUE
C
      ISPA=IIS
      KL=KL+1
      RETURN
      END
```

```
      SUBROUTINE FL(EFE1,EFE2,REFE1,REFE2,E,ERG)                    10
      ERG=EFE1+(EFE2-EFE1)/(REFE2-REFE1)*(E-REFE1)                  20
      RETURN                                                        30
      END                                                           40
```

```
      SUBROUTINE GRUP (I,II,M,ENG,SE,FSE,SF,MOD)                    1C
      DIMENSION ENG(1),SE(M),FSE(M)                                 2C
      DO 1 NI=II,M                                                  3C
      IF( SE(NI).GE.ENG(I+1))  GO TO 2                              4C
    1 CONTINUE                                                      5C
    2 IF(FSE(NI).EQ.1.E20)  GO TO 4                                 6C
      DO 3 MI=1,NI                                                  7C
    3 IF(FSE(MI).EQ.1.E20)  FSE(MI)=0.                              8C
      IF(SF.EQ.1.E20)  SF=0.                                        9C
      MOD=0                                                        10C
    4 RETURN                                                       11C
      END                                                          12C
```

```
C*****SUBROUTINE SCAT.DATE OF LAST CHANGE 21.12. 1976.(LINES 10 TO
C*****3650)
C      CALCULATION OF THE INELASTIC SCATTERING PROBABILITIES
C
       SUBROUTINE SCAT(NX,EG,XNUE,NFE,EF,FI,NE27,KINEM,NIN,NINA,INTYP,X,
      1IX,MMAXX,MFELD)
       REAL*8 NAM,NAM4,NP
       DIMENSION EG(NX),EF(NFE),FI(NFE),X(MMAXX),IX(MMAXX),NP(3),NAM4(3),
      1INTYP(3),MFELDC(3)
       COMMON NAM,ISTRUK,ISPA,NA,LIZ,NANF,NEND,KL
C      AUSDRUCK DER DIMENSIONEN FUER HILFSFELDER
C      WRITE(NA,2000) (EG(IGEN),IGEN=1,NX)
C2000 FORMAT(6E15.9)
       IA=0
       NAB=0
       IAC=0
       NABD=0
       IAC=0
       NABC=0
       IFELD=0
       IT=1
       KI=2
       MFELD=0
       MFELDD=0
       MFELDC(1)=0
       MFELDC(2)=0
       MFELDC(3)=0
    46 DO 44 I=1,MMAXX
       X(I)=0.
    44 IX(I)=0
       CALL DOPW(8HSMTOT   ,NAM4(1))
       CALL DOPW(8HSMTOT2N ,NAM4(2))
       CALL DOPW(8HSMTOT3N ,NAM4(3))
       CALL DOPW(8HPROBSGI ,NP(1))
       CALL DOPW(8HPROBSG2N,NP(2))
       CALL DOPW(8HPROBSG3N,NP(3))
       IF(INTYP(IT).EQ.2.OR.INTYP(IT).EQ.3) GO TO 45
C*****ESTIMATED VALUES OF THE DIMENSIONS OF THE WORKING FIELDS
C*****USED IN SCATD.
       NAEP=0
       ISGP=0
       NISGP=0
       NAE=30
       ISG=200
       NISG=400
C*****ORGANIZATION OF THE WORKING FIELDS FOR SUBROUTINE SCATD.
     7 NAE=NAE+NAEP
       ISG=ISG+ISGP
       NISG=NISG+NISGP
       NAEP=0
       ISGP=0
       NISGP=0
       IF(INTYP(IT).EQ.2) CALL DOPW(8HSG2N    ,TYP)
       IF(INTYP(IT).EQ.3) CALL DOPW(8HSG3N    ,TYP)
C      WRITE(NA,1013) NAE,ISG,NISG,NAEP,ISGP,NISGP
C1013 FORMAT('NAE=',I10,' ISG=',I10,' NISG=',I10,
C     */' NAEP=',I10,' ISGP=',I10,' NISGP=',I10)
C      WIRD MAXIMALE DIMENSION UEBERSCHRITTEN?
       L1=1
       L2=L1+NX*NX
       L3=(L2+NX)/2*2+3
       L4=L3+2*NX
       L5=L4+2*NX
       L6=L5+2*NE27
       L7=L6+2*NAE
       L8=L7+NX
       L9=L8+NX
       L10=L9+ISG
       L11=L10+NAE
       L12=L11+ISG*NAE
       L13=(L12+ISG)/2*2+3
       L14=L13+2*NISG
       MFELDD=L14
C      WRITE(NA,1006) L14,MMAXX
C1006 FORMAT(/' BENOETIGTE FELDLAENGE',I10,
C     */        ' VERFUEGBARE FELDLAENGE',I10)
       IF(L14.LE.MMAXX) GO TO 4
C      WRITE(NA,1014) L14,MMAXX
C1014 FORMAT('OSUMME DER LAENGEN ALLER EINZELNEN HILFSFELDER GLEICH ',
C     *I12,' WORTE'/' DIESE ZAHL UEBERSTEIGT DIE MAXIMALE DIMENSION VON
C     *',I12,' WORTEN.'/' VERGROESSERN SIE DIE REGION UM DIE MAXIMALE DI
C     *MENSION MMAXX UND STARTEN SIE DAS PROGRAMM ERNEUT.')
       MFELDD=L14
       IFELD=1
       NINA=IT
       GO TO 100
    4 CONTINUE
   45 WRITE(NA,9000)
 9000 FORMAT(/////' PROGRAMM KENNZIFFER 5'/)
       WRITE(NA,9001)
 9001 FORMAT('OPROGRAMM ZUR BERECHNUNG VON TRANSFERMATRIZEN FUER '/
     *'   INELASTISCHE STREUUNG, (N,2N) - UND (N,3N) - PROZESSE'/)
       WRITE(NA,9018) NP(INTYP(IT))
 9018 FORMAT(1HO/' ',A8/1X)
       IF(INTYP(IT).EQ.2.OR.INTYP(IT).EQ.3) GO TO 40
       L31=L3-1
       DO 1 L=L1,L31
    1 X(L)=0.
       CALL SCATD(NX,EG,NFE,EF,FI,NE27,X(L1),X(L2),X(L3),
     *X(L4),X(L5),X(L6),X(L7),X(L8),X(L9),X(L10),X(L11),X(L12),
     *X(L13),NISG,NISGP,NAE,NAEP,ISG,ISGP,KINEM,IAD,NABD)
C*****X(L1).....X(L2-1) : NORMALIZED TRANSFER PROBABILITIES
C*****PICGH.X(L2).....X(L3-1) : ENERGY INTEGRAL OF DISCRETE
C*****LEVEL INELASTIC SCATTERING CROSS SECTION MULTIPLIED BY
C*****WEIGHTING FUNCTION SIDG. (G MEANS GROUP NUMBER OF OUT
C*****SCATTERING GROUP,H GROUP NUMBER OF INSCATTERING GROUP)
       IF(NAEP.EQ.0.AND.ISGP.EQ.0.AND.NISGP.EQ.0) GO TO 2
       WRITE(NA,9007) NAE,ISG,NISG,NAEP,ISGP,NISGP
 9007 FORMAT(' NAE=',I6,'ISG=',I6,'NISG=',I6,
     *'NAEP=',I6,'ISGP=',I6,'NISGP=',I6)
```

```
      GO TO 7                                                          1110
    2 IF (IAD.EQ.0.AND.NABD.EQ.0) GO TO 43                             1120
      NX2=NX*NX                                                        1130
C*****IG : EXTERNAL ENERGY GROUP COUNT (1 CORRESPONDS TO ENERGY GROUP  1140
C*****WITH HIGHEST ENERGY                                              1150
      DO 8 IG=1,NX                                                     1160
C*****MG : INTERNAL ENERGY GROUP COUNT (1 CORRESPONDS TO ENERGY GROUP  1170
C*****WITH LOWEST ENERGY.                                              1180
      MG=NE27-IG                                                       1190
C*****NXMH : NUMBER OF DOWNSCATTERING GROUPS INCLUDING OUTSCATTERING    1200
C*****GROUP.                                                           1210
    8 NXMH=NX-IG+1                                                     1220
C*****MH : COUNT OF INSCATTERING (DOWNSCATTERING) GROUPS.MH=1 MEANS    1230
C*****SCATTERING INTO OUTSCATTERING GROUP.MH=2 MEANS SCATTERING INTO    1240
C*****THAT ENERGY GROUP,THAT ENERGETICALLY LIES ONE GROUP BELOW THE     1250
C*****OUTSCATTERING GROUP.MH=3 MEANS SCATTERING INTO THAT ENERGY GROUP, 1260
C*****THAT ENERGETICALLY LIES TWO GROUPS BELOW THE OUTSCATTERING GROUP. 1270
C   8 WRITE(NA,9002) (X(L1+(MH-1)*NX+MG-1),MH=1,NXMH)                  1280
C9002 FORMAT(10E12.5)                                                  1290
      DO 5 IG=1,NX                                                     1300
    5 MG=NE27-IG                                                       1310
C   5 WRITE(NA,9006) MG,IG,X(L2-1+MG)                                  1320
C9006 FORMAT(' MG=',I6,'IG=',I6,'QUOT(IG)=',E12.5)                     1330
C*****CALCULATION OF SIDG*PIDGH.                                       1340
      DO 9 IG=1,NX                                                     1350
      MG=NE27-IG                                                       1360
      NXMH=NX-IG+1                                                     1370
      DO 10 MH=1,NXMH                                                  1380
   10 X(L1+(MH-1)*NX+MG-1)=X(L1+(MH-1)*NX+MG-1)*X(L2-1+MG)             1390
    9 CONTINUE                                                         1400
      DO 11 IG=1,NX                                                    1410
      MG=NE27-IG                                                       1420
      NXMH=NX-IG+1                                                     1430
C  11 WRITE(NA,9002) (X(L1+(MH-1)*NX+MG-1),MH=1,NXMH)                  1440
   11 CONTINUE                                                         1450
      GO TO 43                                                         1460
   40 L1=1                                                             1470
      L2=L1+NX*NX                                                      1480
      L3=(L2+NX)/2*2+3                                                 1490
C*****ESTIMATION OF DIMENSIONS OF WORKING FIELDS USED IN SCATC         1500
   43 NISG=200                                                         1510
      NISGI=300                                                        1520
      NEP=30                                                           1530
      NF=5                                                             1540
      NISGP=0                                                          1550
      NISGIP=0                                                         1560
      NEPP=0                                                           1570
      NFP=0                                                            1580
C*****ORGANIZATION OF THE WORKING FIELDS FOR SUBROUTINE SCATC.          1590
   15 NISG=NISG+NISGP                                                  1600
      NISGI=NISGI+NISGIP                                               1610
      NEP=NEP+NEPP                                                     1620
      NF=NF+NFP                                                        1630
      NISGP=0                                                          1640
      NISGIP=0                                                         1650
      NEPP=0                                                           1660
      NFP=0                                                            1670
      L4=L3+NX*NX                                                      1680
      L5=L4+NX                                                         1690
      L6=L5+NE27                                                       1700
      L7=L6+NISG                                                       1710
      L8=L7+NISG                                                       1720
      L9=L8+NISGI                                                      1730
      L10=L9+NEP                                                       1740
      L11=L10+NEP*NF                                                   1750
      L12=L11+NEP*NF                                                   1760
      L13=L12+NEP*NF                                                   1770
      L14=L13+NEP*NF                                                   1780
      L15=L14+NX                                                       1790
      MFELDC(INTYP(IT))=L15                                            1800
C     WRITE(NA,1006) L15,MMAXX                                         1810
      IF(L15.LE.MMAXX) GO TO12                                         1820
C     WRITE(NA,1014) L15,MMAXX                                         1830
      IFELD=1                                                          1840
      NINA=IT                                                          1850
      GO TO 100                                                        1860
   12 L51=L15-1                                                        1870
      DO 13 L=L3,L51                                                   1880
   13 X(L)=0.                                                          1890
      IR=0                                                             1900
      CALL SCATC(NX,EG,XNUE,NFE,EF,FI,NE27,INTYP(IT),X(L3),X(L4),X(L5), 1910
     *X(L6),X(L7),X(L8),X(L9),X(L10),X(L11),X(L12),X(L13),             1920
     *NISG,NISGP,NISGI,NISGIP,NEP,NEPP,NF,NFP,IAC,NABC,IR)             1930
C*****X(L3).....X(L4-1) : NORMALIZED TRANSFER PROBABILITIES FOR INELAST 1940
C*****IC SCATTERING IN CONNECTION WITH THE EXCITATION OF CONTINUOUS LEVE 1950
C*****LS OF THE RESIDUAL NUCLEUS (OR FOR (N,2N)- OR (N,3N)-REACTIONS    1960
C*****PIDGH.X(L4).....X(L5-1) : ENERGY GROUP INTEGRAL OVER THE PRODUCT  1970
C*****OF CONTINUOUS LEVEL INELASTIC SCATTERING CROSS SECTION (OR (N,2N) 1980
C*****OR (N,3N)-CROSS-SECTION) AND THE WEIGHTING FUNCTION SIGG         1990
      IF (IR.EQ.1) GO TO 50                                            2000
      GO TO 51                                                         2010
   50 KL=KL+1                                                          2020
      GO TO 52                                                         2030
   51 IF(NISGP.EQ.0.AND.NISGIP.EQ.0.AND.NEPP.EQ.0.AND.NFP.EQ.0) GO TO 14 2040
      WRITE(NA,9008) NISG,NISGP,NISGI,NISGIP,NEP,NEPP,NF,NFP           2050
 9008 FORMAT(' NISG=',I6,'NISGP=',I6,'NISGI=',I6,'NISGIP=',I6,        2060
     *'NEP=',I6,'NEPP=',I6,'NF=',I6,'NFP=',I6)                         2070
      GO TO 15                                                         2080
   14 IF(INTYP(IT).EQ.2.OR.INTYP(IT).EQ.3) GO TO 41                    2090
      IF(IAD.EQ.0.AND.NABD.EQ.0) GO TO 41                              2100
      IF(IAC.NE.0) IA= MINO(IAD,IAC)                                   2110
      IF(IAC.EQ.0) IA=IAD                                              2120
      IF(NABC.NE.0) NAB=MAXO(NABD,NABC)                                2130
      IF(NABC.EQ.0) NAB=NABD                                           2140
      GO TO 42                                                         2150
   41 IA=IAC                                                           2160
      NAB=NABC                                                         2170
   42 KD=NAB-IA+1                                                      2180
      IF(NAB.EQ.0.AND.IA.EQ.0) KD=0                                    2190
C     WRITE(NA,9004) IA,NAB,KD,IAD,NABD,IAC,NABC                       2200
```

```
C9004 FORMAT('   IN SCAT IA=',I6,'NAB=',I6,'KD=',I6,'IAD=',I6,'NABD=',I6 2210
C     1,'IAC=',I6,'NABC=',I6)                                           2220
      IF (KD.NE.0) GO TO 48                                             2230
      WRITE(NA,9022) KD,NAM4(INTYP(IT))                                 2240
 9022 FORMAT(//' KD=',I6,'  NO TRANSFER MATRICES FOR TYPE  ',A8,'IN THE 2250
     1 ENERGY REGION REQUIRED BY INPUT'/)                               2260
      GO TO 240                                                         2270
   48 IA7=NE27-IA                                                       2280
      NAB7=NE27-NAB                                                     2290
C     WRITE(NA,9012) IA7,NAB7                                           2300
C9012 FORMAT(' IN SCAT IA7=',I6,'NAB7=',I6)                             2310
      NX2=NX*NX                                                         2320
C*****IG : EXTERNAL ENERGY GROUP COUNT ( 1 CORRESPONDS TO ENERGY GROUP  2330
C*****WITH HIGHEST ENERGY).                                             2340
      DO 16 IG=NAB7,IA7                                                 2350
C*****MG : EXTERNAL ENERGY GROUP COUNT ( 1 CORRESPONDS TO ENERGY GROUP  2360
C*****WITH LOWEST ENERGY).                                              2370
      MG=NE27-IG                                                        2380
C*****NXMH : NUMBER OF DOWNSCATTERING GROUPS INCLUDING OUTSCATTERING     2390
C*****GROUP.                                                            2400
   16 NXMH=NX-IG+1                                                      2410
C*****MH : GROUP COUNT FOR DOWNSCATTERING GROUPS,MH=1 MEANING           2420
C*****INSCATTERING GROUP CORRESPONDS TO OUTSCATTERING GROUP,MH=2         2430
C*****MEANS INSCATTERING GROUP IS THAT ENERGY GROUP,THAT ENERGETICALLY   2440
C*****IS NEXT LOWER TO OUTSCATTERING.MH=3 REFERS TO INSCATTERING         2450
C*****GROUP ENERGETICALLY TWO GROUPS LOWER THAN OUTSCATTERING GROUP.     2460
C  16 WRITE(NA,9002) (X(L3+(MH-1)*NX+MG-1),MH=1,NXMH)                    2470
      DO 17 IG=NAB7,IA7                                                 2480
   17 MG=NE27-IG                                                        2490
C  17 WRITE(NA,9009) MG,X(L4-1+MG)                                       2500
C9009 FORMAT(' MG=',I6,'QUOTC(MG)=',E12.5)                              2510
C*****CALCULATION OF SICG*PICGH                                         2520
      DO 18 IG=NAB7,IA7                                                 2530
      MG=NE27-IG                                                        2540
      NXMH=NX-IG+1                                                      2550
      DO 19 MH=1,NXMH                                                   2560
   19 X(L3+(MH-1)*NX+MG-1)=X(L3+(MH-1)*NX+MG-1)*X(L4-1+MG)              2570
   18 CONTINUE                                                          2580
      DO 20 IG=NAB7,IA7                                                 2590
      MG=NE27-IG                                                        2600
   20 NXMH=NX-IG+1                                                      2610
C  20 WRITE(NA,9002) (X(L3+(MH-1)*NX+MG-1),MH=1,NXMH)                    2620
C*****CALCULATION OF THE COMBINATION OF DISCRETE LEVEL AND CONTINUOUS    2630
C*****LEVEL INELASTIC TRANSFER PROBABILITY :                            2640
C*****PIGH=(PIDGH*SIDG+PICGH*SICG)/(SIDG+SICG).                         2650
      DO 21 IG=NAB7,IA7                                                 2660
      MG=NE27-IG                                                        2670
      NXMH=NX-IG+1                                                      2680
      DO 22 MH=1,NXMH                                                   2690
      X(L1+(MH-1)*NX+MG-1)=X(L1+(MH-1)*NX+MG-1)+X(L3+(MH-1)*NX+MG-1)    2700
      XD=(X(L2-1+MG)+X(L4-1+MG))                                        2710
      IF (XD.NE.0.)                                                     2720
     1X(L1+(MH-1)*NX+MG-1)=X(L1+(MH-1)*NX+MG-1)/XD                      2730
   22 CONTINUE                                                          2740
   21 CONTINUE                                                          2750
      DO 23 IG=NAB7,IA7                                                 2760
      MG=NE27-IG                                                        2770
   23 NXMH=NX-IG+1                                                      2780
C  23 WRITE(NA,9002) (X(L1+(MH-1)*NX+MG-1),MH=1,NXMH)                    2790
      IF(KD.NE.0) GO TO 47                                              2800
      GO TO 240                                                         2810
   47 MZ=0                                                              2820
      WRITE(LIZ) MZ,NAM4(INTYP(IT))                                     2830
C     WRITE(NA,9014) MZ,NAM4(INTYP(IT))                                 2840
C9014 FORMAT(' MZ=',I6,'NAM4=',A8)                                      2850
      KZ=KI+1                                                           2860
      WRITE(LIZ) KZ,NAM,KD                                              2870
      WRITE(NA,9013) KZ,NAM,KD                                          2880
 9013 FORMAT('OKZ=',I6,'NAM=',A8,'KD=',I6)                              2890
C*****IG1 : EXTERNAL ENERGY GROUP COUNT ( 1 CORRESPONDS TO ENERGY GROUP 2900
C*****WITH HIGHEST ENERGY).IG : EXTERNAL ENERGY GROUP COUNT.IG IS       2910
C*****INTRODUCED TO OBTAIN AN OUTPUT ,THAT STARTS WITH THE OUTSCATTERING 2920
C*****GROUP OF LOWEST ENERGY.                                           2930
      DO 24 IG1=NAB7,IA7                                                2940
      IG=IA7+NAB7-IG1                                                   2950
      NNULL=0                                                           2960
C*****THE MEANING OF MG,NXMH AND MH CORRESPONDS TO THE MEANING          2970
C*****THEY HAVE IN THE WRITE COMMANDS AFTER RETURNING FROM SCATD        2980
C*****AND SCATC RESPECTIVELY.                                           2990
      MG=NE27-IG                                                        3000
      NXMH=NX-IG+1                                                      3010
      NXMH1=NXMH                                                        3020
      DO 25 MH=1,NXMH                                                   3030
      MH1=NXMH-MH+1                                                     3040
      IF(X(L1+(MH1-1)*NX+MG-1).LE.0..AND. NNULL.EQ.0) GO TO 26          3050
      NNULL=1                                                           3060
      GO TO 25                                                          3070
   26 NXMH1=NXMH1-1                                                     3080
   25 CONTINUE                                                          3090
      IF(NXMH1.NE.0) GO TO 27                                           3100
      WRITE(NA,9020)                                                    3110
 9020 FORMAT(' ***WARNING 5.10 :THE INELASTIC SCATTERING MATRIX IS FOUND 3120
     1TO BE EQUAL TO ZERO IN AN ENERGY GROUP'/',WHERE THE INELASTIC SCAT 3130
     2TERING CROSS SECTION IS GREATER THAN ZERO.CHECK NUCLEAR DATA       3140
     3KD GETS A WRONG VALUE.')                                          3150
      GO TO 24                                                          3160
   27 NXMH11=NXMH1+1                                                    3170
C     WRITE(NA,9010) IG,NXMH11                                          3180
C9010 FORMAT('aaaaaaIG=',I6,'NXMH11=',I6,'aaaaaaaaaaaa')                3190
C     WRITE(NA,9011) (X(L1+(MH-1)*NX+MG-1),MH=1,NXMH1)                  3200
C9011 FORMAT(10E12.5)                                                   3210
      WRITE (LIZ) NXMH11,IG,(X(L1+(MH-1)*NX+MG-1),MH=1,NXMH1)           3220
C     ORGANIZATION OF THE OUTPUT ON LISTING IN THE FORM OF MAXIMUM 11    3230
C     SCATTERING PROBABILITIES PER LINE STARTING WITH THE OUTSCATTERING  3240
C     GROUP OF LOWEST ENERGY(LARGEST GROUP NUMBER ACCORDING TO ABN-SET)  3250
      NZ=NXMH1                                                          3260
      DO 30 LN=1,NZ                                                     3270
      IX(L14+LN-1)=IG+LN-1                                              3280
   30 CONTINUE                                                          3290
      KJ=NZ/11                                                          3300
      KJJ=KJ*11                                                         3310
      IF(NZ.NE.KJJ)  GOTO 31                                            3320
```

```
      KJ1=KJ                                                            3320
      GOTO 32                                                           3340
   31 KJ1=KJ+1                                                          3350
   32 DO 37 LI=1,KJ1                                                    3360
      IF(LI.NE.1)   GOTO 33                                             3370
      LIM=1                                                             3380
      GO TO 34                                                          3390
   33 LIM=(LI-1)*11+1                                                   3400
      IF(LI.EQ.KJ1)   GOTO 35                                           3410
   34 IF(KJ1.LE.1)   GOTO 35                                            3420
      LII=LI*11                                                         3430
      GO TO 36                                                          3440
   35 LII=NZ                                                            3450
   36 IF(LIM.GT.LII)  GOTO 37                                           3460
      WRITE(NA,9015)   (IX(L14+LM-1),LM=LIM,LII)                        3470
 9015 FORMAT(10X,11(3X,I3,5X))                                          3480
      IF(LI.NE.1)   GOTO 38                                             3490
C     IG-OUTSCATTERING GROUP ACCORDING TO THE COUNTING IN THE ABN-SET    3500
C     I.E. LOWEST GROUP NUMBER CORRESPONDS TO HIGHEST ENERGY BOUNDARIES  3510
C     X(L1+(MH-1)*NX+MG-1)-PROBABILITY FOR INELASTIC SCATTERING OUT OF   3520
C      GROUP IG INTO GROUP (MH+IG-1).                                    3530
      WRITE(NA,9016) IG,(X(L1+(MH-1)*NX+MG-1),MH=1,LII)                 3540
 9016 FORMAT(3X,I2,5X,11(1PE10.3,1X))                                   3550
      GO TO 37                                                          3560
   38 WRITE(NA,9017)(X(L1+(MH-1)*NX+MG-1),MH=LIM,LII)                   3570
 9017 FORMAT(10X,11(1PE10.3,1X))                                        3580
   37 CONTINUE                                                          3590
   24 CONTINUE                                                          3600
C     WRITE(NA,9021) KD,IT,NIN                                          3610
C9021 FORMAT(' AFTER STATEMENT 24 KD=',I6,'IT=',I6,'NIN=',I6)           3620
  240 IT=IT+1                                                           3630
      IF(IT.LE.NIN) GO TO 46                                            3640
    3 KL=KL+1                                                           3650
  100 MFELD=MAXO(MFELDD,MFELDC(1),MFELDC(2),MFELDC(3))                  3660
      IF(IFELD.EQ.1) WRITE(NA,9019) NP(INTYP(NINA))                     3670
 9019 FORMAT(/' *****CALCULATION OF    ',A8/)                           3680
   52 RETURN                                                            3690
      END                                                               3700
```

```
      SUBROUTINE RENUDA(TYP,KONT,SGIZC,EZ,EU,EC,NACT,NISG,              10
     1NISGP)                                                            20
C*****SUBROUTINE READS TYPE SGIZC FROM THE NUCLEAR LIBRARY WITHIN THE EN 30
C*****NERGY LIMITS EU AND EO.                                           40
C     DIMENSION EZ(NISG),SGIZC(NISG),NAME(3),NNAM(3),QUER(2),NN(5)      50
      DIMENSION EZ(NISG),SGIZC(NISG),NAME(6),NNAM(4),QUER(2),NN(5)      60
C     REAL*8 NAM,TYP,NAME,NN,NIVEAU                                     70
      REAL*8 NAM,TYP,NAME,NN,NIVEAU,BEST                                80
      COMMON NAM,ISTRUK,ISPA,NA,LIZ                                     90
      KONTG=1                                                           100
      NISGF=0                                                           110
      NOPT=0                                                            120
      NACT=0                                                            130
      IEW=0                                                             140
      EW=0.                                                             150
      SW=0.                                                             160
```

```
C     WRITE(NA,103) EU,EC                                               170
C 103 FORMAT(' EU=',F12.6,'EC=',E12.6)                                  180
      CALL DOPW(8HSGIZC    ,NN(1))                                      190
      CALL DOPW(8HSGIZ     ,NN(2))                                      200
      CALL DOPW(8HSGI      ,NN(3))                                      210
      CALL DOPW(8HSG2N     ,NN(4))                                      220
      CALL DOPW(8HSG3N     ,NN(5))                                      230
      CALL DOPW(8HBEST     ,BEST)                                       240
      IF(TYP.EQ.NN(1).OR.TYP.EQ.NN(4).OR.TYP.EQ.NN(5)) GO TO 1          250
      IF(TYP.EQ.NN(2)) GO TO 4                                          260
    1 I=1                                                               270
C     NNAM(1)=2                                                         280
      NNAM(1)=3                                                         290
      NAME(1)=NAM                                                       300
      NAME(2)=BEST                                                      310
C     NAME(2)=TYP                                                       320
      NAME(3)=TYP                                                       330
C   19 CALL LOFLOC(KENNZ,NNAM,NAME,QUER)                                340
   19 CALL NOFLOC(KENNZ,NNAM,NAME,NDAT,NCO)                             350
      IF (KENNZ.EQ.0) GO TO 2                                           360
   21 QUER(1)=NAME(4)                                                   370
      QUER(2)=NAME(5)                                                   380
C   21 IF(QUER(1).LT.EU) GO TO 20                                       390
      IF(QUER(1).LT.EU) GO TO 20                                        400
      IF(QUER(1).EQ.EU) GO TO 12                                        410
      IF(QUER(1).GT.EU.AND.QUER(1).LE.EO.AND.EW.GT.0..AND.I.EQ.1.AND.   420
     1NISGF.EQ.0) GO TO 10                                              430
      IF(QUER(1).GE.EO) GO TO 22                                        440
      IF(QUER(1).GT.EU.AND.QUER(1).LT.EC) GO TO 12                      450
   22 NOPT=1                                                            460
      IF(IEW.EQ.1.AND.I.EQ.1) GO TO 10                                  470
      GO TO 12                                                          480
   10 EZ(I)=EW                                                          490
      SGIZC(I)=SW                                                       500
      I=I+1                                                             510
   12 EZ(I)=QUER(1)                                                     520
      SGIZC(I)=QUER(2)                                                  530
      IF(NOPT.EQ.1) GO TO 6                                             540
      I=I+1                                                             550
      IF (I.LE.NISG) GO TO 3                                            560
      GO TO 5                                                           570
C    2 WRITE(NA,100) NAM,TYP                                            580
C 100 FORMAT(' *** FOR THE ISOTOPE  ',A8,'THE DATA TYPE  ',A8,'IS NOT AV 590
C     1AILABLE ON THE NUCLEAR LIBRARY')                                 600
    2 KONT=0                                                            610
      GO TO 9                                                           620
   20 CONTINUE                                                          630
      EW=QUER(1)                                                        640
      SW=QUER(2)                                                        650
      IEW=1                                                             660
C    3 CALL LOFNXT(KENNZ,NNAM,NAME,QUER)                                670
    3 CALL NOFNXT(KENNZ,NNAM,NAME,NDAT,NCO)                             680
      QUER(1)=NAME(4)                                                   690
      QUER(2)=NAME(5)                                                   700
      IF (KENNZ.EQ.0) GO TO 23                                          710
```

```
      GO TO 21                                                          720
   23 I=I-1                                                             730
      GO TO 6                                                           740
    5 I=1                                                               750
      NISGF=NISGF+1                                                     760
      GO TO 3                                                           770
    6 IF(I.GT.1) GO TO 7                                                780
C     WRITE(NA,101) TYP,NAM,EU,EO                                       790
C 101 FORMAT(' ***NO DATA FOR',A8,'OF MATERIAL',A8,'AVAILABLE IN THE ENE 800
C    1RGY REGION',G14.6,G14.6)                                          810
      KCNTG=0                                                           820
      GO TO 9                                                           830
    7 NACT=I                                                            840
      IF(NISGF.NE.0) GO TO 8                                            850
C     IF(KENNZ.EQ.0) NACT=I-1                                           860
      IF (SGIZC(1).EQ.0..AND.SGIZC(2).EQ.0.) GO TO 24                   870
      GO TO 9                                                           880
   24 IF(NACT.GT.2) GO TO 31                                            890
      NACT=0                                                            900
      GO TO 29                                                          910
   31 NACT1=NACT-1                                                      920
      DO 25 NTH=1,NACT1                                                 930
      EZ(NTH)=EZ(NTH+1)                                                 940
   25 SGIZC(NTH)=SGIZC(NTH+1)                                           950
      NACT=NACT1                                                        960
      IF (EZ(1).GE.EO) NACT=0                                           970
      GO TO 9                                                           980
    8 NISGP=I+NISG*(NISGF-1)                                            990
      GO TO 9                                                          1000
    4 E=0.                                                             1010
C     NNAM(1)=3                                                        1020
      NNAM(1)=4                                                        1030
      NAME(1)=NAM                                                      1040
      NAME(2)=BEST                                                     1050
C     NAME(2)=TYP                                                      1060
      NAME(3)=TYP                                                      1070
C     NAME(3)=0                                                        1080
      NAME(4)=0                                                        1090
C     CALL LDFLOC(KENNZ,NNAM,NAME,QUER)                                1100
      CALL NDFLOC(KENNZ,NNAM,NAME,NDAT,NCO)                            1110
      IF(KENNZ.EQ.1) GO TO 13                                          1120
   16 CALL NDFLOC(KENNZ,NNAM,NAME,NDAT,NCO)                            1130
C  16 CALL LDFLOC(KENNZ,NNAM,NAME,QUER)                                1140
      IF(KENNZ.EQ.0) GO TO 17                                          1150
C  12  NIVEAU=NAME(3)                                                  1160
   13  NIVEAU=NAME(4)                                                  1170
   15 QUER(1)=NAME(5)                                                  1180
      QUER(2)=NAME(6)                                                  1190
C  15 E=AMAX1(E,QUER(1))                                               1200
      E=AMAX1(E,QUER(1))                                               1210
C     CALL LDFNXT(KENNZ,NNAM,NAME,QUER)                                1220
      CALL NDFNXT(KENNZ,NNAM,NAME,NDAT,NCO)                            1230
      IF(KENNZ.EQ.1) GO TO 15                                          1240
C     IF(NAME(3).GT.NIVEAU) GO TO 16                                   1250
      IF(NAME(4).GT.NIVEAU) GO TO 16                                   1260
C     GO TO 17                                                         1270
C  14 WRITE(NA,100) NAM,TYP                                            1280
   17 IF(E.GE.EU.AND.E.LE.EO) GO TO 18                                 1290
      KCNTG=0                                                          1300
      TYP=NN(3)                                                        1310
C     WRITE(NA,101) TYP,NAM,EU,EO                                      1320
C  18 WRITE(NA,102) E                                                  1330
C 102 FORMAT(' UPPER ENERGY OF TYPE SGIZ IS',G14.6,'EV')               1340
C     NNAM(1)=2                                                        1350
   18 NNAM(1)=3                                                        1360
C     NAME(2)=NN(3)                                                    1370
      NAME(3)=NN(3)                                                    1380
      TYP=NN(3)                                                        1390
      EU=AMAX1(EU,E)                                                   1400
      I=1                                                              1410
      GO TO 19                                                         1420
    9 IF(EZ(1).GE.EO) NACT=0                                           1430
      IF(SGIZC(1).EQ.0..AND.NACT.GE.2) GO TO 30                        1440
      GO TO 29                                                         1450
   30 IF((EZ(2)-EZ(1))/EZ(2).GT.1.E-2) GO TO 27                        1460
      GO TO 29                                                         1470
   27 IF(NISG.GE.(NACT+2)) GO TO 28                                    1480
      NISGF=NISGF+1                                                    1490
      NISGP=NISGP+2                                                    1500
      GO TO 29                                                         1510
   28 EZ1=(EZ(2)-EZ(1))*0.1+EZ(1)                                      1520
      EZ2=(EZ(2)-EZ(1))*0.1+EZ1                                        1530
      SGIZC1=FIPOLA(EZ(1),EZ1,EZ(2),SGIZC(1),SGIZC(2))                 1540
      SGIZC2=FIPOLA(EZ(1),EZ2,EZ(2),SGIZC(1),SGIZC(2))                 1550
      DO 26 I=2,NACT                                                   1560
      EZ(NACT-I+4)=EZ(NACT-I+2)                                        1570
   26 SGIZC(NACT-I+4)=SGIZC(NACT-I+2)                                  1580
      EZ(2)=EZ1                                                        1590
      EZ(3)=EZ2                                                        1600
      SGIZC(2)=SGIZC1                                                  1610
      SGIZC(3)=SGIZC2                                                  1620
      NACT=NACT+2                                                      1630
C     WRITE(NA,104) (I,EZ(I),SGIZC(I),I=1,NACT)                        1640
C 104 FORMAT(2(' I=',I6,'EZ=',E12.5,'SGIZC=',E12.5))                   1650
   29 RETURN                                                           1660
      END                                                              1670
```

```
C*****SUBROUTINE SCATC.DATE OF LAST CHANGE 21.12.1976.(LINES 3660 TO      10
C*****6460)                                                              20
      SUBROUTINE SCATC(NX,EG,XNUE,NFE,EF,FI,NE27,INTYP,WEINC,QUCTC,ENG,  30
     *EZ,SGIZC,EI,EP,F1,F2,F3,F4,NISG,NISGP,NISGI,NISGIP,NEP,NEPP,NF,NEP 40
     *,IA,NAB,IR)                                                        50
      DIMENSION EG(NX),EF(NFE),FI(NFE),WEINC(NX,NX),CLOTC(NX),ENG(NE27), 60
     *EZ(NISG),SGIZC(NISG),EI(NISGI),EP(NEP),F1(NF,NEP),F2(NF,NEP),      70
     *F3(NF,NEP),F4(NF,NEP),NN(8)                                        80
      COMMON NAM,ISTRUK,ISPA,NA,LIZ,NAAF,NEND,KL                         90
      REAL*8 NAM,TYP,NN                                                 100
      IF (INTYP.EQ.1) WRITE(NA,9000)                                    110
```

```
 9000 FORMAT(////' PROGRAMM ZUR BERECHNUNG INELASTISCHER STREUMATRIZEN '/
     1' IM ENERGIEBEREICH KONTINUIERLICHER ANREGUNGSNIVEAUS DES RESTKERN
     2S'/)
      IA=0
      NAB=0
      EPS=0.01
      EPSSP=0.0001
      A=0.
      NMAX=100000
      KEN=NFE
      IF (NFE.EQ.1) KEN=0
      CALL DOPW(8HSGIZC   ,NN(1))
      CALL DOPW(8HSGIZ    ,NN(2))
      CALL DOPW(8HSGI     ,NN(3))
      CALL DOPW(8HSEDIC   ,NN(4))
      CALL DOPW(8HSG2N    ,NN(5))
      CALL DOPW(8HSED2N   ,NN(6))
      CALL DOPW(8HSG3N    ,NN(7))
      CALL DOPW(8HSED3N   ,NN(8))
      NUGRE=0
      IF (EG(1)-1.E-3) 40,40,25
   40 NE=NX
      DO 26 I=1,NX
   26 ENG(NX)=EG(NX)
      GO TO 41
C****** : ADDING THERMAL GROUP TO INSCATTERING GROUPS
   25 DO 28 I=1,NX
   28 ENG(NE27-I+1)=EG(NX-I+1)
      NE=NE27
      ENG(1)=1.E-3
   41 DO 29 IG=1,NX
      DO 29 IH=1,NX
   29 WEINC(IG,IH)=0.
      IG1=NE27-NANF
      IG2=NE27-NEND
      DO 42 IGE=IG1,IG2
      IF(INTYP.EQ.1) GO TO 5
      ITYP=2*INTYP+1
      GO TO 8
    5 ITYP=1
      GO TO 8
    7 ITYP=ITYP+1
    8 KONT=1
      TYP=NN(ITYP)
    3 REU =ENG(IGE)
      REO=ENG(IGE+1)
      CALL RENUDA (TYP,KONT,SGIZC,EZ,REU,REO,
     *NACT,NISG,NISGP)
C     WRITE(NA,119) NISG,NISGP,KONT
C 119 FORMAT(' NISG=',I6,'NISGP=',I6,'KONT=',I6)
 9002 FORMAT(/' ***WARNING 5.00 : THE CROSS-SECTION-VALUES,GIVEN FOR THE
     1 MATERIAL ',A8,',TYPE ',A8/' ***DO NOT COVER THE ENERGY-GROUP BETW
     2EEN ',E14.6,'EV AND ',E14.6,'EV.THE LOWEST AND HIGHEST VALUES '/'
     3***GIVEN ON KEDAK FOR THIS GROUP ARE  ',E14.6,'EV AND ',E14.6,
     4'EV.'/' ***THE INTEGRATION IN THIS ENERGY-GROUP THEREFORE IS RESTR
     5ICTED.')
      IF(KONT.EQ.0) GO TO 6
      IF(NISGP.NE.0) GO TO 49
      IF (NACT.EQ.0) GO TO 52
      GO TO 51
C   52 WRITE(NA,9003) NAM,TYP,ENG(IGE),ENG(IGE+1)
C9003 FORMAT(' NO ENERGY-POINTS ON KEDAK FOR MATERIAL ',A8,'TYPE ',A8/
C     2' IN THE ENERGY-REGION BETWEEN ',E12.5,'EV AND ',E12.5,'EV')
   52 CONTINUE
      GO TO 42
   51 IF(NISGI.GE.NACT) GO TO 33
      NISGIP=NACT-NISGI
C     IF(NISGIM.GE.NACT) GO TO 35
C     WRITE(NA,117) NACT,NISGIM
C 117 FORMAT(' NISGIM TOO SMALL,NACT=',I6,'NISGIM=',I6)
      GO TO 49
C   35 NISGI=NISGI+NISGIP
C     NISGIP=0
   33 IF(EZ(1).GT.ENG(IGE).OR.EZ(NACT).LT.ENG(IGE+1))
     1WRITE(NA,9002) NAM,TYP,ENG(IGE),ENG(IGE+1),EZ(1),EZ(NACT)
      DO 17 I=1,NACT
   17 EI(I)=EZ(I)
C*****EZ(1)...EZ(NACT) : ENERGY POINTS OF SGIZC
C*****EF(1)...EF(NFE) : ENERGY POINTS OF THE SPECTRUM
C*****EI(1)...EI(KMAX) : SUM OF EZ AND EF AND ENERGY GROUP LIMITS
      GO TO 9
C    1 IF((NISG+NISGP).LE.NISGM  ) GO TO 2
C     WRITE(NA,100) NISGM
C 100 FORMAT(' &&&DIMENSION NISGMAX TOO SMALL')
C     GO TO 49
C    2 NISG=NISG+NISGP
C     NISGP=0
C     KONT=1
C     GO TO 3
    6 IF(ITYP.EQ.1) GO TO 7
      WRITE(NA,9001) NN(ITYP)
 9001 FORMAT(' NO INFORMATION FOR TYPE',A8,'ON THE NUCLEAR LIBRARY')
      GO TO 49
    9 IF(KEN.NE.0) GO TO 14
      KMAX=NACT
      EI(1)=AMAX1(ENG(IGE),EI(1))
      EI(NACT)=AMIN1(ENG(IGE+1),EI(NACT))
      GO TO 12
   14 CALL ENORG(ENG(IGE),ENG(IGE+1),EI,EF,NACT,KMAX,NFE,NISGI,
     *NISGIP)
C     WRITE(NA,107) NISGI,NISGIP
C 107 FORMAT(' NISGI=',I6,'NISGIP=',I6)
      IF(NISGIP.NE.0) GO TO 49
      GO TO 36
C   34 IF((NISGI+NISGIP).LE.NISGIM) GO TO 37
C     WRITE(NA,118) NISGI,NISGIP,NISGIM
C 118 FORMAT('***NISGIM TOO SMALL NISGI=',I6,'NISGIP=',I6,'NISGIM=',I6)
C     GO TO 49
C   37 NISGI=NISGI+NISGIP
C     NISGIP=0
```

```
C      GO TO 14                                                          1220
C   36 WRITE(NA,108) (EI(KS),KS=1,KMAX)                                  1230
C 108 FORMAT(' ',E12.5)                                                  1240
    36 CONTINUE                                                          1250
    12 KONT=1                                                            1260
       CALL REPROB(INTYP,KONT,EP,F1,F2,F3,F4,NEP,NEPP,NF,NFP)            1270
       IF (KONT.EQ.0) GO TO 15                                           1280
       U=F4(1,1)                                                         1290
       GO TO 11                                                          1300
    15 IF (INTYP.EQ.1) TYP=NN(4)                                         1310
       IF (INTYP.EQ.2) TYP=NN(6)                                         1320
       IF (INTYP.EQ.3) TYP=NN(8)                                         1330
       U=F4(1,2)                                                         1340
       IF(A.EQ.F4(1,1)) GO TO 11                                         1350
       A=F4(1,1)                                                         1360
       WRITE(NA,109) TYP,NAM,NN(2*INTYP+1),U,A,XNUE                      1370
   109 FORMAT(/' NO INFORMATION ON THE NUCLEAR DATA LIBRARY FOR TYPE ',A8 1380
      1,'OF MATERIAL',A8,'.AN EVAPORATION MODEL WITH'/' THETA=SQRT(E/(NUE 1390
      2*A)) IS USED.FOR THE NORMALIZATION THE THRESHOLD OF   ',A8,'   IS  1400
      3TAKEN INTO ACCOUNT.'/' U=',E12.5,'EV,A=',E12.5,'NUE=',E12.5/)     1410
    11 IF (EZ(1).LT.U) GO TO 65                                          1420
       IF(NEPP.EQ.0.AND.NFP.EQ.0) GO TO 50                               1430
       GO TO 49                                                          1440
C*****CALCULATION OF SIGMA*WEIGHTING FUNCTION.(SUM) (NM=0)               1450
    50 SUM=0.                                                            1460
       KMAX1=KMAX-1                                                      1470
       NM=0                                                              1480
       IF(KEN.GT.0)GOTO 30                                               1490
       EF1=0.                                                            1500
       EFKEN=1.E+20                                                      1510
       GOTO 31                                                           1520
    30 EF1=EF(1)                                                         1530
       EFKEN=EF(KEN)                                                     1540
    31 CONTINUE                                                          1550
       EMIN=AMAX1(EZ(1),ENG(IGE),EF1)                                    1560
       EMAX=AMIN1(EZ(NACT),ENG(IGE+1),EFKEN)                             1570
       EMINW=AMAX1(ENG(IGE),EF1)                                         1580
       EMAXW=AMIN1(ENG(IGE+1),EFKEN)                                     1590
       DO 16 IE=1,KMAX1                                                  1600
       IF (EI(IE+1).LE.EMIN) GO TO 18                                    1610
       IF(EI(IE).GE.EMAX) GO TO 18                                       1620
       CALL SIMPSI(NUGRE,U,A,XNUE,EI(IE),EI(IE+1),EPS,NMAX,RESINT,N,EZ,  1630
      1SGIZC,EF,FI,ENG,NACT,NFE,NE,NM,EP,F1,F2,F3,F4,NEP,NF,KONT,ERR,INTG 1640
      2)                                                                 1650
       GO TO 19                                                          1660
    18 RESINT=0.                                                         1670
    19 CONTINUE                                                          1680
C      WRITE(NA,9010) IE,EI(IE),EI(IE+1),RESINT,SUM                      1690
C9010 FORMAT(' IE=',I6,'EI(IE)=',E12.5,'EI(IE+1)=',E12.5/                1700
C     1' RESINT=',E12.5,'SUM=',E12.5)                                    1710
    16 SUM=SUM+RESINT                                                    1720
C      WRITE(NA,111) SUM                                                 1730
C 111 FORMAT(' SUM=',E12.5)                                              1740
       NM=2                                                              1750
C*****CALCULATION OF THE INTEGRAL OF THE WEIGHTING SPECTRUM OVER THE OUT 1760

C*****SCATTERING GROUP IGE. (SUMW) (NM=2)                                1770
       SUMW=0.                                                           1780
       IF(KEN.EQ.0) GO TO 60                                             1790
       DO 46 IE=1,KMAX1                                                  1800
       IF(EI(IE+1).LE.EMINW) GO TO 47                                    1810
       IF(EI(IE).GE.EMAXW) GO TO 47                                      1820
C      WRITE(NA,126) EI(IE),EI(IE+1),NM                                  1830
C 126 FORMAT(' ENTER SIMPSI E(IE)=',E12.5,'E(IE+1)=',E12.5,'NM=',I6)     1840
       CALL SIMPSI(NUGRE,U,A,XNUE,EI(IE),EI(IE+1),EPS,NMAX,WINT,N,EZ,    1850
      1SGIZC,EF,FI,ENG,NACT,NFE,NE,NM,EP,F1,F2,F3,F4,NEP,NF,KONT,ERR,    1860
      2INTG)                                                             1870
C      WRITE(NA,127) EI(IE),EI(IE+1),NM,WINT                             1880
C 127 FORMAT(' AFTER SIMPSI EI(IE)=',E12.5,'EI(IE+1)=',E12.5,'NM=',I6,   1890
C     1'WINT=',E12.5)                                                    1900
       GO TO 48                                                          1910
C   47 WRITE(NA,128)                                                     1920
C 128 FORMAT(' 47  47  47 47  47  47  47  47  47')                       1930
    47 WINT=0.                                                           1940
    48 SUMW=SUMW+WINT                                                    1950
C      WRITE(NA,124) SUMW                                                1960
C 124 FORMAT(' &&&&&&SUMW=',E12.5,'&&&&&&')                              1970
C      WRITE(NA,9020) IE,EI(IE),EI(IE+1),WINT,SUMW                       1980
C9020 FORMAT(' IE=',I6,'EI(IE)=',E12.5,'EI(IE+1)=',E12.5/                1990
C     1' WINT=',E12.5,'SUMW=',E12.5)                                     2000
    46 CONTINUE                                                          2010
       GO TO 61                                                          2020
    60 CALL SIMPSI(NUGRE,U,A,XNUE,EMINW,EMAXW,EPSSP,NMAX,WINT,N,EZ,      2030
      1SGIZC,EF,FI,ENG,NACT,NFE,NE,NM,EP,F1,F2,F3,F4,NEP,NF,KONT,ERR,    2040
      2INTG)                                                             2050
C      WRITE (NA,9004) EMINW,EMAXW,WINT                                  2060
C9004 FORMAT(' EMINW=',E12.5,'EMAXW=',E12.5,'WINT=',E12.5)               2070
       SUMW=SUMW+WINT                                                    2080
    61 SUMQQ=SUM/SUMW                                                    2090
       NIGE=NE-IGE                                                       2100
C*****SUMQQ = WEIGHTED GROUP CROSS-SECTION.                              2110
       SUMQ=SUM                                                          2120
C      WRITE(NA,125) SUMQ                                                2130
C 125 FORMAT(' &&&&&&SUMQ=',E12.5,'&&&&&&')                              2140
       IF(INTYP.EQ.2.OR.INTYP.EQ.3) WRITE(NA,115) SUMQQ,NIGE,U,KONT      2150
  115 FORMAT(//' **WEIGHTED GROUP CROSS-SECTION = ',E12.6,' FOR OUTSCATT 2160
     1ERING - GROUP ',I6,' U = ',E12.6,'KONT = ',I6)                     2170
       QUOTC(IGE)=SUMQ                                                   2180
       NM=1                                                              2190
C*****CALCULATION OF THE INTEGRAL OF SIGMA*SPECTRUM*TRANSFER-PROBABILITY 2200
C*****OVER THE OUTSCATTERING GROUP IGE. (PROSUM) (NM=1)                  2210
       PRSUM=0.                                                          2220
       NIE=NE-IGE                                                        2230
       DO 22 NUGR1=NIE,NX                                                2240
       INTG=0                                                            2250
       INTG1=0                                                           2260
       PROSUM=0.                                                         2270
       NUGRE=NE-NUGR1                                                    2280
       DO 20 IE=1,KMAX1                                                  2290
       IF (EI(IE+1).LE.EMIN) GO TO 21                                    2300
       IF (EI(IE).GE.EMAX) GO TO 21                                      2310
```

```
      CALL SIMPSI(NUGRE,U,A,XNUE,EI(IE),EI(IE+1),EPS,AMAX,PRINT,N,EZ,     2320
     1SGIZC,EF,FI,ENG,NACT,NFE,NE,NM,EP,F1,F2,F3,F4,NEP,NF,KONT,ERR,     2330
     2INTG1)                                                             2340
C     WRITE(NA,116) INTG                                                 2350
C 116 FORMAT(' ***************INTG=',I6,'*****************')             2360
      IF (INTG1.EQ.1) INTG=1                                             2370
      IF(N.GE.NMAX.AND.ERR.GT.EPS) INTG=1                                2380
C     WRITE(NA,112) IE,EI(IE),EI(IE+1),NUGRE,PRINT                       2390
  112 FORMAT(' IE=',I6,'EI(IE)=',E12.5,'EI(IE+1)=',E12.5,'NUGRE=',I6,    2400
     1'PRINT=',E12.5)                                                    2410
C     WRITE(NA,112) IE,EI(IE),EI(IE+1),NUGRE,PRINT                       2420
C 112 FORMAT(' IE=',I6,'EI(IE)=',E12.5,'EI(IE+1)=',E12.5,'NUGRE=',I6,    2430
C    1'PRINT=',E12.5)                                                    2440
      GO TO 23                                                           2450
   21 PRINT=0.                                                           2460
C     WRITE(NA,115) EI(IE),EI(IE+1)                                      2470
C 115 FORMAT(' NO CONTRIBUTION TO THE INTEGRAL IN INTERVAL EI(IE)=',     2480
C    1E12.5,'EI(IE+1)=',E12.5)                                           2490
   23 PRCSUM=PROSUM+PRINT                                                2500
C     WRITE(NA,113) PROSUM                                               2510
  113 FORMAT(' PROSUM=',E12.5)                                           2520
   20 CONTINUE                                                           2530
      IF(INTG.EQ.1) WRITE(NA,114) NIE,NUGR1,PROSUM                       2540
  114 FORMAT(' **OUTSCATTERING GROUP = ',I6,' INSCATTERING GROUP = ',I   2550
     16/' TOTAL CONTRIBUTION OF SIGMA*SPECTRUM*TRANSFER-PROBABILITY = ', 2560
     2 1PE14.6/)                                                         2570
      NUGR1=NUGR1-NIE+1                                                  2580
      IF (SUM.EQ.0.) GO TO 55                                            2590
      WEINC(IGE,NUGR1)=PRCSUM/SUM                                        2600
   22 PRSUM=PRSUM+WEINC(IGE,NUGR1)                                       2610
C     WRITE(NA,116) PRSUM                                                2620
C 116 FORMAT('**********PRSUM=',E12.5,'**********')                      2630
      NE1=NE-1                                                           2640
      IF(PRSUM*0.9995.LE.1..AND.PRSUM*1.0005.GE.1.) GO TO 53             2650
      DO 54 INU=1,NE1                                                    2660
   54 WEINC(IGE,INU)=WEINC(IGE,INU)/PRSUM                                2670
C     WRITE(NA,114) (IGR,WEINC(IGE,IGR),IGR=1,NE1)                       2680
C 114 FORMAT(2(' IGR=',I6,'WEINC(IGE,IGR)=',E12.5))                      2690
      GO TO 53                                                           2700
   55 NE1=NE-1                                                           2710
      DO 56 INU=1,NE1                                                    2720
   56 WEINC(IGE,INU)=0.                                                  2730
      GO TO 42                                                           2740
   53 IF(IA.EQ.0) IA=IGE                                                 2750
      NAB=IGE                                                            2760
   42 CONTINUE                                                           2770
C     WRITE(NA,130) IA,NAB                                               2780
C 130 FORMAT('      IA=',I6,'NAB=',I6)                                   2790
      GO TO 49                                                           2800
   49 RETURN                                                             2810
   65 WRITE(NA,131) EZ(1),U                                              2820
  131 FORMAT(//' THE LOWEST ENERGY OF SGIZC (SG2N,SG3N) ON KEDAK , E=',E 2830
     1 12.5,' EV LIES BELOW THE THRESHOLD'/' OF THE CORRESPONDING REACTIO 2840
     2N (GIVEN IN SEDIC (SED2N,SED3N) OR SGI RESPECTIVELY) U=',F12.5,' E 2850
     3V.'/'                          ******CHECK NUCLEAR DATA******')    2860
      IR=1                                                               2870
      RETURN                                                             2880
      END                                                                2890
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      SUBROUTINE REPROB(INTYP,KONT,EP,F1,F2,F3,F4,NEP,NEPP,NF,NFF)        10
      COMMON NAM,ISTRUK,ISPA,NA,LIZ,NANF,NEND,KL                          20
      DIMENSION EP(NEP),F1(NF,NEP),F2(NF,NEP),F3(NF,NEP),F4(NF,NEP),      30
C     1ANSW(4),NAME(3),NNAM(3)                                            40
     1ANSW(4),NAME(8),NNAM(4)                                             50
      COMMON/APOINT/INEP,INF                                              60
C     REAL*8 NAM,NAME,TYP                                                 70
      REAL*8 NAM,NAME,TYP,BEST                                            80
C     KENNZ=0,IN THE CASE,THE REQUIRED DATA SET WAS NOT FOUND,=1 OTHERWI  90
C     NNAM(1)=NUMBER OF NAMES OF THE REQUIRED DATASET.                   100
C     (HAS TO BE SPECIFIED BY THE CALLING PROGRAMM)                      110
C     NNAM(2)=NUMBER OF ARGUMENTS FOR A SINGLE DATA ITEM                 120
C     NNAM(3)=NUMBER OF FUNCTIONAL VALUES FOR A SINGLE DATA ITEM.        130
C     (NNAM(2) AND NNAM(3) ARE FILLED BY LDFLOC.                         140
C     NAM(1)=NAME OF THE ISOTOPE IN ALPHAMERICAL FORM                    150
C     NAM(2)=NAME OF THE DATA TYPE IN ALPHAMERICAL FORM                  160
C     NAM(3)=FLOATING POINT VALUE OF THE FURTHER NAME                    170
C     NAM(1),(2),(3) HAVE TO BE FILLED BY THE CALLING PROGRAM.           180
C     ANSW:FLOATING POINT ARRAY,WHICH IS FILLED BY LDFLOC WITH THE       190
C     FIRST DATA ITEM,BELONGING TO THE NAMES,SUPPLIED IN NAM(I)).        200
C     ANSW(1)=K,ANSW(2)=P,ANSW(3)=THETA,FOR K=1,2                        210
C     =A,FOR K=3,=EC,FOR K=4                                             220
C     ANSW(4)=U FOR K=1,2,B FOR K=3,Q FOR K=4                            230
C*****MAT=MATERIALNAME,TYP=TYPNAME**************************************240
C*****NOPT=1:ES FOLGT NOCH EINE EINGABE*********************************250
C*****NOPT=0:DIESE EINGABE IST DIE LETZTE*******************************260
      KONTG=1                                                            270
      CALL DOPW(8HBEST    ,BEST)                                         280
      IF(INTYP.EQ.1) CALL DOPW(8HSEDIC    ,TYP)                          290
      IF(INTYP.EQ.2) CALL DOPW(8HSED2N    ,TYP)                          300
      IF(INTYP.EQ.3) CALL DOPW(8HSED3N    ,TYP)                          310
      NEPP=0                                                             320
      NFF=0                                                              330
C     NNAM(1)=3                                                          340
      NNAM(1)=4                                                          350
      NAME(1)=NAM                                                        360
      NAME(2)=BEST                                                       370
C     NAME(2)=TYP                                                        380
      NAME(3)=TYP                                                        390
C     NAME(3)=0.                                                         400
      NAME(4)=0.                                                         410
      II=0                                                               420
      I=1                                                                430
C     WRITE(NA  ,9) NAM,TYP                                              440
C    9 FORMAT(///,' ISOTOPENAME=',A9,'      DATA TYPE=',A7//)           450
C     CALL LDFLOC(KENNZ,NNAM,NAME,ANSW)                                  460
      CALL NDFLOC(KENNZ,NNAM,NAME,NDAT,NCO)                              470
      IF (KENNZ.EQ.1) GO TO 2                                            480
    5 SUM=0.                                                             490
C     CALL LDFLOC(KENNZ,NNAM,NAME,ANSW)                                  500
      CALL NDFLOC(KENNZ,NNAM,NAME,NDAT,NCO)                              510
      IF(KENNZ.EQ.0) GO TO 3                                             520
C     GO TO 500                                                          530
      GO TO 2                                                            540
C   3 WRITE(NA  ,6) NAM,TYP                                              550
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C   6 FORMAT(' FOR THE ISOTOPE',A9,' THE DATA TYPE',A7,' IS NOT                 560
C    1AVAILABLE ON THE KEDAK-LIBRARY',///)                                     570
    3 KONT=0                                                                   580
      GO TO 11                                                                 590
    2 II=II+1                                                                  600
      IF(II.LE.NEP) GO TO 23                                                   610
      NEPF=NEPF+1                                                              620
      II=1                                                                     630
C     EP(II)=SNGL(NAME(3))                                                     640
   23 EP(II)=SNGL(NAME(4))                                                     650
C     WRITE(NA   ,7) EP(II),II                                                 660
C   7 FORMAT(/,' EP=',E16.8,'II=',I6)                                          670
C     WRITE(NA   ,13)                                                          680
C  13 FORMAT(/,'         K                 F             THETA/A/EC/           690
C    1U/B/       ')                                                            700
    4 ANSW(1)=NAME(5)                                                          710
      ANSW(2)=NAME(6)                                                          720
      ANSW(3)=NAME(7)                                                          730
      ANSW(4)=NAME(8)                                                          740
C   4 F1(I,II)=ANSW(1)                                                         750
      F1(I,II)=ANSW(1)                                                         760
      F2(I,II)=ANSW(2)                                                         770
      F3(I,II)=ANSW(3)                                                         780
      F4(I,II)=ANSW(4)                                                         790
      IF(F1(I,II).NE.1.0) WRITE(NA,101) EP(II),F1(I,II)                        800
  101 FORMAT(' ***WARNING 5.01 : FOR PRIMARY NEUTRON ENERGY EP=',E14.8,'       810
     1EV ,   K IS EQAL TO ',E10.4)                                             820
      SUM=SUM+ANSW(2)                                                          830
C     CALL LDFNXT(KENNZ,NNAM,NAME,ANSW)                                        840
      CALL NDFNXT(KENNZ,NNAM,NAME,NDAT,NCO)                                    850
      IF (KENNZ.EQ.1) GO TO 24                                                 860
      GO TO 28                                                                 870
   24 I=I+1                                                                    880
      IF(I.LE.NF) GO TO 4                                                      890
      NFF=NFF+1                                                                900
      I=1                                                                      910
      GO TO 4                                                                  920
   28 IF((ABS(SUM)-1.).GT.1.E-4) WRITE(NA   ,12) SUM                           930
   12 FORMAT(' WARNUNG: SUMME ALLER P=', G16.8)                                940
C     WRITE(NA   ,8) (F1(J,II),F2(J,II),F3(J,II),F4(J,II),J=1,I)               950
C   8 FORMAT(4E16.8)                                                           960
      I=1                                                                      970
C     IF(SNGL(NAME(3)).GT.EP(II)) GO TO 5                                      980
      IF(SNGL(NAME(4)).GT.EP(II)) GO TO 5                                      990
      KONT=1                                                                  1000
      IF (NEPF.NE.0) GO TO 25                                                 1010
      INEP=II                                                                 1020
      GO TO 26                                                                1030
   25 NEPP=((NEPF-1)*NEP)+II                                                  1040
   26 IF(NFF.NE.0) GO TO 27                                                   1050
      INF=I                                                                   1060
      GO TO 11                                                                1070
   27 NFF=((NFF-1)*NF)+I                                                      1080
   11 CONTINUE                                                               1090
      IF (KONT.EQ.0) GO TO 14                                                1100
      GO TO 15                                                               1110
   14 IF(INTYP.EQ.1) CALL DOPW(8HSGI     ,TYP)                             1120
      IF(INTYP.EQ.2) CALL DOPW(8HSG2N    ,TYP)                             1130
      IF(INTYP.EQ.3) CALL DOPW(8HSG3N    ,TYP)                             1140
C     NNAM(1)=2                                                              1150
      NNAM(1)=3                                                              1160
      NAME(1)=NAM                                                            1170
C     NAME(2)=TYP                                                            1180
      NAME(3)=TYP                                                            1190
      U=0.                                                                   1200
C     CALL LDFLOC(KENNZ,NNAM,NAME,ANSW)                                      1210
      CALL NDFLOC(KENNZ,NNAM,NAME,NDAT,NCO)                                  1220
      IF (KENNZ.EQ.0) GO TO 3                                                1230
   22 ANSW(1)=NAME(4)                                                        1240
      ANSW(2)=NAME(5)                                                        1250
C  22 IF(ANSW(2).GT.0.) GO TO 16                                             1260
      IF(ANSW(2).GT.0.) GO TO 16                                             1270
      L=ANSW(1)                                                              1280
      GO TO 20                                                               1290
   16 IF(U.NE.0.) GO TO 17                                                   1300
C     WRITE(NA,100) ANSW(1),ANSW(2)                                          1310
C 100 FORMAT(' FIRST VALUES OF E,SGI ON KEDAK:E=',E12.5,'SGI=',E12.5)        1320
      F4(1,2)=ANSW(1)                                                        1330
      GO TO 18                                                               1340
   17 F4(1,2)=U                                                              1350
      GO TO 18                                                               1360
C  20 CALL LDFNXT(KENNZ,NNAM,NAME,ANSW)                                      1370
   20 CALL NDFNXT(KENNZ,NNAM,NAME,NDAT,NCO)                                  1380
      IF (KENNZ.EQ.0) GO TO 21                                               1390
      GO TO 22                                                               1400
   21 F4(1,2)=U                                                              1410
   18 CALL DOPW(8HISOT1   ,TYP)                                             1420
C     NAME(2)=TYP                                                            1430
      NAME(3)=TYP                                                            1440
C     CALL LDFLOC(KENNZ,NNAM,NAME,ANSW)                                      1450
      CALL NDFLOC(KENNZ,NNAM,NAME,NDAT,NCO)                                  1460
      IF(KENNZ.EQ.0) GO TO 3                                                 1470
      ANSW(1)=NAME(4)                                                        1480
      ANSW(2)=NAME(5)                                                        1490
      F4(1,1)=ANSW(1)                                                        1500
      U=F4(1,2)                                                              1510
      A=F4(1,1)                                                              1520
C     WRITE(NA,19) U,A                                                       1530
C  19 FORMAT(' AT THE END OF REPROB U=',E12.5,'A=',E12.5)                    1540
   15 RETURN                                                                 1550
      END                                                                    1560
```

```
      SUBROUTINE ENORG(EU,EO,EI,EF,NACT,KMAX,KEN,NISGI,NISGIP)                10
C*****SUBROUTINE ESTABLISHES ENERGY-FIELD,CONSISTING OF THE ENERGY            20
C*****POINTS OF SGIZC (SGI) AND THE ENERGY POINTS OF THE WEIGHTING SPECT      30
C*****RUM,FOR THE ENERGY REGION OF THE ENERGY-GROUP CALCULATED.               40
      COMMON NAM,ISTRUK,ISPA,NA,LIZ,NANF,NENC,KL                              50
```

```
      REAL*8 NAM                                                        60
      DIMENSION EI(NISGI),EF(KEN)                                       70
      NISGIF=0                                                          80
      EPS=0.0                                                           90
      E1=AMAX1(EF(1),EU)                                               100
      E2=AMIN1(EF(KEN),EO)                                             110
      CALL CUTS(E1,E2,EF,KEN,KA,KE,KMAX1)                              120
C*****KA:EF(KA)=POINT OF SPECTRUM EF WITH LOWEST ENERGY,THAT BELONGS TO 130
C*****THE DESIRED REGION.EF(KE):POINT OF EF WITH HIGHEST ENERGY,WHICH   140
C*****BELONGS TO THE DESIRED REGION.KMAX1=NUMBER OF ENERGY POINTS EF IN 150
C*****THE REGION.                                                       160
C     WRITE(NA,100) KA,KE,KMAX1                                         170
C 100 FORMAT(' AFTER CUT KA=',I6,'KE=',I6,'KMAX1=',I6)                  180
      NISGIF=NACT+KMAX1+2                                               190
      IF(NISGIF.LE.NISGI) GO TO 1                                       200
      NISGIP=NISGIF-NISGI                                               210
      GO TO 10                                                          220
    1 EI(NACT+1)=E1                                                     230
      EI(NACT+2)=E2                                                     240
      NACT2=NACT+2                                                      250
      DO 2 J=1,KMAX1                                                    260
    2 EI(NACT2+J)=EF(KA+J-1)                                            270
      KMAX=NACT+KMAX1+2                                                 280
C     WRITE(NA,102) (I,EI(I),I=1,KMAX)                                  290
C 102 FORMAT(2(' ',I6,E12.6))                                           300
      CALL ORD1(KMAX,E1,E2,EI,NISGI,EPS)                                310
C     WRITE(NA,101) (KS,EI(KS),KS=1,KMAX)                               320
C 101 FORMAT(2(' KS=',I6,'EI=',E12.5))                                  330
   10 RETURN                                                            340
      END                                                               350
```

```
      SUBROUTINE ORD1(KMAX,EMIN,EMAX,FELD,NTT,EPS)                      10
      DIMENSION FELD(NTT)                                               20
C                                                                       30
C  ORD1 ORDNET FELD NACH WACHSENDEN WERTEN                              40
C                                                                       50
      IF(KMAX.LT.2) GOTO 100                                            60
      DO 99 K=2,KMAX                                                    70
      M=K-1                                                             80
      IF(FELD(K).GE.FELD(M)) GOTO 99                                    90
      R=FELD(K)                                                        100
   10 M=M-1                                                            110
      IF(M.EQ.0) GOTO 20                                               120
      IF(R.LT.FELD(M)) GOTO 10                                         130
   20 IA=M+1                                                           140
      IE=K-1                                                           150
      J=IE                                                             160
      DO 30 I=IA,IE                                                    170
      FELD(J+1)=FELD(J)                                                180
   30 J=J-1                                                            190
      FELD(IA)=R                                                       200
   99 CONTINUE                                                         210
  100 IF(KMAX.EQ.0) GOTO 200                                           220
      GOTO 300                                                         230
  200 EMIN=0                                                           240
      EMAX=0                                                           250
      GO TO 800                                                        260
  300 KMAXX=KMAX                                                       270
      DO 500 K=2,KMAX                                                  280
  502 IF(K    .GT.KMAXX) GO TO 501                                     290
      M=K-1                                                            300
      IF((FELD(K)-FELD(M))/FELD(K).LE.EPS) GO TO 600                   310
      GO TO 500                                                        320
  600 KMAXX=KMAXX-1                                                    330
      KMAXS= MAXO(K,KMAXX)                                             340
      DO 700 KK=K,KMAXS                                                350
  700 FELD(KK)=FELD(KK+1)                                              360
      GO TO 502                                                        370
  500 CONTINUE                                                         380
  501 KMAX=KMAXX                                                       390
      EMIN=FELD(1)                                                     400
      EMAX=FELD(KMAX)                                                  410
  800 CONTINUE                                                         420
      RETURN                                                           430
      END                                                              440
```

```
C*****SUBROUTINE SIMPSI.DATE OF LAST CHANGE 15.11.1976.(LINES 10212      10
C*****TO 10790)                                                         20
      SUBROUTINE SIMPSI(NUGRE,U,AW,XNUE,A,B,EPS,NMAXX,RESINT,N,EZ,SGIZC,  30
     1EF,FI,ENG,NACT,NFE,NE,NN,EP,F1,F2,F3,F4,NEP,NF,KONT,ERR,INTG)      40
C*****A,B:LIMITS OF INTEGRATION.NMAXX:MAXIMUM NUMBER OF INTEGRATION POIN 50
C*****TS.FINT: FUNCTION , WHICH IS TO BE INTEGRATED.RESINT:RESULT       60
C*****OF INTEGRATION.FINT(X,..): X=COORDINATE,OVER WHICH THE INTEGRATION 70
C*****IS CARRIED OUT.                                                   80
      COMMON NAM,ISTRUK,ISPA,NA,LIZ,NAAF,NFAD,KL                        90
      REAL*8 NAM                                                       100
      DIMENSION EZ(NACT),SGIZC(NACT),EF(NFE),FI(NFE),ENG(NE),EP(NEP),  110
     1F1(NF,NEP),F2(NF,NEP),F3(NF,NEP),F4(NF,NEP)                      120
      INTG=0                                                           130
      NINT=0                                                           140
       NMAX=NMAXX                                                      150
      IF(ENG(NUGRE+1).LE.101..AND.A.LE.U*1.0005) NMAX=100              160
      IF(ABS((B-A)/B).LE.1.1E-5) GO TO 10                              170
       IF(ABS((B-A)/B).LE.5.E-5) GO TO 5                               180
      GO TO 6                                                          190
    5 NMAX=20                                                          200
    6 N=2                                                            210
      SUM=FINT(A,NUGRE,U,AW,XNUE,EZ,SGIZC,EF,FI,ENG,NACT,NFE,NE,NN,EP, 220
     1F1,F2,F3,F4,NEP,NF,KONT)+4.*                                     230
     2FINT((A+B)*0.5,NUGRE,U,AW,XNUE,EZ,SGIZC,EF,FI,ENG,NACT,NFE,NE,NN, 240
     3EP,F1,F2,F3,F4,NEP,NF,KONT)                                      250
     4+FINT(B,NUGRE,U,AW,XNUE,EZ,SGIZC,EF,FI,ENG,NACT,NFE,NE,NN,       260
     5EP,F1,F2,F3,F4,NEP,NF,KONT)                                      270
      H=SNGL(0.500*(DBLE(B)-DBLE(A)))                                  280
```

```
      SUM4=FINT((A+H),NUGRE,U,AW,XNUE,EZ,SGIZC,EF,FI,ENG,NACT,NFE,NE,NN,
     1EP,F1,F2,F3,F4,NEP,NF,KONT)
      ERR=1.
      RESINT=0.
      IF(SUM.EQ.0.)GOTO 4
    1 CONTINUE
      SUME=SUM
      N2=N
      N=2*N
      H2=H
      H=0.5*H
      IF(H/A.LT..5E-6.AND.N.GT.100) NINT=1
      SUM2=2.*SUM4
      SUM4=0.
      HM=A-H
      DO 2 M=1,N2
      HM=HM+H2
    2 SUM4=FINT(HM,NUGRE,U,AW,XNUE,EZ,SGIZC,EF,FI,ENG,NACT,NFE,NE,NN,
     1EP,F1,F2,F3,F4,NEP,NF,KONT)
     2+SUM4
      SUM=-SUM2+4.*SUM4+SUM
      RESINT=H*SUM/3.
      ERR=ABS(1.-2.*SUME/SUM)
      IF(N.GE.NMAX.OR.NINT.EQ.1)GOTO 3
      IF(N.LT.4.OR.ERR.GT.EPS)GOTO 1

      GOTO 4
    3 IF(ERR.LE.EPS)GOTO 4
      INUGRE=NE-NUGRE
      INTG=1
      WRITE(NA   ,1000)N,NMAX,RESINT,ERR,NN,A,B,INUGRE,H
 1000 FORMAT(/' **SIMPSI, N=',I6,'  NMAX=',I6,'  RESINT=',1PE14.6,' ERR=
     *',F14.6/' NN=',I6,' A=',E14.6,' B=',E14.6,' INUGRE=',I4,
     *' H=',E14.6)
    4 RETURN
   10 RESINT=FINT(A,NUGRE,U,AW,XNUE,EZ,SGIZC,EF,FI,ENG,NACT,NFE,NE,NN,
     1EP,F1,F2,F3,F4,NEP,NF,KONT)+FINT(B,NUGRE,U,AW,XNUE,EZ,SGIZC,EF,FI,
     2ENG,NACT,NFE,NE,NN,EP, F1,F2,F3,F4,NEP,NF,KONT)
      RESINT=RESINT*(B-A)*0.5
      GO TO 4
      END
```

```
      FUNCTION SINPOL(EINT,      EFELD,FELD,NFELD)                          10
C*****FUNCTION CALCULATES VALUE OF FELD AT ENERGY EINT BY LINEAR INTERP     20
C*****CLATION                                                              30
C*****OLATION                                                              40
      DIMENSION EFELD(NFELD),FELD(NFELD)                                   50
      COMMON NAM,ISTRUK,ISPA,NA,LIZ                                        60
      REAL*8 NAM                                                           70
      DO 1 I=1,NFELD                                                       80
      IF(EFELD(I).LT.EINT) GO TO 1                                         90
      IF(EFELD(I).EQ.EINT) GO TO 2                                        100
      IF(EFELD(I).GT.EINT) GO TO 4                                        110
    4 IF(I.EQ.1) GO TO 5                                                  120
      I1=I                                                                130
      GO TO 6                                                             140
    2 I1=I                                                                150
      GO TO 3                                                             160
    1 CONTINUE                                                            170
      IF(ABS(EFELD(NFELD)-EINT)/AMAX1(EFELD(NFELD),EINT).LT.1.E-6)        180
     1GO TO 8                                                             190
      WRITE(NA,101) EFELD(NFELD),EINT                                     200
  101 FORMAT(' INTERPOLATION NOT POSSIBLE,GREATEST VALUE OF FIELD EFFLD   210
     1 IS',E14.7,'EINT=  ',E14.7)                                         220
      SINPOL=0.                                                           230
      GO TO 99                                                            240
    3 SINPOL=FELD(I1)                                                     250
      GO TO 99                                                            260
    5 IF (ABS(EFELD(1)-EINT)/AMAX1(EFELD(1),EINT).LT.1.E-6)GO TO 10       270
      WRITE(NA,100) EFELD(1),EINT                                         280
  100 FORMAT(' INTERPOLATION NOT POSSIBLE.SMALLEST VALUE OF FIELD EFELD=  290
     1= ',E14.7,'EINT=  ',E14.7)                                          300
      SINPOL=0.                                                           310
      GO TO 99                                                            320
    6  SINPOL=FIPOLA(EFELD(I1-1),EINT,EFELD(I1),FELD(I1-1),FELD(I1))      330
C   99 WRITE(NA,102) EINT,SINPOL                                          340
      GO TO 99                                                            350
   10 SINPOL=FELD(1)                                                      360
      GO TO 99                                                            370
    8 SINPOL=FELD(NFELD)                                                  380
C   99 WRITE(NA,102) EINT,SINPOL                                          390
C 102 FORMAT(' END OF SINPOL EINT=',E14.6,'SINPOL=',E14.6)                400
   99 RETURN                                                              410
      END                                                                 420
```

```
      FUNCTION FINT(E,NUGRE,U,AW,XNUE,EZ,SGIZC,EF,FI,ENG,NACT,NFE,NF,NN,    10
     1EP,F1,F2,F3,F4,NEP,NF,KONT)                                           20
      DIMENSION EZ(NACT),SGIZC(NACT),EF(NFE),FI(NFE),ENG(NE),EP(NEP),       30
     1FI(NF,NEP),F2(NF,NEP),F3(NF,NEP),F4(NF,NEP)                           40
      IF (NFE.GT.1) GO TO 1                                                 50
      GO TO 2                                                               60
    1 W=SINPOL(E,EF,FI,NFE)                                                 70
      GO TO 3                                                             80
    2 W=PHI(E)                                                            90
    3 IF(NN.EQ.2) GO TO 7                                                100
      FFINT=SINPOL(E,EZ,SGIZC,NACT)*W                                    110
      IF (NN.EQ.1) GO TO 4                                               120
      GO TO 5                                                            130
    4 FINT=FFINT*PROB(E,NUGRE,U,AW,XNUE,ENG,NF,FP,F1,F2,F3,F4,           140
     1NEP,NF,KONT)                                                       150
C     WRITE(6,100) FINT,E,NUGRE                                         160
C 100 FORMAT(' ***FINT=',E12.5,'E=',F12.5,'NUGRE=',I6)                   170
      GO TO 6                                                            180
    5 FINT=FFINT                                                         190
      GO TO 6                                                            200
```

```
    7 FINT=W                                                              210
    6 RETURN                                                              220
      END                                                                 230
```

```
C*****FUNCTION PROB.DATE OF LAST CHANGE 15.11.76.(LINES 23970             10
C*****TO 24560)                                                           20
      FUNCTION PROB(E,NUGR,U,A,XNUE,ENG,NE,EP,F1,F2,F3,F4,                30
     1NEP,NF,KONT)                                                        40
C*****SUBROUTINE CALCULATES PROBABILITY FOR INELASTIC SCATTERING FROM      50
C*****ENERGY E TO GROUP NUGR. AN EVAPORATION MODEL IS USED. U IS THE       60
C*****THRESHOLD OF THE INELASTIC SCATTERING PROCESS.                       70
C*****NUGR=GROUP NUMBER,ENG(NUGR)=LOWER ENERGY LIMIT OF GROUP,            80
C*****ENG(NUGR+1)=UPPER ENERGY LIMIT OF GROUP.                            90
      REAL*8 ELD,EUD,EXEM,EINS,SU1,SU2,EMD,WD,EXEL,EXD,                   100
     1     NAM,      EMAX,W,SW                                          110
      DIMENSION ENG(NE),EP(NEP),F1(NF,NEP),F2(NF,NEP),F3(NF,NEP),         120
     1F4(NF,NEP)                                                          130
      COMMON NAM,ISTRUK,ISPA,NA,LIZ                                       140
C     XNUE IS THE ADJUSTABLE PARAMETER FOR THE CALCULATION OF THE         150
C     NUCLEAR TEMPERATURE AND IS AN INPUT QUANTITY.                       160
      ETHR=E-U                                                            170
      IF(ETHR.LE.ENG(NUGR)) GO TO 1                                       180
      ELP=AMIN1(ENG(NUGR),ETHR)                                           190
      ELP=AMIN1(ENG(NUGR+1),ETHR)                                         200
      IF(KONT.EQ.1) GO TO 3                                               210
      XN=XNUE*A                                                           220
      THE=THETA(E,XN)                                                     230
      GO TO 2                                                             240
    3 THE=TEMP(E,EP,F3,NEP,NF)*0.000001                                   250
      IF(THE.EQ.0.) GO TO 1                                               260
      GO TO 2                                                             270
    1 PROB=0.                                                             280
      GO TO 99                                                            290
    2 THE2=THE**2                                                         300
      EL=ELP/THE*0.000001                                                 310
      EU=EUP/THE*0.000001                                                 320
      EM=EU-EL                                                            330
      ELD=DBLE(EL)                                                        340
      EUD=DBLE(EU)                                                        350
      EMD=DBLE(EM)                                                        360
      EINS=DBLE(1.0)                                                      370
      IF(EM-0.01)600,600,601                                              380
C     IF (E(H)/THETA-E(H+1)/THETA) LESS OR EQUAL 0.01,(STATEMENT          390
C     NUMBER 600),EXD IS USED TO CALCULATE THE TRANSITION PROBABILITIES,   400
C     OTHERWISE(STATEMENT NUMBER 601) THE DOUBLE PRECISION EXPONENTIAL     410
C     FUNCTION IS SUFFICIENT.                                             420
  600 WD=-ELD*EXD(-EMD)-EMD*EXD(-EMD)-EXC(-EMD)-EMD                       430
C     EXEL=DEXP(-ELD)                                                     440
C     WD=EXEL*WD                                                          450
      GO TO 602                                                           460
  601 EXEM=DEXP(-EMD)                                                     470
      SU1=EINS*ELD                                                        480
      SU2=EINS+EUD                                                        490
      SU2=SU2*EXEM                                                        500
      WD=SU1-SU2                                                          510
  602 EXEL=DEXP(-ELD)                                                     520
      WD=EXEL*WD                                                          530
      W    =WD*DBLE(THE2)                                                 540
C*****WN:PROBABILITY FOR INELASTIC SCATTERING FROM ENERGY E ,INTEGRATED   550
C*****OVER ALL POSSIBLE FINAL ENERGIES.                                   560
C*****NORMALIZATION OF PROBABILITIES TO 1.                                570
      ARG=(E-U)/THE*0.000001                                              580
      WN=THE2*(1.-EXP(-ARG)*(1.+ARG))                                     590
      PROB=SNGL(W)/WN                                                     600
   99 RETURN                                                              610
      END                                                                 620
```

```
      DOUBLE PRECISION FUNCTION EXC(X)                                     10
C     EXD CALCULATES THE SERIES EXP(X)-1.                                  20
      REAL*8 X,XN,DNFAK,XN1                                                30
      N=1                                                                  40
    1 XN=X**N/DNFAK(N)                                                     50
      IF(DABS(XN).LE.1.D-50) GO TO 2                                       60
      N=N+1                                                                70
      GO TO 1                                                              80
    2 IF(N.EQ.1) GO TO 4                                                   90
      N1=N-1                                                              100
      EXD  =XN                                                            110
      DO 3 K=1,N1                                                         120
      XN1=XN*DFLOAT(N-K+1)/X                                              130
      EXD = EXD  +XN1                                                     140
    3 XN=XN1                                                              150
      GO TO 5                                                             160
    4 EXC=XN                                                              170
    5 RETURN                                                              180
      END                                                                 190
```

```
      FUNCTION THETA(E,XN)                                                 10
C*****FUNCTION CALCULATES NUCLEAR TEMPERATURE OF RESIDUAL NUCLEUS IN MEV    20
      THETA=SQRT(E/XN)*0.001                                               30
      RETURN                                                               40
      END                                                                  50
```

```
      DOUBLE PRECISION FUNCTION DNFAK(NN)                                  10
C     DNFAK CALCULATES N*(N-1)*(N-2)*.......*(N-(N-1)) FOR THE             20
C     SERIES DEVELOPED IN EXC.                                             30
      REAL*8 N                                                             40
      N=DFLOAT(NN)                                                         50
```

```
      DNFAK=N                                                           60
    1 IF(N.LE.(1.D0+1.D-5))RETURN                                       70
      N=N-1.D0                                                          80
      DNFAK=DNFAK*N                                                     90
      GO TO 1                                                          100
      END                                                              110
```

```
C                                                                       10
C                                                                       20
      FUNCTION TEMP(EFS,EP,F3,NEP,NF)                                   30
      COMMON NAM,ISTRUK,ISPA,NA,LIZ,NANF,NEND,KL                        40
      DIMENSION EP(NEP),F3(NF,NEP)                                      50
      REAL*8 NAM                                                        60
      COMMON/APOINT/INEP,INF                                            70
      DO 4 I=1,INEP                                                     80
      IF(EP(I)-EFS)1,2,3                                                90
    1 GO TO 4                                                          100
    3 IF(I.EQ.1) GO TO 9                                               110
      I1=I                                                             120
      GO TO 5                                                          130
    2 TEMP=F3(1,I)                                                     140
      GO TO 7                                                          150
    4 CONTINUE                                                         160
      TEMP=F3(1,INEP)                                                  170
    8 CONTINUE                                                         180
C   8 WRITE (NA,100) EFS,EP(1),EP(NT)                                  190
C 100 FORMAT(' DIE GEWUENSCHTE ENERGIE EFS=',E16.8,'LIEGT AUSSERHALB   200
C    1 DES VORGEGEBENEN ENERGIEBEREICHS'/,' E(1)=',E16.8,'EN(T)=',E16.8)210
      GO TO 7                                                          220
    9 TEMP=F3(1,1)                                                     230
C   9 TEMP=0.                                                          240
      GO TO 8                                                          250
    5 TEMP=(F3(1,I1)-F3(1,I1-1))/(EP(I1)-EP(I1-1))*(EFS-EP(I1-1))      260
     1+F3(1,I1-1)                                                      270
    7 GO TO 6                                                          280
C   7 WRITE(NA,101 ) EFS,TEMP                                          290
C 101 FORMAT(' EFS=',E16.8,'TEMP=',E16.8)                              300
    6 RETURN                                                           310
      END                                                              320
```

```
C     IN THE FOLLOWING FUNCTION FIPOLD(XAD,YA)                          10
C     AND (XCD,YD) ARE THE STARTING POINTS AND                          20
C     (XBD,FIPOLD) IS THE INTERPOLATED POINT.                           30
      FUNCTION FIPOLD(XAD,XBD,XCD,YA,YC)                                40
      REAL*8 XAD,XBD,XCD                                                50
      DX1=SNGL(XBD-XAD)                                                 60
      DX2=SNGL(XCD-XBD)                                                 70
      DX=SNGL(XCD-XAD)                                                  80
      IF(DX.LT.1.E-30) GO TO 1                                          90
      FIPOLD=(YA*DX2+YC*DX1)/DX                                        100
      GO TO 2                                                          110
    1 FIPOLD=(YA+YC)/2.                                                120
    2 RETURN                                                           130
      END                                                              140
```

```
C*****SUBROUTINE SCATD.DATE OF LAST CHANGE 14.10.1976.(LINES 6532 TO    10
C*****10210)                                                            20
C     CALCULATIONS OF THE INELASTIC SCATTERING PROBABILITIES            30
C                                                                       40
      SUBROUTINE SCATD(NX,EG,NFE,EF,FI,NE27,WEIN,QUOT,WAHR,VW,          50
     1E,AE,SU,LBA,SGIT,IANF,SGIP,WERT,EZ,                               60
     2NISG,NISGP,NAE,NAEP,ISG,ISGP,KINEM,NEA,NAB)                       70
      REAL*8 NAM,ISOT,NAM4,EC,EU,DIFF,AE,EMIN,EMAX,F,SUM,WAHR,          80
     1WAI,VW,UWA,EH,AB,EZ,FE,FA                                         90
      REAL*8 WITHP,WITH/'WITH    '/,WITHC/'WITHOUT'/                    100
      DIMENSION AE(NAE),SGIP(ISG,NAE),WERT(ISG),                       110
     1EG(NX),EF(NFE),FI(NFE),NN(4),SU(NX),QUOT(NX),WAHR(NX),           120
     2LBA(NX),VW(NX),E(NE27),SGIT(ISG),                                130
     3ISCT(2),IANF(NAE),EZ(NISG),WEIN(NX,NX)                           140
      COMMON NAM,ISTRUK,ISPA,NA,LIZ,NANF,NEND,KL                       150
      DATA ISOT/'BEST ','ISOT1'/                                       160
      WRITE (NA    ,9001)                                              170
 9001 FORMAT(///' PROGRAMM ZUR BERECHNUNG INELASTISCHER STREUMATRIZEN'/  180
     1 VON DISKRETEN ANREGUNGSNIVEAUS.'/)                              190
C     WRITE(NA,9002)                                                   200
C9002 FORMAT(1HO/' PROBSGIZ'/1X)                                       210
      IF(KINEM.EQ.0)GOTO 20                                            220
      XM=1.008665                                                      230
      WITHP=WITH                                                       240
      GOTO 21                                                          250
   20 XM=0.                                                            260
      WITHP=WITHO                                                      270
C  21 WRITE(NA,9003)WITHP                                              280
C9003 FORMAT(///' CALCULATION  ',A8,'  KINEMATIC',/' ',32('-'))        290
   21 NN(1)=3                                                          300
      AE(1)=NAM                                                        310
      AE(2)=ISOT(1)                                                    320
      AE(3)=ISOT(2)                                                    330
      CALL NDFLOC (I,NN,AE,K,K)                                        340
      IF(I.EQ.0)  GO TO 999                                            350
      A=AE(4)                                                          360
      NE=NX                                                            370
C     IF NOT CONTAINED IN EG(NX) THE THERMAL GROUP                     380
C     IS ADDED.THIS RESULTS IN E(NE27).                                390
      IF(EG(1)-1.E-3)305,301,307                                       400
  305 WRITE (NA,304)                                                   410
  304 FORMAT(                                                          420
     1' ***ERROR 5.01 : THE LOWER BOUNDARY OF THE LOWEST ENERGY'      /  430
     2' GROUP HAS TO BE LARGER OR EQUAL TO 1.E-3,WHICH IS THE LOWEST' /  440
     3' ENERGY ON KEDAK FOR ALL DATA TYPES.THIS IS NOT FULFILLED')     450
      GO TO 999                                                        460
```

```
  307 NE=NE27                                                          470
      E(1)=1.0-3                                                       480
      DO 302 I=2,NE27                                                  490
  302 E(I)=EG(I-1)                                                     500
      GO TO 303                                                        510
  301 DO 300  I=1,NE                                                   520
      E(I)=EG(I)                                                       530
  300 CONTINUE                                                         540
C     WRITE(NA,9200) (I,E(I),I=1,NE)                                   550
C9200 FORMAT(3(' I=',I6,' E=',E15.9))                                  560
C     DETERMINATION OF THE EFFECTIVE INITIAL ENERGY GROUP OUT OF WHICH  570
C     INELASTIC SCATTERING OCCURS AND OF THE LAST GROUP UP TO WHICH     580
C     THE TRANSITION PROBABILITIES ARE REQUIRED                        590
  303 NE1=NE-1                                                         600
      DO 37  IM=1,NE1                                                  610
   37 QUOT(IM)=0.0                                                     620
      INF=NE-NANF                                                      630
      IE=NE-NEND                                                       640
      KI=2                                                             650
      KEN=NFE                                                          660
      IF(NFE.EQ.1) KEN=0                                               670
      IA=0                                                             680
      IC=0                                                             690
      NAB1=NE27-1                                                      700
      NAB=NAB1                                                         710
      NISGP=0                                                          720
      NISGF=0                                                          730
      NAEP=0                                                           740
      NAEF=0                                                           750
      ISGP=0                                                           760
      ISGF=0                                                           770
      JMAT=0                                                           780
C     WRITE(NA,9010) IC,NISG,NISGF,NISGP,NAE,NAEF,NAEF,ISG,            790
C    1JMAT                                                             800
 9010 FORMAT(' IC=',I6,'NISG=',I6,'NISGF=',I6,'NISGP=',I6/'NAE=',I6,   810
     1'NAEF=',I6,'NAEP=',I6,'ISG=',I6,'JMAT=',I6)                      820
      DO 90 I=INF,IE                                                   830
      CALL DAORG(I,KEN,EZ,E,AE,EF,FI,JMAT,LMAX,NISG,NISGF,NISGP,       840
     *NE27,NAE,NAEF,NAEP,ISG,ISGF,ISGP,IA,NAB,&998)                    850
C     WRITE(NA,9012) IA,NAB,I,NAB1                                     860
 9012 FORMAT(' IA=',I6,'NAB=',I6,'I=',I6,'NAB1=',I6)                   870
      GO TO 997                                                        880
  998 NEA=0                                                            890
      NAB=0                                                            900
      GO TO 999                                                        910
  997 IF(IA.GT.I) GO TO 91                                             920
      IF(NISGF.NE.0.OR.NAEF.NE.0.OR.ISGF.NE.0) RETURN                  930
   91 IF(NAB.EQ.NAB1) GO TO 9C                                         940
      GO TO 92                                                         950

   90 CONTINUE                                                         960
C  92 WRITE(NA,9011) IA,NAB                                            970
 9011 FORMAT('IA=',I6,'NAB=',I6)                                       980
   92 IF(IA.GE.I NF)  GOTC 205                                         990
      NEA=I NF                                                        1000
      GOTO 206                                                        1010

  205 NEA=IA                                                          1020
      IF(IA.LE.IF)  GOTO 206                                          1030
      WRITE(NA,179)                                                   1040
  179 FORMAT(                                                         1050
     1' ***ERROR 5.04 : WITH INCIDENT NEUTRON ENERGIES OUT OF THE'    / 1060
     2' ENERGY GROUPS REQUESTED IN THE INPUT INELASTIC SCATTERING'    / 1070
     3' FROM DISCRETE LEVELS CANNOT OCCUR.')                          1080
      NEA=0                                                           1090
      NAB=0                                                           1100
      GO TO 999                                                       1110
  206 KC=IE-NEA+1                                                     1120
      MZ=C                                                            1130
      CALL DOPW (8HSMTOT   ,NAM4)                                     1140
C  26 WRITE(LIZ) MZ,NAM4                                              1150
   26 CONTINUE                                                        1160
C     IF(EZ(1).LT.E(IA+1))  GOTO 39                                   1170
C 2C4 KD=KD-1                                                         1180
   39 KZ=KI+1                                                         1190
C     WRITE (LIZ) KZ,NAM,KC                                           1200
C     LOOP OVER ALL OUTSCATTERING GROUPS TO BE CONSIDERED             1210
      DO 1  I=NEA,IE                                                  1220
C     WRITE(NA,9016) I,NAB,NEA,IE,NFE                                 1230
 9016 FORMAT(' I=',I6,'NAB=',I6,'NEA=',I6,'IE=',I6,'NFE=',I6)        1240
      CALL AKED(I,E,EZ,SGIP,JMAT,LMAX,SU,QUCT,WERT,AE,                1250
     1IA,NAB,IE,INF,NFE,EF,FI,NE,NX,SGIT,NAE,                         1260
     2NAEP,ISG,ISGP,IANF,NISG,NISGP)                                  1270
      IF (LMAX.EQ.0) GO TO 995                                        1280
      EMIN=EZ(1)                                                      1290
      EMAX=EZ(LMAX)                                                   1300
C     WRITE(NA,9050)JMAT,I,SU(I)                                      1310
C9050 FORMAT(' AFTER AKED JMAT=',I6,'I=',I6,'SU=',E12.6)              1320
C     DO 310 J=1,JMAT                                                 1330
C 310 AE(J)=AE(J)*((A+XM)/A)                                          1340
      NFI=NE-I                                                        1350
      IF(E(I+1).LE.EZ(1))   GOTO 1                                    1360
   10 GES=0.                                                          1370
      IF(I-NAB)83,85,1002                                             1380
   85 EH=EMAX                                                         1390
      GO TO 89                                                        1400
   83 EH=E(I+1)                                                       1410
   89 NE1=NF-1                                                        1420
C     LOOP OVER ALL INSCATTERING GROUPS                               1430
      DO 2 K=1,I                                                      1440
      SUM=0.DO                                                        1450
C     LOOP OVER ALL INELASTIC EXCITATION LEVELS OF THE MATERIAL CONSIDER 1460
      DO 3 J=1,JMAT                                                   1470
C     WRITE(NA,9014)J,IANF(J),EZ(1),LMAX                              1480
C9C14 FORMAT(' J=',I6,'IANF(J)=',I6,'EZ(1)=',G14.6,'LMAX=',I6)        1490
      IF(J.NE.1)    GOTO 6                                            1500
C     KMIN=0                                                          1510
      KMIN=IANF(J)-1                                                  1520
      GO TO 8                                                         1530
    6 KMIN=IANF(J)-1                                                  1540
C     DETERMINATION OF THE LIMITS EU,EO FOR INTEGRATION OVER THE      1550
C     OUTSCATTERING GROUP                                             1560
```

```
    8 FE=1.DO                                                              1570
      FA=1.DO                                                              1580
      IF(KINEM.EQ.2) GO TO 5                                               1590
      IF (KINEM.EQ.1) GO TO 201                                            1600
      GO TO 200                                                            1610
  201 FA=DBLE((A+XM)/A)                                                    1620
      GO TO 200                                                            1630
    5 EINMIN=(A*A+XM*A)/(A*A+XM*XM)*SNGL(AE(J))                            1640
C     WRITE(NA,9051) J,AE(J),EINMIN                                        1650
C9051 FORMAT(' J=',I6,'AE=',D14.6,'EINMIN=',E14.6)                         1660
      FE=DBLE((A*A+XM*XM)/((A+XM)*(A+XM)))                                 1670
      FA=DBLE(A/(A+XM))                                                    1680
  200 IF((E(K)+FA*AE(J)).LT.FE*E(I))  GOTO 9                               1690
      IF((E(K)+FA*AE(J)).GE.FE*EH)    GOTO  88                             1700
      EU=(E(K)+FA*AE(J))/FE                                                1710
      GO TO 44                                                             1720
    9 IF((E(K+1)+FA*AE(J)).LT.FE*E(I))    GOTO 3                           1730
      EU=E(I)                                                              1740
   44 IF((E(K+1)+FA*AE(J)).GE.FE*EH)    GOTO 61                           1750
      EO=(E(K+1)+FA*AE(J))/FE                                              1760
      GO TO 62                                                             1770
   61 EO=EH                                                                1780
C     DETERMINATION OF SIGMA AND THE WEIGHTING FUNCTION AT EU,EO           1790
   62 KJ=LMAX-IANF(J)+1                                                    1800
C     WRITE(NA,9100) I,K,EO,EU                                             1810
C9100 FORMAT(' I=',I6,'K=',I6,'EO=',D20.6,'EU=',D20.6)                     1820
      IAB=0                                                                1830
      IAF=0                                                                1840
      IF1=IAF+1                                                            1850
      IB=IAB+1                                                             1860
      FI1=0.                                                               1870
      FI2=0.                                                               1880
      SGP1=0.                                                              1890
      SGP2=0.                                                              1900
      IF(KJ.LE.0)GOTO 80                                                   1910
      DO 4 IG=1,KJ                                                         1920
      KM=KMIN+IG                                                           1930
      IF(EZ(KM).GE.EU)   GOTO 66                                           1940
   65 IAB=IG                                                               1950
      IAF=IG                                                               1960
      IF(EZ(KM+1).LT.EO)    GOTO 4                                         1970

      IF(EZ(KM+1).GE.EO)   GOTO 67                                         1980
   66 IF(IG.NE.1)   GOTO 72                                                1990
      SGP1=SGIP(1,J)                                                       2000
      CALL TRA(EU,FI1,NFE,EF,FI)                                           2010
      IAF=1                                                                2020
      IF(EZ(KM).LT.EO)  GOTO 4                                             2030
  164 SGP2=SGIP(1,J)                                                       2040
      CALL TRA(EO,FI2,NFE,EF,FI)                                           2050
      GO TO 80                                                             2060
   72 IF(IAB.NE.0)     GOTO 70                                             2070
   73 IF(EZ(KM).GE.EO)   GOTO 75                                           2080
   76 IAF=IG                                                               2090
      GO TO 4                                                              2100
   70 IF(EZ(KM).LT.EO)   GOTO 74                                           2110

   75 IF1=IAF+1                                                            2120
      KMF=KMIN+IF1                                                         2130
      KMAF=KMIN+IAF                                                        2140
      SGP2=FIPOLD(EZ(KMAF),EO,EZ(KMF),                                     2150
     1SGIP(IAF,J),SGIP(IF1,J))                                             2160
C     SGP2=SGIP(IAF,J)+(SGIP(IF1,J)-SGIP(IAF,J))*(EO-EZ(KMAF))/(EZ(KMF)-   2170
C    1EZ(KMAF))                                                            2180
      CALL TRA(EO,FI2,NFE,EF,FI)                                           2190
      GO TO 80                                                             2200
   74 IAF=IG                                                               2210
   67 IB=IAB+1                                                             2220
      KMB=KMIN+IB                                                          2230
      KMAB=KMIN+IAB                                                        2240
      SGP1=FIPOLD(EZ(KMAB),EU,EZ(KMB),                                     2250
     1SGIP(IAB,J),SGIP(IB,J))                                              2260
      CALL TRA(EU,FI1,NFE,EF,FI)                                           2270
C     SGP1=SGIP(IAB,J)+(SGIP(IB,J)-SGIP(IAB,J))*(EU-EZ(KMAB))/(EZ(KMB)-    2280
C    1EZ(KMAB))                                                            2290
      GO TO 4                                                              2300
    4 CONTINUE                                                             2310
C   4 WRITE(NA,9052) SGP1,SGP2,FI1,FI2                                     2320
C9052 FORMAT(' SGP1=',E12.6,'SGP2=',E12.6,'FI1=',E12.6,'FI2=',E12.6)       2330
C     CALCULATION OF THE INTEGRAL BETWEEN EU AND EO BY TRAPEZOIDAL RULE    2340
   80 IF(IAB.EQ.0)    GOTO 79                                             2350
   78 KMB=KMIN+IB                                                          2360
      IF(EZ(KMB).NE.EU)  GOTO 82                                           2370
   81 IB1=IB                                                               2380
      LIE=IAF                                                              2390
      GO TO 77                                                             2400
   82 IB1=IAB                                                              2410
      LIE=IAF                                                              2420
      GO TO 77                                                             2430
   79 IB1=1                                                                2440
      IF(IF1.EQ.IAF)  GOTO 185                                             2450
      LIE=IF1                                                              2460
      KMB1=KMIN                                                            2470
      GOTO 182                                                             2480
  185 LIE=IAF                                                              2490
   77 KMB1=KMIN+IB1                                                        2500
  182 KMAF=KMIN+IAF                                                        2510
C     WRITE(NA,9054) KMB1,KMAF,EZ(KMB1+1),EZ(KMAF)                         2520
C9054 FORMAT(' KMB1=',I6,'KMAF=',I6,'EZ(KMB1+1)=',E12.6,'EZ(KMAF)=',E12.   2530
C    16)                                                                   2540
      DO 60  L=IB1,LIE                                                     2550
      IF(IAB.NE.0)     GOTO 183                                            2560
      IF(IF1.EQ.IAF)     GOTO 183                                          2570
      KML=KMIN+L-1                                                         2580
      GOTO 184                                                             2590
  183 KML=KMIN+L                                                           2600
  184 IF(IB1.LT.LIE)  GOTO 63                                              2610
   64 F1=SGP1*FI1                                                          2620
      F2=SGP2*FI2                                                          2630
      DIFF=EO-EU                                                           2640
      GO TO 45                                                             2650
   63 IF(L.NE.IB1)   GOTO 49                                               2660
```

```
   48 F1=SGP1*FI1                                                          2670
      DIFF=EZ(KMB1+1)-EU                                                   2680
      GC TO 43                                                             2690
   49 IF(L.NE.LIE)  GOTO 46                                                2700
   47 F1=F2                                                                2710
      DIFF=EO-EZ(KMAF)                                                     2720
      F2=SGP2*FI2                                                          2730
      GC TO 45                                                             2740
   46 F1=F2                                                                2750
      DIFF=EZ(KML+1)-EZ(KML)                                               2760
   43 IF(IAB.EQ.0)    GOTO 181                                             2770
      F2=SGIP(L+1,J)*WERT(KML+1)                                           2780
      GOTO 45                                                              2790
  181 F2=SGIP(L,J)*WERT(KML+1)                                             2800
   45 SUM=SUM+DIFF*(DBLE(F1)+DBLE(F2))/2.DO                                2810
C  60 WRITE(NA,9053) L,KML,EZ(KML),EZ(KML+1)                               2820
C9053 FORMAT(' L=',I4,'KML=',I4,'EZ(KML)=',E12.6,'EZ(KML+1)=',E12.6)       2830
   60 CONTINUE                                                             2840
C     SUMMATION LOOP FOR INTEGRAL CLOSED                                   2850
    3 CONTINUE                                                             2860
C     LOOP OVER EXCITAION LEVELS J CLOSED                                  2870
   88 IF(SU(I).EQ.0.0)    GOTO 42                                          2880
   51 WAHR(K)=SUM/DBLE(SU(I))                                              2890
      GC TO 52                                                             2900
   42 WAHR(K)=0.DO                                                         2910
   52 GES=GES+SNGL(WAHR(K))                                                2920
C   2 WRITE(NA,9101) I,K,WAHR(K)                                           2930
C9101 FORMAT(' I=',I6,'K=',I6,'WAHR=',E12.6)                               2940
    2 CONTINUE                                                             2950
C     LOOP OVER ALL INSCATTERING GROUPS K CLOSED                           2960

 1002 GC TO 111                                                            2970
  111 QUC=0.                                                               2980
      KE=0                                                                 2990
      DC 55 LK=1,I                                                         3000
      LB=I+1-LK                                                            3010
  130 IF(GES.EQ.0.0)    GOTO 54                                            3020
   53 WAHR(LK)=WAHR(LK)/DBLE(GES)                                          3030
      GO TO 56                                                             3040
   54 WAHR(LK)=0.DO                                                        3050
   56 QUO=QUO+SNGL(WAHR(LK))                                               3060
      VW(LB)=WAHR(LK)                                                      3070
   55 CONTINUE                                                             3080
      NZ=1                                                                 3090
      DO 170 KV=1,I                                                        3100
      WAHR(KV)=VW(KV)                                                      3110
      AB=0.DO                                                              3120
      IF(WAHR(KV).LE.AB)  GOTO 170                                         3130
  171 NZ=KV                                                                3140
  170 CONTINUE                                                             3150
      IF(KE.NE.1)   GOTO 136                                               3160
C     CONCERNS ONLY THE SCATTERING PROBABILITIES IN THE DISCRETE REGION    3170
  145 DC 137 KO=1,I                                                        3180
      IF(QUO.NE.0.0)    GOTO 161                                           3190
  162 UWA=0.DO                                                             3200
      GOTO 163                                                             3210
  161 UWA=WAHR(KO)/DBLE(QUO)                                               3220
  163 WAHR(KO)=UWA                                                         3230
  137 CONTINUE                                                             3240
C     ORGANIZATION OF THE OUTPUT ON LISTING IN THE FORM OF MAXIMUM 11      3250
C     SCATTERING PROBABILITIES PER LINE STARTING WITH THE OUTSCATTERING    3260
C     GROUP OF LOWEST ENERGY(LARGEST GROUP NUMBER ACCORDING TO ABN-SET)    3270
  136 DC 126 LN=1,NZ                                                       3280
      LBA(LN)=NEI+LN-1                                                     3290
  126 CONTINUE                                                             3300
      GO TO 146                                                            3310
C     KI=NZ/11                                                             3320
C     KII=KI*11                                                            3330
C     IF(NZ.NE.KII)  GOTO 168                                              3340
C 167 KII=KI                                                               3350
C     GOTO 169                                                             3360
C 168 KII=KI+1                                                             3370
C 169 DC 146 LI=1,KII                                                      3380
C     IF(LI.NE.1)   GOTO 147                                               3390
C 148 LIM=1                                                                3400
C     GO TO 149                                                            3410
C 147 LIM=(LI-1)*11+1                                                      3420
C     IF(LI.EQ.KII)   GOTC 150                                             3430
C 149 IF(KII.LE.1)   GOTO 150                                              3440
C 154 LII=LI*11                                                            3450
C     GO TO 151                                                            3460
C 150 LII=NZ                                                               3470
C 151 IF(LIM.GT.LII)  GOTC 146                                             3480
C     WRITE(NA,125)   (LBA(LM),LM=LIM,LII)                                 3490
C 125 FORMAT(10X,11(3X,I3,5X))                                             3500
C     IF(LI.NE.1)   GOTO 153                                               3510
C     NEI-OUTSCATTERING GROUP ACCORDING TO THE COUNTING IN THE ABN-SET     3520
C     I.E. LOWEST GROUP NUMBER CORRESPONDS TO HIGHEST ENERGY BOUNDARIES    3530
C     WAHR-PROBABILITY FOR INELASTIC SCATTERING OUT OF GROUP I  INTO K     3540
C 152 WRITE(NA,124) NEI,(WAHR(LM),LM=1,LII)                                3550
C 124 FORMAT(3X,I2,5X,11(1PE10.3,1X))                                      3560
C 153 WRITE(NA,129)(WAHR(LM),LM=LIM,LII)                                   3570
C 129 FORMAT(10X,11(1PE10.3,1X))                                           3580
  146 CONTINUE                                                             3590
      NZ1=NZ+1                                                             3600
      DO 500 K=1,NZ                                                        3610
  500 WEIN(I,K)=SNGL(WAHR(K))                                              3620
C     WRITE(LIZ) NZ1,NEI,(WEIN(I,K),K=1,NZ)                                3630
C     WRITE(NA,9100) NZ1,NEI,I                                             3640
C9100 FORMAT(' NZ1=',I6,'NEI=',I6,'I=',I6)                                 3650
C     WRITE(NA,9110) (WEIN(I,K),K=1,NZ)                                    3660
C9110 FORMAT(1CE12.5)                                                      3670
    1 CONTINUE                                                             3680
  999 RETURN                                                               3690
      END                                                                  3700
```

```
      SUBROUTINE AKED (I,E,EZ,SGIP,JMAT,LMAX,SU,CUOT,WERT,AE,
     1IA,NAB,IE,INF,NFE,EF,FI,NE,NX,SGIT,NAE,
     2NAEP,ISG,ISGP,IANF,NISG,NISGP)
      REAL*8   NAM,FELC,KFEL,NAM2,NAM3,AE,EMAX,E,EMIN,EZ
      DIMENSION  FELD(6),KFEL(6),NFEL(6),SU(NX),CUOT(NX),E(NE),
     1AE(NAE),WERT(ISG),SGIP(ISG,NAE),SGIT(ISG),
     2EF(NFE),FI(NFE),IANF(NAE),EZ(NISG)
      COMMON NAM,ISTRUK,ISPA,NA,LIZ
      EQUIVALENCE  (FELD(1),KFEL(1))
      EPSI=.001
      NISGF=0
      NISGP=0
      NAEF=0
      ISGF=0
      NAEP=0
      ISGP=0
      ISGP=0
      KEN=NFE
      IF(NFE.EQ.1)  KEN=0
      CALL DADRG(I,KEN,EZ,E,AE,EF,FI,JMAT,LMA,NISG,NISGF,NISGP,
     1NE27,NAE,NAEF,NAEP,ISG,ISGF,ISGP,IA,NAB,
     2&1000)
C     WRITE(NA,9002) JMAT,LMA
 9002 FORMAT('&&&&AFTER DACRG JMAT=',I6,'LMA=',I6)
      CALL SIORG(I,EZ,AE,SGIP,SGIT,IANF,JMAT,LMA,NISG,
     1ISG,NAE)
C     WRITE(NA,9001) JMAT,LMA
C9001 FORMAT('&&&&AFTER SIORG JMAT=',I6,' LMA=',I6)
      IF (LMA.EQ.0) GO TO 200
      GO TO 167
  200 NAB=I-1
      LMAX=LMA
      GO TO 1000
  167 NE1=NE-1
  180 FORMAT(
     1' ***ERROR 5.03 : ONE OF THE BOUNDARIES OF THE ENERGY RANGE,IN'   /
     2' WHICH INELASTIC SCATTERING IS POSSIBLE : EMAX ( - UPPER'        /
     3' ENERGY LIMIT OF THE DISCRETE REGION) OR EMIN ( - LAST KEDAK'    /
     4' ENERGY,AT WHICH THE TOTAL INELASTIC SCATTERING CROSS SECTION'   /
     5' IS STILL EQUAL TO ZERO) IS NOT CONTAINED IN ANY OF THE ENERGY'  /
     6' GROUPS OF THE GIVEN GROUP STRUCTURE.THAT MEANS THE GIVEN'       /
     7' STRUCTURE OF ENERGY GROUPS DOES NOT COVER THE WHOLE ENERGY'     /
     8' RANGE')
C     DETERMINATION OF THE ENERGY GROUP IA, IN WHICH EMIN IS LYING, AND
C     OF THE ENERGY GROUP NAB, IN WHICH EMAX IS LYING.
      IA=MAXO(INF,IA)
      NAB=MINO(IE,NAB)
      IF(EZ(LMA).LT.E(NAB+1))   GOTO 315
      DO 313 L=1,LMA
      LMAB=L
      IF(EZ(L).GE.E(NAB+1))  GOTO 314
  313 CONTINUE
C     LMAX - (NUMBER OF KEDAK ENERGIES + 1) BETWEEN EMIN AND THE UPPER
C     ENERGY LIMIT E(NAB+1) OF GROUP NAB
  314 LMAX=LMAB
      GOTO 316
  315 LMAX=LMA
C     INTERPOLATION OF THE WEIGHTING FUNCTION AT THE KEDAK ENERGY POINTS
  316 KEN1=KEN-1
      IF(LMAX.LE.ISG)  GO TO 15
      ISGP=LMAX-ISG+1
      RETURN
C 306 IF(KEN.EQ.0)  GOTO 156
   15 DO 32 LF=1,LMAX
      WERT(LF)=0.
      EA=EZ(LF)
      CALL TRA(EA,FIS,NFE,EF,FI)
   32 WERT(LF)=FIS
C     INTERPOLATION OF SIGMA TOTAL AND THE WEIGHTING FUNCTION AT THE
C     ENERGY GROUP BOUNDARIES
   39  II=I
      NE1=NE-1
C     CRITICAL CASES
      IF(E(IA+1).GT.EZ(1))  GOTO 7
    8  IF(II.EQ.IA)   GOTO 50
    9  IA1=IA+1
      IF(II-IA1)  90,108,90
    7  IF(II-IA) 90,108,90
  108 IF(E(II).GE.EZ(1))   GOTO 112
  109 LA=1
      SG1=0.
      EA=E(II)
      CALL TRA(EA,FHI1,NFE,EF,FI)
      GO TO 91
  112 IF(E(II).EQ.EZ(1))   GOTO 116
C     GO TO 1000
      GO TO 90
  116 LA=1
      SG1=SGIT(1)
      FHI1=WERT(1)
      EA=E(II)
      GO TO 91
   90 LA=0
   91 SL(II)=0.
      SUMM=0.
      LMX1=LMAX-1
      DO 40 LL=1,LMX1
      IF(LA.NE.0)  GOTO 102
  101 IF(E(II).LT.EZ(LL))  GOTO 40
  118 IF(E(II).GE.EZ(LL+1))  GOTO 40
  117 LA=LL
      SG1=FIPOLO(EZ(LL),E(II),EZ(LL+1),
     1SGIT(LL),SGIT(LL+1))
C     SG1=SGIT(LL)+(SGIT(LL+1)-SGIT(LL))*(E(II)-EZ(LL))/(EZ(LL+1)-EZ(LL)
C     1)
      EA=E(II)
      CALL TRA(EA,FHI1,NFE,EF,FI)
  102 IF(E(II+1).GT.EZ(LL))  GOTO 122
      GO TO 40
C     THE END GROUP IS THE CASE IN QUESTION
```

```
  122 IF(II.NE.NAB)   GOTO 107                                          1110
 123  NE1=NE-1                                                          1120
      IF(NAB.NE.NE1)   GOTO 107                                         1130
  124 IF(E(NAB+1).LT.EZ(LMAX))  GOTO 107                                1140
  126 EE=EZ(LMAX)                                                       1150
      LE=LMAX                                                           1160
      SG2=SGIT(LMAX)                                                    1170
      FHI2=WERT(LMAX)                                                   1180
      GO TO 100                                                         1190
  107 IF(E(II+1).GT.EZ(LL+1))  GO TO 128                                1200
      GO TO 127                                                         1210
  128 IF (LMX1.GT.LL) GO TO 40                                          1220
  127 LE=LL+1                                                           1230
      EE=DMIN1(E(II+1),EZ(LMAX))                                        1240
      SG2=FIPOLD(EZ(LL),EE,EZ(LL+1),                                    1250
     1SGIT(LL),SGIT(LL+1))                                              1260
C     SG2=SGIT(LL)+(SGIT(LL+1)-SGIT(LL))*(E(II+1)-EZ(LL))/(EZ(LL+1)-EZ(L 1270
C    1L))                                                               1280
      CALL TRA(EE,FHI2,NFE,EF,FI)                                       1290
      GO TO 100                                                         1300
   40 CONTINUE                                                          1310
C     IF (LMAX.GT.0) WRITE(NA,3000) II,E(II+1),EZ(LMAX),LMAX            1320
C3000 FORMAT(' II=',I10,'  E(II+1)=',1PD14.6,'  EZ(LMAX)=',1PD14.6,     1330
C    1'LMAX=',I6)                                                       1340
      GO TO 41                                                          1350
C     CALCULATION OF THE INTEGRAL OVER THE WEIGHTING FUNCTION AND THE   1360
C     INTEGRAL OVER SIGMA TOTAL*WEIGHTING FUNCTION BY TRAPEZOIDAL RULE  1370
C 100 WRITE(NA,9101) II,LMAX,LA,LE,E(II),E(II+1)                        1380
C9101 FORMAT(' II=',I6,'LMAX=',I6,'LA=',I6,'LE=',I6,'E=',E15.9,'E1=',E15 1390
C    1.9)                                                               1400
C     WRITE(NA,9102) (SGIT(ISR),EZ(ISR),ISR,ISR=1,LMAX)                 1410
C9102 FORMAT(2(' SGIT=',E12.6,'EZ=',E15.9,'ISR=',I6))                   1420
  100 LE1=LE-1                                                          1430
      DO 30 IL=LA,LE1                                                   1440
      IF(LA.NE.LE1)  GOTO 104                                           1450
    3 IF(E(II).GE.EZ(1))   GOTO 103                                     1460
   44 FU1=SGIT(LA)*WERT(LA)                                             1470
      FU2=SG2*FHI2                                                      1480
      DIF1=EZ(LA)-EA                                                    1490
      DIFF=EE-EZ(LA)                                                    1500
      SUP=DIF1*(WERT(LA)+FHI1)/2.+DIFF*(FHI2+WERT(LA))/2.               1510
      GOTO 28                                                           1520
  103 FU1=SG1*FHI1                                                      1530
      FU2=SG2*FHI2                                                      1540
      DIFF=EE-EA                                                        1550
      SUP=DIFF*(FHI2+FHI1)/2.                                           1560
      GO TO 28                                                          1570
  104 IF(IL.NE.LA)   GOTO 19                                            1580
    5 IF(E(II).GE.EZ(1))    GOTO 34                                     1590
    6 FU1=SGIT(LA)*WERT(LA)                                             1600
      DIF1=EZ(LA)-EA                                                    1610
      DIFF=EZ(LA+1)-EZ(LA)                                              1620
      SUP=DIF1*(WERT(LA)+FHI1)/2.+DIFF*(WERT(LA+1)+WERT(LA))/2.         1630
      GOTO 35                                                           1640
   34 FU1=SG1*FHI1                                                      1650
      DIFF=EZ(LA+1)-EA                                                  1660
      SUP=DIFF*(WERT(LA+1)+FHI1)/2.                                     1670
      GO TO 35                                                          1680
   19 IF(IL.NE.LE1)  GOTO 26                                            1690
   27 FU1=FU2                                                           1700
      DIFF=EE-EZ(LE1)                                                   1710
      SUP=DIFF*(FHI2+WERT(LE1))/2.                                      1720
      FU2=SG2*FHI2                                                      1730
      GO TO 28                                                          1740
   26 FU1=FU2                                                           1750
      DIFF=EZ(IL+1)-EZ(IL)                                              1760
      SUP=DIFF*(WERT(IL+1)+WERT(IL))/2.                                 1770
   35 FU2=SGIT(IL+1)*WERT(IL+1)                                         1780
   28 SUMM=SUMM+DIFF*(FU1+FU2)/2.                                       1790
      SU(II)=SU(II)+SUP                                                 1800
   30 CONTINUE                                                          1810
   41 IF(SU(II).EQ.0.)   GOTO 31                                        1820
C  29 QUOT(II)=SUMM/SU(II)                                              1830
   29 QUOT(II)=SUMM                                                     1840
      GO TO 50                                                          1850
   31 QUOT(II)=0.                                                       1860
C  50 WRITE(NA,9100) II,QUOT(II),SUMM,SU(II)                            1870
C9100 FORMAT(' II=',I6,'QUOT=',E12.6,'SUMM=',E12.6,'SU=',E12.6)         1880
   50 CONTINUE                                                          1890
 1000 RETURN                                                            1900
      END                                                               1910
```

```
      SUBROUTINE TRA(EFI,FIS,NF,EF,FI)                                    10
      DIMENSION EF(NF),FI(NF)                                             20
      KEN=NF                                                              30
      IF(NF.EQ.1)KEN=0                                                    40
      KUA=0                                                               50
      IF(KEN.NE.0)GOTO 2                                                  60
    1 FIS=PHI(EFI)                                                        70
      GOTO 3                                                              80
    2 DO 105 KI=1,KEN                                                     90
      IF(EF(KI).GE.EFI)GOTO 114                                          100
  113 KUA=KI                                                             110
      GOTO 105                                                           120
  114 KAB=KUA+1                                                          130
      GOTO 106                                                           140
  105 CONTINUE                                                           150
  106 FIS=FIPOLA(EF(KUA),EFI,EF(KAB),FI(KUA),FI(KAB))                    160
    3 RETURN                                                             170
      END                                                                180
```

```
C*****SUBROUTINE NOREAD.DATE OF LAST CHANGE 14.10.1976.(LINES 10792
C*****12660)
      SUBROUTINE NDREAD(I,EZ,E,AE,XLEVEL,J,KMAX,NENRE,NISG,
     1NISGF,NISGP,NE27,NAE,NAEF,NAEP,NETMAX,IL,IB,IP,*)
C*****SUBROUTINE READS ENERGY SCALE OF EXCITATION CROSS-SECTIONS,
C*****WHICH COVER ENERGY GROUP I,WITH LOWER ENERGY LIMIT E(I) AND
C*****UPPER ENERGY LIMIT E(I+1).
      DIMENSION EZ(NISG),AE(NAE),E(NE27),FELD(6),KFEL(6),NFEL(6)
      REAL*8 NAM,NAM2,NAM3,KFEL,FELD,XLEVEL,AE,E,EZ,ENN,XLEV
      COMMON NAM,ISTRUK,ISPA,NA,LIZ
      EQUIVALENCE (FELD(1),KFEL(1))
      CALL DOPW(8HBEST     ,NAM2)
      CALL DOPW(8HSGIZ     ,NAM3)
      KFEL(1)=NAM
      KFEL(2)=NAM2
  170 FORMAT(' FELD(5)=',G16.8)
      KFEL(3)=NAM3
      NFEL(1)=4
      FFLD(4)=XLEVEL
      ISN=0
      K=1
      KK=0
      IF(J.NE.0) GO TO 9
      NETMAX=1
      KMAX=0
C*****FINDING EXCITATION CROSS-SECTION TABLE WITH EXCITATION ENERGY
C*****GREATER THAN FELD(4).
    9 NANRE=0
      NENRE=0
      CALL NDFLOC(N,NFEL,FELD,NDAT,NCO)
      IF(N.EQ.1) GO TO 2
C*****NANRE=0 (NENRE=0):FIRST (LAST) ENERGY POINT BELONGING TO GROUP
C*****I HAS NOT YET BEEN FOUND.NANRE=1 (NENRE=1) : FIRST (LAST)
C*****ENERGY POINT BELONGING TO I HAS BEEN FOUND.
C*****NENRE=2: ALL EXCITATION CROSS-SECTIONS INFLUENCING GROUP I
C*****HAVE BEEN READ.
      CALL NDFLOC(N,NFEL,FELD,NDAT,NCO)
      IF(N.EQ.0) GO TO 30
      GO TO 2
   30 CONTINUE
      GO TO 3
C    3 WRITE(NA,110) NAM,NAM3,FELD(4)
C  110 FORMAT(' FOR THE ISOTOPE',A8,'THE DATA TYPE',A8,'IS NOT AVAILABLE
C     1FOR EXCITATION ENERGIES ABOVE',G16.8,'EV KEDAK')
    3 IF (J.EQ.0) GO TO 1000
      IL=1
      GO TO 57
C*****IL=1 MEANS : LAST EXCITATION LEVEL OF THE KEDAK LIBRARY
C*****HAS BEEN REACHED.
    2 J=J+1
      IF(J.LE.NAE) GO TO 22
C     J=1
      NAEF=NAEF+1
   22 AE(J)=FELD(4)
      XLEV=AE(J)
      IF(AE(J).GT.E(I+1)) GO TO 55
      GO TO 6
   55 NENRE=2
      J=J-1
      IF(J.EQ.0) IB=1
      GO TO 57
C*****FINDING AT THE BEGINNING OF THE TABLE OF EXCITATION CROSS-SECTIONS
C*****LAST ENERGY POINT EN  WITH CROSS-SECTION VALUE EQUAL TO ZERO.
    6 IF(FELD(6).NE.0.) GO TO 11
      EN=FELD(5)
      CALL NDFNXT(N,NFEL,FELD,NDAT,NCO)
      IF(N.EQ.1) GO TO 6
      WRITE(NA,112) J,AE(J)
  112 FORMAT(' *** WARNING 5.20 : FOR LEVEL J= ',I6,'AE(J) = ',E12.6,'
     1ALL EXCITATION CROSS SECTIONS ARE EQUAL TO ZERO.')
      J=J-1
      NENRE=2
      GO TO 57
C*****CHECK WHETHER EN BELONGS TO THE ENERGY SCALE NEEDED FOR ENERGY
C****GROUP I
   11 CONTINUE
      IF(EN.GE.E(I).AND.EN.LT.E(I+1)) GO TO 19
      IF(FELD(5).GE.E(I).AND.FELD(5).LT.E(I+1)) GO TO 18
      IF(EN.LT.E(I)) GO TO 19
      IF(EN.GT.E(I+1)) GO TO 40
C*****FOLLOWING CONDITION,THAT LEADS TO STATEMENT NUMBER 18. (EN OR
C*****FELD(5) BETWEEN LOWER AND UPPER LIMIT OF GROUP I)
   18 KK=KMAX+K
      IF(KK.LE.NISG) GO TO24
      NISGF=NISGF+1
      KK=1
   24 CONTINUE
      EZ(KK)=EN
      K=K+1
      KK=KMAX+K
      IF(KK.LE.NISG) GO TO 50
      NISGF=NISGF+1
      KK=1
   50 CONTINUE
      EZ(KK)=FELD(5)
      NANRE=1
      GO TO 42
C*****FOLLOWING CONDITION , THAT LEADS TO STATEMENT NUMBER 19 ( EN IS
C*****LESS THAN THE LOWER LIMIT OF GROUP I)
   19 ISN=1
      ENN=FELD(5)
      GO TO 42
C*****FOLLOWING CONDITION,THAT LEADS TO STATEMENT NUMBER 40 ( EN IS
C*****GREATER THAN UPPER LIMIT OF GROUP I)
   40 NENRE=2
      IF (J.EQ.1) IB=1
C*****IB=1 : LOWEST ENERGY POINT OF FIRST INELASTIC CROSS-SECTION
C*****IS GREATER THAN THE UPPER ENERGY LIMIT OF GROUP I
      GO TO 57
C*****FINDING FURTHER ENERGY POINTS OF CROSS-SECTION TABLE
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   42 CONTINUE                                                          1110
      CALL NDFNXT(N,NFEL,FELD,NDAT,NCO)                                 1120
      IF(N.EQ.0) GO TO 51                                               1130
      IF(FELD(5).GE.E(I).AND.FELD(5).LE.E(I+1)) GO TO 43                1140
      IF(FELD(5).LT.E(I)) GO TO47                                       1150
      IF(FELD(5).GT.E(I+1)) GO TO 48                                    1160
C*****FOLLOWING CONDITION LEADING TO STATEMENT NUMBER 43.(FELD(5)        1170
C*****WITHIN ENERGY LIMITS OF GROUP I)                                  1180
   43 K=K+1                                                             1190
      KK=KMAX+K                                                         1200
      IF(KK.LE.NISG) GO TO 44                                           1210
      NISGF=NISGF+1                                                     1220
      KK=1                                                              1230
   44 IF(NANRE.EQ.0) GO TO 45                                           1240
      EZ(KK)=FELD(5)                                                    1250
      GO TO 42                                                          1260
   45 NANRE=1                                                           1270
      K=MAXO((K-1),1)                                                   1280
      KK=KMAX+K                                                         1290
      EZ(KK)=ENN                                                        1300
      K=K+1                                                             1310
      KK=KMAX+K                                                         1320
      IF(KK.LE.NISG) GO TO 46                                           1330
      NISGF=NISGF+1                                                     1340
      KK=1                                                              1350
   46 EZ(KK)=FELD(5)                                                    1360
      GO TO 42                                                          1370
C*****FOLLOWING CONDITION,LEADING TO STATEMENT NUMBER 47(FELD(5)        1380
C*****IS LESS THAN THE LOWER ENERGY OF GROUP I)                         1390
   47 ISN=1                                                             1400
      ENN=FELD(5)                                                       1410
      K=MAXO((K-1),0)                                                   1420
      GO TO 42                                                          1430
C*****FOLLOWING CONDITION,THAT LEADS TO STATEMENT NUMBER 48(FELD(5)     1440
C*****IS LARGER THAN THE UPPER ENERGY OF GROUP I)                       1450
   48 K=K+1                                                             1460
      KK=KMAX+K                                                         1470
      IF(K.EQ.1.AND.ISN.EQ.1.AND.NANRE.EQ.0) GO TO 70                   1480
      GO TO 71                                                          1490
   70 NANRE=1                                                           1500
      EZ(KK)=ENN                                                        1510
      K=K+1                                                             1520
      KK=KMAX+K                                                         1530
   71 IF(KK.LE.NISG) GO TO 49                                           1540
      NISGF=NISGF+1                                                     1550
      KK=1                                                              1560
   49 EZ(KK)=FELD(5)                                                    1570
C*****LAST ENERGY OF CROSS-SECTION TABLE ,CORRESPONDING TO EXCITATION   1580
C*****ENERGY FELD(4),THAT INFLUENCES ENERGY GROUP I,HAS BEEN READ.      1590
   51 IF(XLEV.LT.FELD(4))                                               1600
     1IH=1                                                              1610
      IF(NISGF.NE.0) GO TO 52                                           1620
C     IF(NAEF.NE.0) GO TO 53                                            1630
      GO TO 54                                                          1640
   52 NISGF=NISGF+NISG                                                  1650
      NISGP=NISGF-NISG                                                  1660
      GO TO 57                                                          1670
C  53 NAEP=(NAEF-1)*NAE+J+4                                             1680
C     GO TO 57                                                          1690
 1000 WRITE(NA,111) J,FELD(4)                                           1700
  111 FORMAT(' J=',I6,'FELD=',G16.8)                                    1710
      RETURN 1                                                          1720
   54 XLEVEL=FELD(4)                                                    1730
      IF (NENRE.EQ.2) GO TO 57                                          1740
      KMAX1=KMAX                                                        1750
      KMAX=KK                                                           1760
   62 IF(EZ(KMAX-1).EQ.E(I+1)) GO TO 56                                 1770
      GO TO 59                                                          1780
   56 KMAX=KMAX-1                                                       1790
   59 IF(EZ(KMAX1+2).EQ.E(I)) GO TO 60                                  1800
      GO TO 58                                                          1810
   60 KMAX11=KMAX1+1                                                    1820
      KMAX=KMAX-1                                                       1830
      DO 61 IO=KMAX11,KMAX                                              1840
   61 EZ(IO)=EZ(IO+1)                                                   1850
   58 CONTINUE                                                          1860
      NETMAX=MAXO(NETMAX,K)                                             1870
   57 RETURN                                                            1880
      END                                                               1890
```



```
      SUBROUTINE DAORG(I,KEN,EZ,E,AE,EF,FI,J,KMAX,NISG,NISGF,NISGP        10
     1,NE27,NAE,NAEF,NAEP,ISG,ISGF,ISGP,IA,NAB,*                          20
     2)                                                                   30
C*****SUBROUTINE CONSTRUCTS ENERGY FIELD EZ,CONSISTING OF ALL ENERGIES    40
C*****CONTAINED IN THE CROSS-SECTIONS TABLES OF THE EXCITATION            50
C*****CROSS-SECTIONS,BELONGING TO DIFFERENT EXCITATION ENERGIES.          60
      DIMENSION EZ(NISG),AE(NAE),E(NE27),EF(KEN),FI(KEN)                  70
      REAL*8 EZ,AE,E,NAM,XLEVEL,E1,E2                                     80
      COMMON NAM,ISTRUK,ISPA,NA,LIZ                                       90
C*****IH=1:LAST ENERGY POINT ,FOR WHICH SGIZ ARE STORED FOR              100
C*****LEVEL AE(J) HAS BEEN READ.IH=0:LAST ENERGY POINT,FOR               110
C*****WHICH VALUES OF SGIZ ARE STORED FOR LEVEL AE(J) HAS                120
C*****NOT YET BEEN READ.IH=0,IF LAST ENERGY POINT FOR SGIZ               130
C*****OF HIGHEST EXCITATION LEVEL HAS BEEN READ.                         140
      NABL=0                                                             150
      IB=0                                                               160
      IL=0                                                               170
      IH=0                                                               180
      J=0                                                                190
      EPS=0.0                                                            200
      EPSI=0.001                                                         210
C     EPSI=1.                                                            220
      KMAX=0                                                             230
      KMAXC=0                                                            240
      XLEVEL=0.D0                                                        250
    1 CALL NDREAD(I,EZ,E,AE,XLEVEL,J,KMAX,NENRE,NISG,NISGF,NISGP,NE27,   260
     1NAE,NAEF,NAEP,NETMAX,IL,IB,IH,& 1000)                              270
```

```
C       IF(NAEF.NE.0) GO TO 10                                          280
        KMAXC=MAXO(KMAXC,KMAX)                                          290
        IF(IL.EQ.1.AND.KMAXC.EQ.0) GO TO 26                             300
        IF(IL.EQ.1) GO TO 24                                            310
        IF(IB.EQ.1) GO TO 23                                            320
C*****IA=0 MEANS : CROSS-SECTIONS OF TYPE SGIZ ARE AVAILABLE FOR THE    330
C*****LOWEST ENERGY REQUIRED BY INPUT. IA.NE.0 : CROSS-SECTIONS ARE     340
C*****AVAILABLE STARTING FROM GROUP IA.                                 350
        IF(NISGF.NE.0.AND.J.NE.1) GO TO 10                              360
        IF(J.EQ.1.AND.NENRE.NE.2) GO TO 3                               370
        IF(NENRE.EQ.2) GO TO 11                                         380
        CALL ORDNEN(KMAX,EMIN,EMAX,EZ,NISG,EPS)                         390
     3  IF (IH.EQ.0)                                                    400
      1XLEVEL=XLEVEL*(1.D0+1.D-5)                                       410
        IH=0                                                            420
        GO TO 1                                                         430
    11  CONTINUE                                                        440
C*****ADDING THE ENERGY POINTS OF THE WEIGHTING FUNCTION.               450
    25  IF(KEN.EQ.0) GO TO 12                                           460
        E1=DMAX1(EZ(1),E(I))                                            470
        E2=DMIN1(EZ(KMAX),E(I+1))                                       480
        CALL CUTS(SNGL(E1),SNGL(E2),EF,KEN,KA,KE,KMAX1)                 490
        DO 13 K=KA,KE                                                   500
        KK=KMAX+K-KA+1                                                  510
        IF(KK.LE.NISG) GO TO 13                                         520
        NISGF=KK                                                        530
        KK=1                                                            540
    13  EZ(KK)=EF(K)                                                    550
        IF(NISGF.NE.0) GO TO 15                                         560
        GO TO 16                                                        570
    15  NISGP=NISGF-NISG                                                580
        RETURN                                                          590
    16  KMAX=KMAX+KMAX1                                                 600
    20  CALL ORDNEN(KMAX,EMIN,EMAX,EZ,NISG,EPS)                         610
        IF (NABL.EQ.1) GO TO 27                                         620
        GO TO 28                                                        630
    27  DO 29 IS=1,KMAX                                                640
        ISS=IS                                                          650
        IF (EZ(IS).LE.E2) GO TO 29                                      660
        IF (EZ(IS).GT.E2) GO TO 30                                      670
    29  CONTINUE                                                        680
        GO TO 28                                                        690
    30  KMAX=MAXO(1,ISS-1)                                              700
C       WRITE(NA,1010) (IS,EZ(IS),IS=1,KMAX)                            710
C1010  FORMAT(2(' IS=',I6,'EZ=',E12.6))                                720
    28  IF(KMAX.LE.ISG) GO TO 17                                        730
        ISGF=MAXO(KMAX,NETMAX)                                          740
        ISGP=ISGF-ISG                                                   750
    17  IF(NISG.LT.(KMAX+NETMAX)) GO TO 18                              760
        GO TO 21                                                        770
    18  NISGF=KMAX+NETMAX                                               780
        NISGP=NISGF-NISG                                                790
    21  IF(NAEF.NE.0) NAEP=NAEF                                         800
        GO TO 10                                                        810
  1000  IA=0                                                            820
        NAB=0                                                           830
        RETURN 1                                                        840
C*****WEIGHTING FUNCTION GIVEN AS AN ANALYTICAL FUNCTION.               850
    12  CALL SPECT1(KMAX,EZ,NISG,NISGF,NISGP,EPSI,EPS)                 860
C       WRITE(NA,105) NISG,NISGF,NISGP                                  870
   105  FORMAT(' NISG=',I6,'NISGF=',I6,'NISGP=',I6)                     880
        IF(NISGF.NE.0) GO TO 19                                         890
        GO TO 20                                                        900
    19  NISG=NISG+NISGP                                                 910
        GO TO 10                                                        920
C   24  WRITE(NA,107) IL,J,XLEVEL                                       930
C  107  FORMAT(' IL=',I6,'J=',I6,'LAST EXCITATION LEVEL=',G14.6)        940
    24  NABL=1                                                          950
        IF (EZ(KMAX).LT.E(I+1).AND.EZ(KMAX).GE.E(I)) NAB=I              960
        IF(EZ(KMAX).EQ.E(I)) NAB=I-1                                    970
C       WRITE(NA,108) NAB                                               980
C  108  FORMAT(' LAST ENERGY POINT OF SGIZ LIES WITHIN GROUP NAB=',I6)  990
        GO TO 25                                                       1000
C   23  WRITE(NA,106) IB,I,E(I+1)                                      1010
C  106  FORMAT(' IB=',I6,'ALL ENERGY POINTS OF THE FIRST INELASTIC LEVEL 1020
C     1LIE ABOVE THE UPPER GROUP LIMIT FO GROUP I.'/' I=',I6,          1030
C     2'E(I+1)=',G14.6)                                                1040
    23  CONTINUE                                                       1050
    26  IA=I+1                                                         1060
C       WRITE(NA,109) I,IA                                             1070
C  109  FORMAT(' NO CONTRIBUTION TO DISCRETE INELASTIC LEVELS           1080
C     1IN GROUP I=',I6,'.IA IS SET EQUAL TO IA=',I6)                   1090
    10  RETURN                                                         1100
        END                                                            1110
```

```
        SUBROUTINE SPECT1(KMAX,EZ,NISG,NISGF,NISGP,EPSI,EPS)              10
        DIMENSION EZ(NISG)                                                20
        COMMON NAM,ISTRUK,ISPA,NA,LIZ                                     30
        REAL*8 NAM,EZ                                                     40
        NA=6                                                              50
        IO=1                                                              60
        KMAX1=KMAX-1                                                      70
      4 DO 1 I=IO,KMAX1                                                   80
        EI=SNGL((EZ(I)+EZ(I+1)))*0.5                                      90
        PHIE=PHI(EI)                                                     100
        E1=SNGL(EZ(I))                                                   110
        E2=SNGL(EZ(I+1))                                                 120
        PHI1=PHI(E1)                                                     130
        PHI2=PHI(E2)                                                     140
        PHII=FIPOLA(E1,EI,E2,PHI1,PHI2)                                  150
        ERR=ABS((PHII-PHIE)/PHIE)                                        160
        IF(ERR.LT.EPSI) GO TO 1                                          170
        IS=I                                                             180
        GO TO 2                                                          190
      1 ISS=I                                                            200
        GO TO 5                                                          210
      2 KMAX=KMAX+1                                                      220
```

```
      IF (KMAX.LE.NISG) GO TO 3                                          230
      NISGF=NISGF+10                                                     240
      NISGP=NISGP+10                                                     250
      KMAX=NISG                                                          260
      IC=IS                                                              270
      KMAX1=KMAX-1                                                       280
      GO TO 6                                                            290
    3 EZ(KMAX)=DBLE(EI)                                                  300
      CALL ORDNEN(KMAX,EMIN,EMAX,EZ,NISG,EPS)                            310
      IC=IS                                                              320
      KMAX1=KMAX-1                                                       330
      GO TO 4                                                            340
    5 CONTINUE                                                           350
    6 RETURN                                                             360
      END                                                                370
```

```
      SUBROUTINE ORDNEN(KMAX,EMIN,EMAX,FELD,NTT,EPS)                      10
      DIMENSION FELD(NTT)                                                 20
      REAL*8 FELD                                                         30
C                                                                         40
C  ORDNEN ORDNET FELD NACH WACHSENDEN WERTEN                              50
C                                                                         60
      IF(KMAX.LT.2) GOTO 100                                              70
      DO 99 K=2,KMAX                                                      80
      M=K-1                                                               90
      IF(FELD(K).GE.FELD(M)) GOTO 99                                     100
      R=FELD(K)                                                          110
   10 M=M-1                                                              120
      IF(M.EQ.0) GOTO 20                                                 130
      IF(R.LT.FELD(M)) GOTO 10                                           140
   20 IA=M+1                                                             150
      IE=K-1                                                             160
      J=IE                                                               170
      DO 30 I=IA,IE                                                      180
      FELD(J+1)=FELD(J)                                                  190
   30 J=J-1                                                              200
      FELD(IA)=R                                                         210
   99 CONTINUE                                                           220
  100 IF(KMAX.EQ.0) GOTO 200                                             230
      GOTO 300                                                           240
  200 EMIN=0                                                             250
      EMAX=0                                                             260
      GO TO 800                                                          270
  300 KMAXX=KMAX                                                         280
      DO 500 K=2,KMAX                                                    290
  502 IF(K    .GT.KMAXX) GO TO 501                                       300
      M=K-1                                                              310
      IF(SNGL(DABS((FELD(K)-FELD(M))/FELD(K))).LE.EPS) GO TO 600         320
      GO TO 500                                                          330
  600 KMAXX=KMAXX-1                                                      340
      KMAXS= MAXO(K,KMAXX)                                               350
      DO 700 KK=K,KMAXS                                                  360
  700 FELD(KK)=FELD(KK+1)                                                370
      GO TO 502                                                          380
  500 CONTINUE                                                           390
  501 KMAX=KMAXX                                                         400
      EMIN=FELD(1)                                                       410
      EMAX=FELD(KMAX)                                                    420
  800 CONTINUE                                                           430
      RETURN                                                             440
      END                                                                450
```

```
C       SUBROUTINE CUTS CUTS ARRAY FELD AT ENERGIES                       10
C       UGG - LOWER VALUE,OGG - UPPER VALUE                               20
      SUBROUTINE CUTS(     UGG,OGG,FELD,NFE,KA,KE,KMAX1)                  30
      DIMENSION FELD(NFE)                                                40
C     WRITE(6,101) UGG,OGG                                               50
C 101 FORMAT(' UGG=',E12.6,'OGG=',E12.6)                                 60
      KA=1                                                               70
      KE=NFE                                                             80
      UG=AMAX1(UGG,FELD(1))                                              90
      OG=AMIN1(OGG,FELD(NFE))                                           100
      DO 1 K=1,NFE                                                      110
      IF(FELD(K).LT.UG) GO TO 1                                         120
      KA=K                                                              130
      IF(FELD(K).GT.UG) KA=MAXO((K-1),1)                                140
      GO TO 2                                                           150
    1 CONTINUE                                                          160
      KMAX1=0                                                           170
      GO TO 7                                                           180
    2 KMAX1=NFE-KA+1                                                    190
      K=NFE                                                             200
      DO 4 I=1,NFE                                                      210
      IF(FELD(K).LT.OG) GO TO 5                                         220
      K=K-1                                                             230
    4 CONTINUE                                                          240
      GO TO 7                                                           250
    5 KE=K+1                                                            260
      KD=NFE-KE                                                         270
      KMAX1=KMAX1-KD                                                    280
      RETURN                                                            290
    7 WRITE(6,100) UG,OG,FELD(1),FELD(NFE)                              300
  100 FORMAT(' CUTS : UG=',E12.6,'OG=',E12.6,'FELD(1)=',E12.6,          310
     *'FELD(NFE)=',E12.6)                                               320
      RETURN                                                            330
      END                                                               340
```

```
C      IN THE FOLLOWING FUNCTION FIPOLA (XA,YA)                          10
C      AND (XC,YC) ARE THE STARTING POINTS AND                           20
C      (XB,FIPOLA) IS THE INTERPOLATED POINT                             30
       FUNCTION FIPOLA(XA,XB,XC,YA,YC)                                   40
       DX1=XB-XA                                                         50
       DX2=XC-XB                                                         60
       DX=XC-XA                                                          70
       IF(DX.LT.1.E-30) GO TO 1                                          80
       FIPOLA=(YA*DX2+YC*DX1)/DX                                         90
       GO TO 2                                                          100
     1 FIPOLA=(YA+YC)/2.                                                110
     2 RETURN                                                           120
       END                                                              130
```

```
C*****SUBROUTINE SIORG PERFORMS INTERPOLATION OF SGIZ FOR LEVEL          10
C*****XLEVEL INTO ENERGY FIELD EZ(1).....EZ(KMAX),PROVIDED BY DAORG.     20
C*****SGIT HAS TWO MEANINGS:FIRST IT IS USED TO STORE THE PARTIAL        30
C*****INELASTIC CROSS-SECTIONS FROM KEDAK.IN THE SECOND PLACE IT IS      40
C*****USED TO CONTAIN THE SUM OVER THE PARTIAL INELASTIC CROSS-SECTIONS  50
C*****AT THE ENERGIES OF THE ENERGY FIELD EZ(1)...EZ(KMAX).THIS LAST     60
C*****QUANTITY IS NEEDED IN AKED.                                       70
C*****KMAX:DIMENSION OF ENERGY FIELD EZ(1)...EZ(KMAX).(KMAX1-KMAX) :    80
C*****DIMENSION OF ENERGY FIELD OF PARTIAL INELASTIC CROSS-SECTION ON    90
C*****KEDAK.                                                           100
       SUBROUTINE SIORG(I,EZ,AE,SGIP,SGIT,IANF,JMAX,KMAX,NISG,ISG,     110
      1 NAE)                                                           120
       DIMENSION EZ(NISG),AE(NAE),SGIT(ISG),SGIP(ISG,NAE),IANF(NAE)    130
       REAL*8 EZ,AE,XLEVEL,NAM                                         140
       COMMON NAM,ISTRUK,ISPA,NA,LIZ                                   150
C*****IB=1:THRESHOLD OF INELASTIC SCATTERING LIES ABOVE UPPER LIMIT     160
C*****OF ENERGY FIELD UNDER CONSIDERATION.                             170
C*****IL=1:LAST EXCITATION LEVEL OF MATERIAL UNDER CONSIDERATION       180
C*****HAS BEEN REACHED.                                                190
       IB=0                                                            200
       IL=0                                                            210
       IH=0                                                            220
       J=0                                                             230
       J1=J                                                            240
       XLEVEL=0.D0                                                     250
     2 CALL SGINT(EZ,AE,SGIT,KMAX,KMAX1,XLEVEL,J,NISG,NAE,ISG,NENRE,IH)260
       IF (J.EQ.J1) GO TO 7                                            270
       J1=J                                                            280
       IF(KMAX1.GT.KMAX) GO TO 1                                       290
       IANF(J)=1                                                       300
       DO 8 KS=1,ISG                                                   310
     8 SGIP(KS,J)=0.                                                   320
       GO TO 9                                                         330
     1 NETACT=KMAX1-KMAX                                               340
       CALL XINPOL(EZ,SGIT,SGIP(1,J),NISG,NETACT,KMAX,KANF,KEND)       350
       IANF(J)=KANF                                                    360
     9 IF(NENRE.EQ.2) GO TO 3                                          370
       IF(IH.EQ.0)      XLEVEL=XLEVEL*(1.D0+1.D-5)                     380
       IH=0                                                            390
       GO TO 2                                                         400
C      KMAXJ=KMAX-IANF(J)+1                                            410
C*****KMAXJ=DIMENSION OF ENERGY FIELD NEEDED FOR CROSS-SECTION         420
C*****BELONGING TO LEVEL J.                                            430
     3 JMAX=J-1                                                        440
C    7 WRITE(NA,100) JMAX, AE(JMAX),KMAX,I                             450
C  100 FORMAT(//' HIGHEST CALCULATED LEVEL JMAX=',I6,'AE(JMAX)=',1PD14.6460
C     1,'KMAX=',I6,'I=',I6)                                            470
       DO 4 N=1,KMAX                                                   480
       SGIT(N)=0.                                                      490
       DO 5 JJ=1,JMAX                                                  500
       IF(IANF(JJ).LE.N) GO TO 6                                       510
       GO TO 5                                                         520
     6 SGIT(N)=SGIT(N)+SGIP(N-IANF(JJ)+1,JJ)                           530
     5 CONTINUE                                                        540
     4 CONTINUE                                                        550
       SNULL=0                                                         560
       DO 11 IZ=1,KMAX                                                 570
       IF (SGIT(IZ).EQ.0.) GO TO 11                                    580
       SNULL=1                                                         590
       GO TO 12                                                        600
    11 CONTINUE                                                        610
    12 IF (SNULL.EQ.0) KMAX=0                                          620
C      WRITE(NA,1000) KMAX                                             630
C1000 FORMAT(' KMAX=',I6)                                              640
C      WRITE(NA,1001) (IM,SGIT(IM),EZ(IM),IM=1,KMAX)                   650
C1001 FORMAT(2(' IM=',I6,'SGIT=',E12.6,'EZ=',E15.8))                   660
    10 RETURN                                                          670
       END                                                             680
```

```
       SUBROUTINE SGINT(EZ,AE,SGIT,KMAX,KMAX1,XLEVEL,J,NISG,NAE,ISG,    10
      1NENRE,IH)                                                        20
       DIMENSION EZ(NISG),AE(NAE),SGIT(ISG),FELD(6),KFEL(6),NFEL(6)     30
       REAL*8 NAM,NAM2,NAM3,KFEL,FELD,AE,EZ,EN,EAA,XLEVEL,XLEV          40
       COMMON NAM,ISTRUK,ISPA,NA,LIZ                                    50
       EQUIVALENCE(FELD(1),KFEL(1))                                     60
       CALL DOPW(8HBEST     ,NAM2)                                      70
       CALL DOPW(8HSGIZ     ,NAM3)                                      80
       KFEL(1)=NAM                                                      90
       KFEL(2)=NAM2                                                    100
       KFEL(3)=NAM3                                                    110
       NFEL(1)=4                                                       120
       FELD(4)=XLEVEL                                                  130
       K=1                                                             140
       KK=0                                                            150
       KMAX1=KMAX                                                      160
       NANRE=0                                                         170
       NENRE=0                                                         180
       EN=0.D0                                                         190
       EAA=0.D0                                                        200
       SGIN=0.0                                                        210
```

```
      SGINN=0.0                                                          220
      CALL NDFLOC(N,NFEL,FELD,NDAT,NCO)                                  230
      IF(N.EQ.1) GO TO 2                                                 240
      CALL NDFLOC(N,NFEL,FELD,NDAT,NCO)                                  250
      IF(N.EQ.0) GO TO 30                                                260
      GO TO 2                                                            270
   30 CONTINUE                                                           280
      GO TO 3                                                            290
C    3 WRITE(NA,110) NAM,NAM3,FELD(4)                                    300
C  110 FORMAT(' FOR THE ISOTOPE',A8,'THE DATA TYPE',A8,'IS NOT AVAI=     310
C     1LABLE FOR EXCITATION ENERGIES ABOVE',G16.8,'ON  KEDAK')           320
    3 IF(J.EQ.0) GO TO 1000                                              330
      IL=1                                                               340
      GO TO 57                                                           350
C*****IL=1 MEANS : LAST EXCITATION LEVEL OF THE KEDAK LIBRARY            360
C*****HAS BEEN REACHED.                                                  370
    2 J=J+1                                                              380
      AE(J)=FELD(4)                                                      390
      XLEV=AE(J)                                                         400
      IF(AE(J).GT.EZ(KMAX)) GO TO 55                                     410
      GO TO 6                                                            420
   55 NANRE=2                                                            430
      IF(J.EQ.1) IB=1                                                    440
C*****IB=1 MEANS : THRESHOLD FOR INELASTIC SCATTERING LIES ABOVE         450
C*****THE UPPER ENERGY LIMIT OF ENERGY FIELD EZ(1)     EZ(KMAX).          460
      GO TO 57                                                           470
C*****FINDING AT THE BEGINNING OF THE TABLE OF EXCITATION CROSS          480
C*****SECTIONS HIGHEST ENERGY POINT EN WITH CROSS-SECTION VALUE          490
C*****EQUAL TO ZERO.                                                     500
    6 CONTINUE                                                           510
      IF(FELD(6).NE.0.) GO TO 11                                         520
      EN=FELD(5)                                                         530
      SGIN=FELD(6)                                                       540
      CALL NDFNXT(N,NFEL,FELD,NDAT,NCO)                                  550
      IF(N.EQ.1) GO TO 6                                                 560
      GO TO 54                                                           570
C*****CHECK,WHETHER EN BELONGS TO ENERGY SCALE NEEDED FOR THE            580
C*****ENERGY REGION EZ(1).....EZ(KMAX)                                   590
   11 CONTINUE                                                           600
      IF(EN.GE.EZ(1).AND.EN.LT.EZ(KMAX)) GO TO 18                        610
      IF(FELD(5).GE.EZ(1).AND.FELD(5).LT.EZ(KMAX)) GO TO 18              620
      IF(EN.LT.EZ(1)) GO TO 19                                           630
      IF(EN.GT.EZ(KMAX)) GO TO 40                                        640
C*****FOLLOWING CONDITION , THAT LEADS TO STATEMENT NUMBER 18.           650
C*****(EN OR FELD(5) BETWEEN LOWER AND UPPER LIMIT OF FIELD EZ).         660
   18 CONTINUE                                                           670
      KK=KMAX1+K                                                         680
      EZ(KK)=EN                                                          690
      SGIT(K)=SGIN                                                       700
      K=K+1                                                              710
      KK=KMAX1+K                                                         720
      EZ(KK)=FELD(5)                                                     730
      SGIT(K)=FELD(6)                                                    740
      NANRE=1                                                            750
      GO TO 42                                                           760
C*****FOLLOWING CONDITION,THAT LEADS TO STATEMENT NUMBER 19(EN IS        770
C*****LESS THAN THE LOWER LIMIT OF ENERGY FIELD EZ).                     780
   19 ENN=FELD(5)                                                        790
      SGINN=FELD(6)                                                      800
      GO TO 42                                                           810
C*****FOLLOWING CONDITION , THAT LEADS TO STATEMENT NUMBER 40            820
C*****(EN IS GREATER THAN EZ(KMAX))                                      830
   40 NANRE=2                                                            840
      IF(J.EQ.1) IB=1                                                    850
      GO TO 57                                                           860
C*****FINDING FURTHER ENERGY POINTS OF CROSS-SECTION TABLE               870
   42 CONTINUE                                                           880
      CALL NDFNXT(N,NFEL,FELD,NDAT,NCO)                                  890
      IF(N.EQ.0) GO TO 54                                                900
      IF(FELD(5).GE.EZ(1).AND.FELD(5).LE.EZ(KMAX)) GO TO 43              910
      IF (FELD(5).LT.EZ(1)) GO TO 47                                     920
      IF (FELD(5).GT.EZ(KMAX)) GO TO 48                                  930
C*****  FOLLOWING CONDITION LEADING TO STATEMENT NUMBER 43(FELD(5)       940
C*****WITHIN ENERGY LIMITS OF FIELD EZ)                                  950
   43 CONTINUE                                                           960
      K=K+1                                                              970
      KK=KMAX1+K                                                         980
      IF(NANRE.EQ.0) GO TO 45                                            990
      EZ(KK)=FELD(5)                                                    1000
      SGIT(K)=FELD(6)                                                   1010
      GO TO 42                                                          1020
   45 NANRE=1                                                           1030
      K=MAXO((K-1),1)                                                   1040
      KK=KMAX1+K                                                        1050
      EZ(KK)=ENN                                                        1060
      SGIT(K)=SGINN                                                     1070
      K=K+1                                                             1080
      KK=KMAX1+K                                                        1090
      EZ(KK)=FELD(5)                                                    1100
      SGIT(K)=FELD(6)                                                   1110
      GO TO 42                                                          1120
C*****FOLLOWING CONDITION,THAT LEADS TO STATEMENT NUMBER 47.(FELD(5)     1130
C*****IS LESS THAN THE LOWER ENERGY LIMIT OF FIELD EZ)                   1140
   47 ENN=FELD(5)                                                       1150
      SGINN=FELD(6)                                                     1160
      K=MAXO((K-1),0)                                                   1170
      GO TO 42                                                          1180
C*****FOLLOWING CONDITION,THAT LEADS TO STATEMENT NUMBER 48.(FELD(5)     1190
C*****IS LARGER THAN THE UPPER ENERGY OF FIELD EZ)                       1200
   48 CONTINUE                                                          1210
      K=K+1                                                             1220
      KK=KMAX1+K                                                        1230
      EZ(KK)=FELD(5)                                                    1240
      SGIT(K)=FELD(6)                                                   1250
C*****LAST ENERGY OF CROSS-SECTION TABLE,BELONGING TO EXCITATION         1260
C*****ENERGY FELD(4),THAT INFLUENCES ENERGY FIELD EZ(1)...EZ(KMAX)       1270
C*****HAS BEEN READ                                                     1280
      GO TO 54                                                          1290
 1000 WRITE(NA,111) J,FELD(4)                                           1300
  111 FORMAT(' J=',I6,'FELD=',G16.8)                                    1310
```

```
      RETURN 1                                                          1320
   54 IF(XLEV.LT.FELD(4)) IH=1                                          1330
      XLEVEL=FELD(4)                                                    1340
      IF(NENRE.EQ.2) GO TO 57                                           1350
C*****CUTTING ENDS OF ENERGY FIELD,IF EZ(1) OR EZ(KMAX) ARE CONTAINED   1360
C*****IN EZ(KMAX2).....EZ(KMAX1).                                       1370
      KMAX2=KMAX1                                                       1380
      KMAX1=KK                                                          1390
C     IF(EZ(KMAX1-1).EQ.EZ(KMAX)) GO TO 56                              1400
C     GO TO 59                                                          1410
C  56 KMAX1=KMAX1-1                                                     1420
C  59 IF(EZ(KMAX2+2).EQ.EZ(1)) GO TO 60                                 1430
C     GO TO 58                                                          1440
C  60 KMAX21=KMAX2+1                                                    1450
C     KMAX1=KMAX1-1                                                     1460
C     DO 61 IO=KMAX21,KMAX1                                             1470
C  61 EZ(IO)=EZ(IO+1)                                                   1480
   58 KMAX22=KMAX2+1                                                    1490
   57 NET=KMAX1-KMAX2                                                   1500
      RETURN                                                            1510
      END                                                               1520
```

```
C     XINPOL PERFORMS LINEAR INTERPOLATION OF THE EXCITATION             10
C     CROSS-SECTIONS OF EACH LEVEL IN THE ENERGY FIELD EZ.               20
C     SGIT - VALUES READ FROM KEDAK,SGP - INTERPOLATED VALUES.           30
      SUBROUTINE XINPOL(EZ,SGIT,SGP,NISG,NETACT,KMAX,KANF,KEND)          40
      REAL*8 NAM,EZ                                                      50
      DIMENSION EZ(NISG),SGIT(NETACT),SGP(KMAX)                          60
      COMMON NAM,ISTRUK,ISPA,NA,LIZ                                      70
C     WRITE(6,100)((J,EZ(KMAX+J),SGIT(J)),J=1,NETACT)                    80
C 100 FORMAT(2(' J=',I6,'EK=',G16.8,'SK=',G16.8))                        90
      DO 1 I=1,KMAX                                                     100
      DO 2 J=1,NETACT                                                   110
      JA=J                                                              120
      IF(EZ(KMAX+J).LT.EZ(I)) GO TO 2                                   130
      IF(EZ(KMAX+J).EQ.EZ(I)) GO TO 7                                   140
      IF(EZ(KMAX+J).GT.EZ(I).AND.J.EQ.1) GO TO 3                        150
      SGP(I)=FIPOLD(EZ(KMAX+J-1),EZ(I),EZ(KMAX+J),                      160
     1SGIT(J-1),SGIT(J))                                                170
C     SGP(I)=SGIT(J-1)+SNGL((EZ(I)-EZ(KMAX+J-1))/(EZ(KMAX+J)-EZ(KMAX+J-1  180
C    1))*(SGIT(J)-SGIT(J-1))                                             190
      GO TO 1                                                           200
    2 CONTINUE                                                          210
    3 SGP(I)=0.                                                         220
      GO TO 1                                                           230
    7 SGP(I)=SGIT(JA)                                                   240
    1 CONTINUE                                                          250
      KANF=1                                                            260
      KEND=KMAX                                                         270
      DO 4 K=1,KMAX                                                     280
      IF(SGP(K).EQ.0.) GO TO 5                                          290
      IF(K.EQ.1) GO TO 4                                                300
      IF(SGP(K-1).EQ.0.)KANF=K-1                                        310
      GO TO 4                                                           320
    5 IF(K.EQ.KANF) GO TO 6                                             330
      IF(K.LT.KMAX.AND.KEND.GT.K) KEND=K                                340
      GO TO 4                                                           350
    6 KANF=K+1                                                          360
    4 CONTINUE                                                          370
      IF(KANF.GT.KMAX) KANF=KMAX                                        380
C     WRITE(NA,121) KANF,KEND                                           390
C 121 FORMAT(' KANF=',I6,'KEND=',I6)                                    400
      KMAXX=ISG-KANF+1                                                  410
      DO 9 I=1,KMAX                                                     420
    9 SGP(I)=SGP(KANF+I-1)                                              430
C 120 FORMAT(3(' I=',I6,'EZ=',G14.8,'SGP=',G14.8))                      440
C     DO 8 I=1,KMAXX                                                    450
C   8 SGIT(I)=SGP(I)                                                    460
      RETURN                                                            470
      END                                                               480
```

```
      SUBROUTINE FLUMMI(A,B,EA,EB,E,EN,SGN,ECO,SCO,V,W,F,AR,FU,ABN,INT,   10
     1                  GR,FEKOE,EG,R,RSP,ESP,SPEK,SGNC,FEKC,ELSIG,       20
     2                  ELTOT,ET,ST,MAT,DAT,ALA,NLE,ISEL,NMAX,NX,NE27,    30
     3                  NSPEK,LSPEK,MAZ,NTK,KT,NTTT,NTTP,ICOS,ICOSP,      40
     4                  NECU,NECUP,ISM,ISMP,ISD,ISDP,ISCO,ISCOP,ISEC,     50
     5                  ISECP,KIM,NS,NK,AR,GE,SG,SGTOT)                   60
C                                                                        70
C                                                                        80
C************************************************************************ 90
C                                                                       100
C                    F L U M M I                                        110
C                                                                       120
C************************************************************************ 130
C                                                                       140
C                                                                       150
C*****ELASTISCHE STREUMATRIX BIS ZUR 5. ORDNUNG************************** 160
C*****UND TOTALE GRUPPENQUERSCHNITTE MIT MOMENTABHAENGIGER WICHTUNG      170
C                                                                       180
C                                                                       190
      REAL*8 STOFF,MAT                                                  200
      DIMENSION A(ISM),B(ISM),EA(ISM),EB(ISM),E(ISM),                   210
     1          EN(ISD),SGN(ISD),ECO(ISD),SCO(ISD),V(ISD),W(ISD),F(ISD),220
     2          AR(ICOS),FU(ICOS),                                      230
     3          ABN(NE27),INT(NE27),GR(NE27),FEKOE(NE27),               240
     4          EG(NX),R(NX),RSP(6,NX),                                 250
     5          ESP(NSPEK),SPEK(LSPEK),                                 260
     6          NST(6),LEG(6),MAZ(2),                                   270
     7          SGNC(ICOS,ISM),FEKO(ISM,NECU),ELSIG(6,NECU,NX),         280
     8          ELTOT(2,NX),                                            290
     9          MAT(KT),DAT(KT),                                        300
     A          ET(NTTT),ST(NTTT),                                      310
     B          GE(ISD),SG(ISD),SGTOT(6,NX)                             320
      COMMON STOFF,ISTRUK,ISPA,NOUT,KPR,IM,IL,KL                        330
```

```
C                                                                       340
      DATA NST/81,81,161,161,321,321/                                   350
C     NST(L)= ANZAHL DER AEQUIDISTANTEN STREUKOSINUSSTUETZPUNKTE DER    360
C             SGNC IM L-SYSTEM FUER DAS (L-1)-TE MOMENT                 370
      DATA LEG/2,1,3,4,5,6/                                             380
C     LEG   = REIHENFOLGE BEI DER MOMENTENBERECHNUNG                    390
C                                                                       400
      WRITE (NOUT ,9000)                                                410
 9000 FORMAT(1HO/1HO/' PROGRAMM KENNZIFFER 6')                          420
      WRITE (NOUT ,9001)                                                430
 9001 FORMAT(' PROGRAMM ZUR BERECHNUNG ELASTISCHER STREUMATRIZEN'/)      440
      CALL FSPIE                                                        450
C                                                                       460
C*****SETZEN INTERNER KONSTANTEN*************************************** 470
C     ISM   = ANZAHL DER ENERGIESTUETZPUNKTE PRO MAKROGRUPPE IM GROBNETZ 480
C     ISD   = MAXIMALE ANZAHL DER ENERGIESTUETZPUNKTE PRO MAKROGRUPPE   490
C             IM FEINNETZ                                               500
C     NK    = ANZAHL VON GRUNDPUNKTEN IM UEBERSTREUBEREICH              510
C     NR    = MAXIMALZAHL VON GRUNDPUNKTEN IM NICHT-UEBERSTREUBEREICH   520
C     NS    = MAXIMALE FEINGRUPPENZAHL PRO GROBGRUPPE                   530
      PP    = 1                                                         540
C     PP    = ANTEIL VON MUEL BEI DER KORREKTUR DES 1. MOMENTES         550
C     NECU  = MAXIMALE STREUBREITE                                      560
C     NMAX  = MAXIMALER LEGENDRE-APPROXIMATIONSGRAD                     570
C     NOUT  = UNIT-NUMMER DER AUSGABE-DATEI                             580
C     ICOS  = ANZAHL DER AEQUIDISTANTEN STREUKOSINUSSTUETZPUNKTE DER VON 590
C             KNOF GELESENEN DIFFERENTIELLEN STREUQUERSCHNITTE (SGNC)   600
      NF    = 10                                                        610
C     NF    = SPEICHEREINHEIT FUER ENERGIEDIFF. LEGENDRE-KOEFF.         620
C                                                                       630
C*****INITIALISIERUNG INTERNER GROESSEN******************************** 640
      NCT = 1                                                           650
      KIM = 0                                                           660
      NEN = 0                                                           670
      ITA = 0                                                           680
      ISC=1                                                             690
      NSTIS = NST(6)                                                    700
      NUEB = NECU                                                       710
      CO = 2./(ICOS-1)                                                  720
      NCS=0                                                             730
      NECUP=0                                                           740
      ISCP=0                                                            750
      ISMP=0                                                            760
      ICOSP=0                                                           770
      ISCOP=0                                                           780
      ISECP=0                                                           790
      NTTP=0                                                            800
      KSPE=1                                                            810
C                                                                       820
C*****LESEN DES ATOMGEWICHTES****************************************** 830
      CALL LOOKO(XMAT,MASSE,COM,&1001)                                  840
      ALFA = ((XMAT-1.)/(XMAT+1.))**2                                   850
C                                                                       860
C*****UMSORTIEREN DER GRUPPENGRENZEN*********************************** 870
      KSPEK=NSPEK                                                       880
      IF(NSPEK.GT.1)  GO TO 305                                         890
      KSPE=0                                                            900
      KSPEK=0                                                           910
  305 DO 302 I=1,NX                                                     920
      II=NX-I+1                                                         930
  302 ABN(I)=EG(II)                                                     940
C                                                                       950
      IF(ABN(NX)-1.E-3)301,303,304                                      960
  301 WRITE(NOUT,350)                                                   970
  350 FORMAT(//' ***ERROR 6.8 : THE SMALLEST GROUP BOUNDARY MUST BE GREA 980
     1TER THAN OR EQUAL TO 1.E-3')                                      990
      GO TO 8000                                                       1000
  304 NEGR=NE27                                                        1010
      ABN(NEGR)=AMAX1(1.E-3, .99*ABN(NX))                              1020
      GO TO 4                                                          1030
  303 NEGR=NX                                                          1040
C                                                                      1050
C*****BESTIMMUNG DER GRUPPENLETHARGIEN********************************* 1060
    4 NGR = NEGR-1                                                     1070
      ALFA = AMAX1(ALFA,ABN(NEGR)/ABN(1))                              1080
      ALLN = ALOG(ALFA)                                                1090
      CA = ABN(1)/ABN(2)                                               1100
      DO 5  I = 1,NGR                                                  1110
    5 R(I)=ALOG(ABN(I)/ABN(I+1))                                       1120
C                                                                      1130
C*****LESEN DER SGNC-ENERGIEN UND BESTIMMUNG DER STREUBREITE*********** 1140
      IF(MASSE.EQ.1)   GOTO 6                                          1150
      CALL LOOK3(NEN,EB,ISC,NGR,ABN,ISM,ISMP,GR,NEGR,ISEL,ISGNC)       1160
      IF(ISGNC.EQ.1)  GO TO 8000                                       1170
      CALL LOOK2(1,EB,ICOS,ICOSP,AR,ISM,SGNC)                          1180
      ES = EB(1)                                                       1190
      GOTO 7                                                           1200
    6 ES = ABN(1)                                                      1210
      I = 100*ALOG10(ABN(1)/ABN(NEGR))                                 1220
      NK = MAXO(I,NK)                                                  1230
    7 NUE=2                                                            1240
      DO 10  I = 2,NGR                                                 1250
      AM = ALFA*ABN(I)                                                 1260
      IP = I+1                                                         1270
      DO 9  II = IP,NEGR                                               1280
      IF(ABN(II).LE.AM)   GOTO 10                                      1290
    9 CONTINUE                                                         1300
      II = NEGR                                                        1310
   10 NUE = MAXO(NUE,II-I+1)                                           1320
      IF(NUE.LE.NUEB)   GOTO 8                                         1330
      NECUP=NUE-NUEB                                                   1340
    8 NUEB = NUE                                                       1350
      ISCOP=NUEB*ISC-ISCO                                              1360
      IF(ISCOP.LT.0)  ISCOP=0                                          1370
      ISECP=ISD-ISEC                                                   1380
      IF(ISECP.LT.0)  ISECP=0                                          1390
      IF(ISMP+ICOSP+NECUP+ISCOP+ISECP.GT.0)   RETURN                   1400
C                                                                      1410
C*****BESTIMMUNG DER MAKROGRUPPENEINTEILUNG***************************** 1420
   12 KIM = MINO(NGR-IM,NUEB-1)                                        1430
      IM = IM+KIM                                                      1440
```

```
      CALL MAKRO(ALFA,ALLN,ISC,IL,IM,NGR,ABN,R,ISO,ISM,ISCP,NS,NK,NR,     1440
     -           NEN,NECU,NUEB,V,W,F,ELTOT,INTT,INT,NEGR,KSPE,NSPEK,     1450
     -           ESP,NTK,KT,MAT,NTTT,NTTP,NF,ISEL,ISCT)                  1460
       IF(ISGT.EQ.1)  GO TO 8000                                         1470
       IF(ISOP+NTTP.GT.0)   RETURN                                       1480
C                                                                        1490
   13  NEK = NEN                                                         1500
       IF(NEN.EQ.0)   GOTO 16                                            1510
       IF(EB(NEN).GE.ABN(IL))   GOTO 16                                  1520
       WRITE(NOUT,913)   STOFF,EB(NEN)                                   1530
       STOP                                                              1540
   16  CONTINUE                                                          1550
C                                                                        1560
C                                                                        1570
C***** M A K R O G R U P P E N R E C H N U N G ************************** 1580
C                                                                        1590
       IR = 1                                                            1600
   20  NANF = INT(IR)+1                                                  1610
       IF(IR.EQ.1)   NANF = NANF-1                                       1620
       NEND = INT(IR+1)                                                  1630
       NEN = NEK                                                         1640
       ISCT = 1                                                          1650
C                                                                        1660
C**** BESTIMMUNG DES EINSTREUINTERVALLES********************************* 1670
       EANF = ABN(NENO+1)                                                1680
   22  EEND=ABN(NANF)                                                    1690
       IF(MASSE.GT.1)   GOTO 28                                          1700
       NEN = 1                                                           1710
       EA(1) = ABN(IL)                                                   1720
   28  IF(MASSE.EQ.1)   GOTO 62                                          1730
       DO 60  NE = 1,NEN                                                 1740
   60  EA(NE) = EB(NE)                                                   1750
   62  CONTINUE                                                          1760
C                                                                        1770
C*****MAKROSKOPISCHER TOTALER QUERSCHNITT FUER FEINSTRUKTURWICHTUNG***** 1780
       NTT=1                                                             1790
       IF(NTK.EQ.1) CALL MIXSGT(KT,MAT,DAT,NTTT,NTTP,NTT,ET,ST,EANF,EEND, 1800
      1ISGT)                                                             1810
       IF(ISGT.EQ.1)  GO TO 8000                                         1820
       IF(NTTP.GT.0)  RETURN                                             1830
C                                                                        1840

C*****EINORDNEN DES AUSSTREUINTERVALLES UND LESEN DER SGNC************** 1850
       IF(EA(1).GE.EEND)   GOTO 88                                       1860
       DO 64  NE = 1,NEN                                                 1870
       NI = NE                                                           1880
       IF(EA(NE).GE.EANF)  GOTO 66                                       1890
   64  CONTINUE                                                          1900
   66  DO 68  NE = 1,NEN                                                1910
       NO = NEN-NE+1                                                     1920
       IF(EA(NO).LE.EEND)  GOTO 70                                       1930
   68  CONTINUE                                                          1940
C                                                                        1950
   70  IF(NI.EQ.1)   GOTO 78                                             1960
       NO=MINO(NO+2,NEN)                                                 1970
       NI=MAXO(NI-2,1)                                                   1980
       NEN = NO-NI+1                                                     1990
       DO 74  NE = NI,NO                                                 2000
   74  A(NE) = EA(NE)                                                    2010
       DO 76  NE = 1,NEN                                                 2020
   76  EA(NE) = A(NE+NI-1)                                               2030
       CALL LOOK2(NEN,EA,ICOS,ICOSP,AR,ISM,SGNC)                         2040
       IF(ICOSP.NE.0)   RETURN                                           2050
       IF(EA(NEN).GE.EEND)   GOTO 100                                    2060
       NEN = NEN+1                                                       2070
       EA(NEN) = EEND                                                    2080
       DO 77  IP = 1,ICOS                                                2090
   77  SGNC(IP,NEN) = SGNC(IP,NEN-1)                                     2100
       GOTO 100                                                          2110
C                                                                        2120
   78  NEN=MINO(NO+2,NEN)                                                2130
       CALL LOOK2(NEN,EA,ICOS,ICOSP,AR,ISM,SGNC)                         2140
       IF(ICOSP.NE.0)   RETURN                                           2150
       IF(ES.LE.EANF)  GO TO 100                                         2160
       DO 84  NE = 1,NEN                                                 2170
       NA = NEN-NE+1                                                     2180
       NU = NEN-NE+2                                                     2190
       EA(NU) = EA(NA)                                                   2200
       DO 84  IP = 1,ICOS                                                2210
   84  SGNC(IP,NU) = SGNC(IP,NA)                                         2220
       EA(1) = EANF                                                      2230
       NEN = NEN+1                                                       2240
       DO 86  IP = 1,ICOS                                                2250
   86  SGNC(IP,1) = 0.7957747E-01                                        2260
       GOTO 100                                                          2270
C                                                                        2280
C*****KOSINUS UND ENERGIEN BEI ISOTROPIE IM CM-SYSTEM******************** 2290
   88  DO 90  IP = 1,ICOS                                               2300
   90  AR(IP) = (IP-1)*CO-1.                                             2310
       NEN = 0                                                           2320
       CALL PUNK(NGR,NEGR,ABN,NANF,NEND,NEN,ALFA,NK,NR,                  2330
     -           ISM,ISMP,ISN,E,R,ALLN)                                  2340
       IF(ISMP.GT.0)   RETURN                                            2350
       ISCT = 0                                                          2360
       GOTO 115                                                          2370
C                                                                        2380
C*****TRANSFORMATION DER SGNC******************************************* 2390
  100  A1 = ABS(AR(1)+1.)                                                2400
       A2 = ABS(AR(ICOS)-1.)                                             2410
       IF(A1.LT.1.E-5.AND.A2.LT.1.E-5)   GOTO 102                        2420
  101  WRITE(NOUT,920)   (AR(IP),IP=1,ICOS)                              2430
       GOTO 8000                                                         2440
  102  DO 103   IP = 2,ICOS                                             2450
       IF(AR(IP).LE.AR(IP-1))  GO TO 101                                 2460
  103  CONTINUE                                                          2470
       CALL TRAFO(ICOS,NEN,ISM,SGNC,XMAT,ALFA,AR)                        2480
C                                                                        2490
C*****ENERGIEINTERPOLATION DER SGNC************************************* 2500
       CALL PUNK(NGR,NEGR,ABN,NANF,NEND,NEN,ALFA,NK,NR,                  2510
     -           ISM,ISMP,ISN,E,R,ALLN)                                  2520
       IF(ISMP.GT.0)   RETURN                                            2530
```

```
      CALL PUSUM(ISM,NEN,EA,ISN,E,V)                                    2540
      NU=0                                                              2550
      NC=0                                                              2560
  104 IF(E(NU+1).GE.EANF)  GO TO 106                                    2570
      NU=NU+1                                                           2580
      GO TO 104                                                         2590
  106 IF(E(ISN-NO).LE.EEND)  GO TO 108                                  2600
      NC=NO+1                                                           2610
      GO TO 106                                                         2620
  108 ISK=ISN-NU-NO                                                     2630
      DO 111  IP = 1,ICOS                                               2640
      DO 110  NE = 1,NEN                                                2650
  110 B(NE) = SGNC(IP,NE)                                               2660
      CALL IPOLA(NEN,EA,B,ISN,E,A,F)                                    2670
      DO 111 NE=1,ISK                                                   2680
      NC=NE+NU                                                          2690
      IF(E(NO).LE.ES)  A(NO)=A(1)                                       2700
  111 SGNC(IP,NE)=A(NO)                                                 2710
      DO 113 NE=1,ISK                                                   2720
  113 E(NE)=E(NE+NU)                                                    2730
      ISK = ISK                                                         2740
C                                                                       2750
C*****ENERGIEDIFFERENTIELLE LEGENDRE-KOEFFIZIENTEN ********************* 2760
  115 CALL LECAL (MASSE,XMAT,ALFA,ISOT,LEG,NLE,NANF,NEND,NUEB,IL,IM,    2770
     1            NEGR,ABN,ICOS,AR,ISN,E,SGNC,NST,NSTIS,ISM,ISD,NECU,    2780
     2            ITA,NF,GR,FEKOE,FU,A,ECO,SCO,V,W,F,FEKO)               2790
C                                                                       2800
C*****LESEN DER SGT, SGN UND MUEL******************************************2810
      IF(IABS(ISEL).EQ.1.AND.ISOT.EQ.0)   GOTO 120                      2820
      CALL LOOK1(ISC,M,ECO,SCC,EANF,EEND,1,ISGT)                        2830
      IF(ISGT.EQ.1)  GO TO 8000                                         2840
      AM = ECO(M)                                                       2850
      IF(M.LT.ISD)   GOTO 117                                           2860
  116 ISDP = ISD*(ALOG(EEND/AM)/ALOG(AM/EANF))                          2870
      RETURN                                                            2880
  117 IF(MASSE.GT.1.OR.EANF.GT.10.)   GOTO 119                          2890
      DO 118  J = 1,M                                                   2900
      IF(ECO(J).GT.10.)    GOTO 119                                     2910
  118 SCO(J) = .6667                                                    2920
  119 CALL LOOK1(ISC,K,EN,SGN,EANF,EEND,0,ISGT)                         2930
      IF(ISGT.EQ.1)  GO TO 8000                                         2940
      IF(NGT.EQ.0)   GOTO 130                                           2950
      CALL LOOK1(ISD,NGG,GE,SG,EANF,EEND,2,ISGT)                        2960
      IF(ISGT.EQ.1)  GO TO 8000                                         2970
      AM = GE(NGG)                                                      2980
      IF(NGG.GE.ISD)   GOTO 116                                         2990
      GOTO 130                                                          3000
C                                                                       3010
  120 IF(NGT.EQ.0)   GOTO 122                                           3020
      NGG = 2                                                           3030
      GE(1) = EANF                                                      3040
      GE(2) = EEND                                                      3050
      SG(1) = 1.                                                        3060
      SG(2) = 1.                                                        3070
  122 K = 2                                                             3080
      EN(1) = EANF                                                      3090
      EN(2) = EEND                                                      3100
      SGN(1) = 1.                                                       3110
      SGN(2) = 1.                                                       3120
      M=2                                                               3130
      ECO(1)=EANF                                                       3140
      ECO(2)=EEND                                                       3150
      SCO(1)=COM                                                        3160
      SCO(2)=COM                                                        3170
      IF(NGS.EQ.0)   NGS=NANF                                           3180
C                                                                       3190
C*****MULTIGRUPPEN-ENERGIEINTEGRATION*********************************** 3200
  130 CALL GRUPIN (MASSE,XMAT,ALFA,COM,ISOT,PM,LEG,NLE,NANF,NEND,NUEB,   3210
     1             IL,IM,NGR,NEGR,ABN,ISN,E,K,EN,SGN,M,ECO,SCO,NTT,ET,   3220
     2             ST,MAT,KSPE,KSPEK,FSP,SPEK,NSPEK,LSPEK,ISM,ISC,       3230
     3             NECU,ISCO,ISEC,NF,F,A,GR,SGNC,FEKO,V,W,ISTT,RSP,      3240
     4             ELSIG,NGT,NGG,GE,SG,SGTOT)                            3250
C                                                                       3260
C*****ALSGABE VON INFORMATIONEN***************************************** 3270
      IF(ISEL.LT.0)   CALL INFORM(ALFA,NEGR,ABN,R,IL,IM,INTT,INT,       3280
     1                            NST,NSTIS,IR,ISTT,K,NTK,NTT,NOUT)     3290
C                                                                       3300
      IF(IR+1.GE.INTT)   GOTO 290                                       3310
      IR = IR+1                                                         3320
      GOTO 20                                                           3330
C                                                                       3340
C*****MULTIGRUPPENKONSTANTEN******************************************** 3350
  290 CALL MUKON(ELSIG,ELTOT,NLE,NECU,NUEB,IL,IM,NGR,MASSE)             3360
C                                                                       3370
C*****AUSDRUCKEN DER ERGEBNISSE***************************************** 3380
      IM = IM-KIM                                                       3390
  300 CALL PRINT(ELSIG,ELTOT,ALA,NLE,NECU,NUEB,ISEL,NGR,KSPE,MAT,NTK,   3400
     -           KIM,NGT,SGTOT,RSP,MASSE,NGS)                           3410
      GO TO 8000                                                        3420
C                                                                       3430
 1001 WRITE (NOUT,1002) STOFF                                           3440
 8000 KL = KL+1                                                         3450
      RETURN                                                            3460
C                                                                       3470
C                                                                       3480
  909 FORMAT(1HO)                                                       3490
  913 FORMAT(//' ***ERROR 6.1 : FOR  ',A8,' SCATTERING MATRICES CANNOT B 3500
     1E CALCULATED'/16X'FOR ENERGIES ABOVE ',1PE10.3,' EV FOR LACK OF SGN 3510
     2C ON KEDAK')                                                      3520
  920 FORMAT(//' ***ERROR 6.8  :  THE FOLLOWING SGNC-COSINE-MESH FOUND C 3530
     -N KEDAK CANNOT BE USED'//(10E12.3))                               3540
 1002 FORMAT(//' ***ERROR 6.7 : FOR  ',A8,' SCATTERING MATRICES CANNOT B 3550
     1E CALCULATED FOR'/16X,'LACK OF ISOTI (ATOMIC WEIGHT) ON KEDAK')   3560
C                                                                       3570
      END                                                               3580
```

```
      SUBROUTINE SUM(M,A,S)                                              10
C                                                                        20
C*****SUMMATION*****************************************************   30
C                                                                        40
      REAL*8  SP,SN                                                      50
      DIMENSION  A(M)                                                    60
C                                                                        70
      IF(M.LE.2)   GOTO 13                                               80
C*****SORTIEREN*****************************************************   90
      N = 1                                                             100
      IA = 2                                                            110
      KK = 0                                                            120
    1 K = 0                                                             130
      DO 2  I = IA,M,2                                                  140
      IB = I-1                                                          150
      IF(A(IB).LE.A(I))   GOTO 2                                        160
      B = A(I)                                                          170
      A(I) = A(IB)                                                      180
      A(IB) = B                                                         190
      K = 1                                                             200
    2 CONTINUE                                                          210
      N = -N                                                            220
      IA = IA-N                                                         230
      IF(K.EQ.1)   GOTO 1                                               240
      IF(KK.EQ.1)   GOTO 3                                              250
      KK = 1                                                            260
      GOTO 1                                                            270
C                                                                       280
C*****SUMMIEREN*****************************************************   290
    3 SP = 0.                                                           300
      SN = 0.                                                           310
      IF(A(1).GE.0.)   GOTO 8                                           320
      IF(A(M).LE.0.)   GOTO 10                                          330
      DO 4  I = 2,M                                                     340
      IF((A(I-1).LE.0.).AND.(A(I).GE.0.))   GOTO 5                      350
    4 CONTINUE                                                          360
    5 IA = I                                                            370
      IB = I-1                                                          380
      DO 6  I = IA,M                                                    390
    6 SP = SP+DBLE(A(I))                                                400
      DO 7  I = 1,IB                                                    410
    7 SN = SN+DBLE(A(IA-I))                                             420
      GOTO 12                                                           430
    8 DO 9  I = 1,M                                                     440
    9 SP = SP+DBLE(A(I))                                                450
      GOTO 12                                                           460
   10 MP = M+1                                                          470
      DO 11  I = 1,M                                                    480
   11 SN = SN+DBLE(A(MP-I))                                             490
   12 S = SNGL(SN+SP)                                                   500
      RETURN                                                            510
   13 S = A(1)                                                          520
      IF(M.EQ.2)   S = S+A(2)                                           530
      RETURN                                                            540
C                                                                       550
      END                                                               560
```

```
      SUBROUTINE IPOLA(M,A,B,N,X,Y,T)                                    10
C                                                                        20
C     KUBISCH-QUADRATISCH-LINEARE INTERPOLATION                          30
C     UNTER VERMEIDUNG ZUSAETZLICHER EXREMWERTE                          40
C                                                                        50
      DIMENSION  A(M),B(M),T(M),X(N),Y(N)                                60
C                                                                        70
C     TANGENTEN                                                          80
      T(1) = (B(2)-B(1))/(A(2)-A(1))                                     90
      T(M) = (B(M)-B(M-1))/(A(M)-A(M-1))                                100
      MN = M-1                                                          110
      DO 2  J = 2,MN                                                    120
      JP = J+1                                                          130
      JM = J-1                                                          140
      T(J) = 0.                                                         150
      IF(B(JP).GT.B(J).AND.B(J).GT.B(JM))                               160
     -T(J) = (B(JP)-B(JM))/(A(JP)-A(JM))                                170
      IF(B(JP).LT.B(J).AND.B(J).LT.B(JM))                               180
     -T(J) = (B(JP)-B(JM))/(A(JP)-A(JM))                                190
    2 CONTINUE                                                          200
C                                                                       210
C     INTERPOLATION                                                     220
      Y(1) = B(1)                                                       230
      Y(N) = B(M)                                                       240
      NM = N-1                                                          250
      J = 1                                                             260
      DO 16  I = 2,NM                                                   270
    4 IF(X(I)-A(J))   6,8,10                                            280
    6 S = X(I)-A(K)                                                     290
      Y(I) = A0+(A1+(A2+A3*S)*S)*S                                      300
      GOTO 16                                                           310
    8 Y(I) = B(J)                                                       320
      GOTO 16                                                           330
   10 K = J                                                             340
      J = J+1                                                           350
      U = A(J)-A(K)                                                     360
      V = B(J)-B(K)                                                     370
      R = V-T(K)*U                                                      380
      W = U*(T(J)-T(K))                                                 390
      A0 = B(K)                                                         400
      A1 = T(K)                                                         410
      A2 = (3*R-W)/(U*U)                                                420
      A3 = (W-2*R)/(U*U*U)                                              430
      IF(T(K).EQ.0..AND.T(J).EQ.0.)   GOTO 4                            440
      IF(ABS(A3).LT.1.E-30)   GOTO 4                                    450
      XW = -A2/(3*A3)                                                   460
      IF(XW.LE.0..OR.XW.GE.U)   GOTO 4                                  470
      A3 = 0.                                                           480
      IF(T(J).EQ.0.)   GOTO 12                                          490
      IF(T(K).EQ.0.)   GOTO 14                                          500
      A2 = R/(U*U)                                                      510
```

```
      T(J) = 2*V/U-T(K)                                                 520
      IF(ABS(A2).LT.1.E-30)   GOTO 4                                    530
      XW = -A1/(2*A2)                                                   540
      IF(XW.LE.0..OR.XW.GE.U)   GOTO 4                                  550
      A1 = V/U                                                          560
      A2 = 0.                                                           570
      T(J) = A1                                                         580
      GOTO 4                                                            590
   12 A1 = 2*V/U                                                        600
      A2 = -V/(U*U)                                                     610
      GOTO 4                                                            620
   14 A1 = 0.                                                           630
      A2 = V/(U*U)                                                      640
      GOTO 4                                                            650
   16 CONTINUE                                                          660
      RETURN                                                            670
C                                                                       680
      END                                                               690
```

```
      SUBROUTINE PUSUM(ISD,KA,A,KE,E,B)                                  10
C                                                                        20
C*****STUETZPUNKTMENGEN VEREINIGEN*****************************************30
C                                                                        40
      DIMENSION  A(ISD),E(ISD),B(ISD)                                    50
C                                                                        60
      DO 2  K = 1,KE                                                     70
    2 B(K) = E(K)                                                        80
C                                                                        90
      J=1                                                               100
      I=1                                                               110
      K=1                                                               120
    3 IF(J.GT.ISD)   GOTO 18                                            130
      IF(K.GT.KA)   GOTO 10                                             140
      IF(I.GT.KE)   GOTO 14                                             150
      IF(A(K)-B(I))   4,5,6                                             160
    4 E(J) = A(K)                                                       170
      J = J+1                                                           180
      K = K+1                                                           190
      GOTO 3                                                            200
    5 E(J) = A(K)                                                       210
      J = J+1                                                           220
      I = I+1                                                           230
      K = K+1                                                           240
      GOTO 3                                                            250
    6 E(J) = B(I)                                                       260
      J = J+1                                                           270
      I = I+1                                                           280
      GOTO 3                                                            290
   10 IF(I.GT.KE)  GO TO 18                                             300
      DO 12 K=I,KE                                                      310
      E(J)=B(K)                                                         320
      J = J+1                                                           330
      IF(J.GT.ISD)   GOTO 18                                            340
   12 CONTINUE                                                          350
      GO TO 18                                                          360
   14 DO 16 I=K,KA                                                      370
      E(J)=A(I)                                                         380
      J = J+1                                                           390
      IF(J.GT.ISD)   GOTO 18                                            400
   16 CONTINUE                                                          410
   18 KE=J-1                                                            420
      RETURN                                                            430
C                                                                       440
      END                                                               450
```

```
      SUBROUTINE MAKRO(ALFA,ALLN,ISD,IL,IM,NGR,ABN,R,ISD,ISM,ISDP,NS,NK,  10
     -                 NR,NEN,NECU,NUEB,V,W,F,LST,INTT,INT,NEGR,          20
     -                 KSPE,NSPEK,ESP,NTK,KT,MAT,NTT1,NTTP,NF,ISEL,ISGT)  30
C                                                                        40
C*****BESTIMMUNG EINER DEN QUERSCHNITTS- UND SPEKTRUMSSTUETZSTELLEN UND  50
C     DER ANZAHL DER GRUNDPUNKTE ANGEPASSTEN MAKROGRUPPEN-EINTEILUNG     60
C                                                                        70
      REAL*8  STOFF,MAT,STM                                              80
      REAL URAN/'U 23'/                                                  90
      DIMENSION  ABN(NEGR),R(NGR), INT(NEGR),LST(2,NGR),V(ISD),W(ISD),  100
     -           F(ISD),ESP(NSPEK),MAT(KT)                              110
      COMMON STOFF,ISTRUK,ISPA,NOUT                                     120
C                                                                       130
C*****ANZAHL DER SGT-STUETZSTELLEN (MISCHUNG) PRO GRUPPE **************  140
      DO 2  N = IL,IM                                                   150
    2 LST(1,N) = 0                                                      160
      IF(NTK.GT.1)   GOTO 46                                            170
      IF(NTK.EQ.0)   GOTO 24                                            180
      DO 4  K = 1,KT                                                    190
      A = MAT(K)                                                        200
      IF(A.NE.URAN)   GOTO 4                                            210
      STM = MAT(K)                                                      220
      MAT(K) = MAT(1)                                                   230
      MAT(1) = STM                                                      240
    4 CONTINUE                                                          250
      STM = STOFF                                                       260
      EA = ABN(IM+1)                                                    270
      EE = ABN(IL)                                                      280
    6 STOFF = MAT(1)                                                    290
      CALL LOOK1(ISD,K,V,W,EA,EE,2,ISGT)                                300
      IF(ISGT.EQ.1)   RETURN                                            310
      V(1) = EA                                                         320
      IF(KT.EQ.1)   GOTO 10                                             330
      DO 8  MM = 2,KT                                                   340
      STOFF = MAT(MM)                                                   350
      CALL LOOK1(ISD,I,F,W,EA,V(K),2,ISGT)                              360
      IF(ISGT.EQ.1)   RETURN                                            370
      F(1) = EA                                                         380
      CALL PUSUM(ISD,I,F,K,V,W)                                         390
```

```
    8 CONTINUE                                                          400
   10 NN = IM-IL+1                                                      410
      K1 = 1                                                            420
      DO 16  N = 1,NN                                                   430
      I = IM-N+1                                                        440
      A = ABN(I)                                                        450
      DO 12  MM = K1,K                                                  460
      IF(V(MM).GE.A)   GOTO 14                                          470

   12 CONTINUE                                                          480
      MM = K+1                                                          490
   14 LST(1,I) = LST(1,I)+MM-K1                                         500
      K1 = MM                                                           510
      IF(K1.GT.K)   GOTO 18                                             520
   16 CONTINUE                                                          530
   18 IF(K.LT.ISD)   GOTO 20                                            540
      EA = V(K)                                                         550
      GOTO 6                                                            560
   20 STOFF = STM                                                       570
      IF(ISEL.LT.0)   WRITE(NOUT,110)                                   580
      DO 22  N = IL,IM                                                  590
      LST(1,N) = LST(1,N)+3                                             600
      IF(ISEL.LT.0)   WRITE(NOUT,102)   N,LST(1,N)                      610
   22 NTTP = MAXO(NTTP,LST(1,N)-NTTT)                                   620
   24 CONTINUE                                                          630
C                                                                       640
C*****ANZAHL SGN-,MUEL-,SGT- UND MAKROWICHTUNGSSPEKTRUM-STUETZSTELLEN   650
C      PRO GRUPPE                                                       660
      IMM = IM                                                          670
      IF(IABS(ISEL).EQ.1)   IMM = MINO(IM,ISC-1)                        680
      DO 26  N = IL,IM                                                  690
   26 LST(2,N) = 2                                                      700
      IF(IMM.LT.IL)   GOTO 44                                           710
      EA = ABN(IMM+1)                                                   720
      EE = ABN(IL)                                                      730
   28 CALL LOOK1(ISD,K,V,W,EA,EE,0,ISGT)                                740
      IF(ISGT.EQ.1)   RETURN                                            750
      V(1) = EA                                                         760
      CALL LOOK1(ISD,I,F,W,EA,V(K),1,ISGT)                              770
      IF(ISGT.EQ.1)   RETURN                                            780
      F(1) = EA                                                         790
      CALL PUSUM(ISD,K,V,I,F,W)                                         800
      CALL LOOK1(ISC,K,V,W,EA,F(I),2,ISGT)                              810
      IF(ISGT.EQ.1)   RETURN                                            820
      V(1) = EA                                                         830
      CALL PUSUM(ISD,I,F,K,V,W)                                         840
      NN = IMM-IL+1                                                     850
      K1 = 1                                                            860
      DO 34  N = 1,NN                                                   870
      I = IMM-N+1                                                       880
      A = ABN(I)                                                        890
      DO 30  MM = K1,K                                                  900
      IF(V(MM).GE.A)   GOTO 32                                          910
   30 CONTINUE                                                          920
      MM = K                                                            930
   32 LST(2,I) = LST(2,I)+MM-K1                                         940
      K1 = MM+1                                                         950
      IF(K1.GT.K)   GOTO 36                                             960
   34 CONTINUE                                                          970
   36 IF(K.LT.ISD)   GOTO 38                                            980
      EA = V(K)                                                         990
      GOTO 28                                                          1000
   38 IF(ISEL.LT.0)   WRITE(NOUT,100)                                  1010
      ISDP = 0                                                         1020
      DO 42  N = IL,IMM                                                1030
      LST(2,N) = LST(2,N)-2                                            1040
      IF(ISEL.LT.0.AND.LST(2,N).NE.0)   WRITE(NOUT,102)   N,LST(2,N)   1050
      IF(KSPE.EQ.0)   GOTO 42                                          1060
      A = ABN(N+1)                                                     1070
      B = ABN(N)                                                       1080
      DO 40  MM = 1,NSPEK                                              1090
      IF(A.LT.ESP(MM).AND.ESP(MM).LT.B)   LST(2,N) = LST(2,N)+1        1100
   40 CONTINUE                                                         1110
   42 ISDP = MAXO(ISDP,ISM+LST(2,N)-ISC)                               1120
C                                                                      1130
   44 IF(NTTP+ISDP.EQ.0)   GOTO 48                                     1140
      NTK = IABS(NTK)+2                                                1150
      WRITE(NF)   ((LST(N,K),K=IL,IM),N=1,2)                           1160
      REWIND NF                                                        1170
      RETURN                                                           1180
   46 READ(NF)   ((LST(N,K),K=IL,IM),N=1,2)                            1190
      NTK = NTK-2                                                      1200
      REWIND NF                                                        1210
C                                                                      1220
C*****MAKROGRUPPENEINTEILUNG*************************************     1230
   48 IT = ISD                                                         1240
      ID = ISD-ISM                                                     1250
      INT(1) = IL-1                                                    1260
      IR = 2                                                           1270
   50 II = INT(IR-1)+1                                                 1280
      IW = 0                                                           1290
      IS = 0                                                           1300
      JS = 0                                                           1310
      DO 52  I = II,IM                                                 1320
      IW = IW+LST(1,I)                                                 1330
      IS = IS+LST(2,I)                                                 1340
      J = NK+NR                                                        1350
      A = -R(I)/ALLN                                                   1360
      IF(A.LT.1.)   J = A*NK                                           1370
      JS = JS+J                                                        1380
      IF(IS.GE.ID.OR.JS.GE.ISM-NEN.OR.I+1-II.GT.NS.OR.IW.GT.NTTT)GOTO 56 1390
      IF(I.NE.IT)   GOTO 52                                            1400
      IF(I.EQ.IM.OR.I.EQ.II)   GOTO 52                                 1410
      IT = 0                                                           1420
      GOTO 56                                                          1430
   52 CONTINUE                                                         1440
      INT(IR) = IM                                                     1450
   54 INT(1) = IL                                                      1460
      INTT = IR                                                        1470
      IE = IR-1                                                        1480
      GOTO 58                                                          1490
```

```
   56 INT(IR) = MAXO(II,I-1)                                          1500
      IF(INT(IR).EQ.IM)   GOTO 54                                     1510
      IR = IR+1                                                       1520
      GOTO 50                                                         1530
C                                                                     1540
C*****SCHREIBEN DER MAKROGRUPPENEINTEILUNG*************************** 1550

   58 IF(ISEL.GT.0)   RETURN                                          1560
      WRITE(NOUT,94)                                                  1570
      DO 60  I = 1,IE                                                 1580
      IP = INT(I)+1                                                   1590
      IF(I.EQ.1)   IP = IP-1                                          1600
   60 WRITE(NOUT,96)   I,IP,INT(I+1)                                  1610
C                                                                     1620
      RETURN                                                          1630
C                                                                     1640
   94 FORMAT(///11X,'M A K R O G R U P P E N'//)                      1650
   96 FORMAT(1HO,2X,I2,'. MAKROGRUPPE',5X,I3,'. BIS ',I3,'. FEINGRUPPE') 1660
  100 FORMAT(///5X,'STUETZSTELLEN FUER SGN, MUEL, SGT UND MAKROSPEKTRUM' 1670
     -//10X,'GRUPPE',11X,'ANZAHL'/)                                   1680
  102 FORMAT(9X,I6,11X,I6)                                            1690
  110 FORMAT(///5X,'STUETZSTELLEN FUER SGT (MISCHUNG FEINSTRUKTURWICHTUN 1700
     -G)'//10X,'GRUPPE',11X,'ANZAHL'/)                                1710
C                                                                     1720
      END                                                             1730
```

```
      SUBROUTINE MIXSGT(KT,MAT,DAT,NTT,NTP,NT,ET,ST,EA,EE,ISGT)        10
C                                                                      20
C*****TOTALER QUERSCHNITT EINER MISCHUNG*************************      30
C                                                                      40
      REAL*8  MAT(KT),A(5),STOFF                                       50
      DIMENSION  DAT(KT),ET(NTT),ST(NTT),NW(4),NAD(2)                  60
      COMMON STOFF,ISTRUK,ISPA,NOUT                                    70
      DATA NW(1),A(2),A(3) /3,'BEST ','SGT  '/                         80
C                                                                      90
      ISGT=0                                                          100
      DO 10  K = 1,KT                                                 110
      D = DAT(K)                                                      120
      A(1) = MAT(K)                                                   130
      NU = 0                                                          140
      CALL NDFLOC(KP,NW,A,NAD,KC)                                     150
      IF(KP.NE.1)   GOTO 12                                           160
      E = A(4)                                                        170
      S = A(5)                                                        180
      IF(E-EA)   6,4,14                                               190
    4 CALL ADD(K,NTT,NTP,NT,ET,ST,NU,D,E,S,EV,SV,EW,SW,EA,EE)         200
      IF(NTP.GT.0)   RETURN                                           210
    6 EV = E                                                          220
      SV = S                                                          230
      CALL NDFNXT(KP,NW,A,NAD,KC)                                     240
      IF(KP.EQ.1)   GOTO 7                                            250
      E = EE                                                          260
      S = SV                                                          270
      GOTO 8                                                          280
    7 E = A(4)                                                        290
      S = A(5)                                                        300
      IF(E-EA)   6,4,8                                                310
    8 CALL ADD(K,NTT,NTP,NT,ET,ST,NU,D,E,S,EV,SV,EW,SW,EA,EE)         320
      IF(NTP.GT.0)   RETURN                                           330
      IF(E.LT.EE)   GOTO 6                                            340
   10 CONTINUE                                                        350
      RETURN                                                          360
C                                                                     370
   12 WRITE(NOUT,20)   MAT(K)                                         380
      ISGT=1                                                          390
      RETURN                                                          400
   14 WRITE(NOUT,22)   MAT(K),EA                                      410
      ISGT=1                                                          420
      RETURN                                                          430
C                                                                     440
   20 FORMAT(//' ***ERROR 6.5 : FOR  ',A8,' IN THE FINE-STRUCTURE MIXTUR 450
     1E NO SGT'/16X,'ARE ON KEDAK')                                   460
   22 FORMAT(//' ***ERROR 6.6 : FOR  ',A8,' IN THE FINE-STRUCTURE MIXTUR 470
     1E NO SGT'/16X,'ARE ON KEDAK FOR ENERGIES BELOW',1PE10.3,' EV')   480
C                                                                     490
      END                                                             500
```

```
      SUBROUTINE ADD(K,NTT,NTP,NT,ET,ST,NU,D,E,S,EV,SV,EW,SW,EA,EE)    10
C                                                                      20
      DIMENSION  ET(NTT),ST(NTT)                                       30
C                                                                      40
C*****ERSTES MATERIAL*********************************************     50
      IF(K.GT.1)   GOTO 10                                             60
      IF(NU.GT.0)   GOTO 6                                             70
      IF(E.GT.EA)   GOTO 2                                             80
      ET(1) = E                                                        90
      ST(1) = S*D                                                     100
      GOTO 4                                                          110
    2 T = (S-SV)/(E-EV)                                               120
      ET(1) = EA                                                      130
      ST(1) = D*(S+T*(EA-E))                                          140
    4 NU = 1                                                          150

      NT = 1                                                          160
      IF(E.LT.EE)   RETURN                                            170
      ET(2) = EE                                                      180
      ST(2) = D*(S+T*(EE-E))                                          190
      NU = 2                                                          200
      NT = 2                                                          210
      RETURN                                                          220
    6 NU = NU+1                                                       230
      NT = NT+1                                                       240
      IF(NT.GT.NTT)   GOTO 22                                         250
      IF(E.LE.EE)   GOTO 8                                            260
      ET(NU) = EE                                                     270
      ST(NU) = ST(NU-1)                                               280
```

```
      RETURN                                                            250
    8 ET(NU) = E                                                        260
      ST(NU) = S*D                                                      270
      RETURN                                                            280
C                                                                       290
C*****WEITERE MATERIALIEN*************************************************300
   10 IF(NU.GT.0)   GOTO 12                                             310
      EW = ET(1)                                                        320
      SW = ST(1)                                                        330
      IF(E.GT.EA)   GOTO 12                                             340
      ST(1) = ST(1)+D*S                                                 350
      EV = E                                                            360
      SV = S                                                            370
      NU = 1                                                            380
      RETURN                                                            390
   12 T = (S-SV)/(E-EV)                                                 400
      NP = NU+1                                                         410
      DO 14  I = NP,NT                                                  420
      IF(ET(I).GT.E)   GOTO 16                                          430
      Z = SV+T*(ET(I)-EV)                                               440
      EW = ET(I)                                                        450
      SW = ST(I)                                                        460
   14 ST(I) = ST(I)+D*Z                                                 470
      RETURN                                                            480
   16 IF(E.EQ.ET(I-1))   GOTO 20                                        490
      Z = SW+(ST(I)-SW)/(ET(I)-EW)*(E-EW)                               500
      IF(NT+1.EQ.NTT)   GOTO 22                                         510
      DO 18  J = I,NT                                                   520
      JJ = NT+I-J                                                       530
      ET(JJ+1) = ET(JJ)                                                 540
   18 ST(JJ+1) = ST(JJ)                                                 550
      NT = NT+1                                                         560
      ET(I) = E                                                         570
      ST(I) = Z+D*S                                                     580
      NU = I                                                            590
      EV = E                                                            600
      SV = S                                                            610
      RETURN                                                            620
   20 NU = I-1                                                          630
      EV = E                                                            640
      SV = S                                                            650
      RETURN                                                            660
C                                                                       670
   22 NTP = 1000                                                        680
      RETURN                                                            690
C                                                                       700
      END                                                               710
```

```
      SUBROUTINE TRAFO(IC,NE,ISM,S,XM,AL,A)                             10
C                                                                       20
C*****TRANSFORMATION DER SGNC INS L-SYSTEM*****************************30
C                                                                       40
      DIMENSION A(IC),S(IC,ISM)                                         50
C                                                                       60
      XMM = XM-1                                                        70
      XMP = XM+1                                                        80
      CM = XM*XM                                                        90
      DO 2  I = 1,IC                                                   100
      V = SQRT(0.5*(1.+AL+(1.-AL)*A(I)))                               110
      A(I) = 0.5*(XMP*V-XMM/V)                                         120
      B = SQRT(A(I)*A(I)+CM-1.)                                        130
      F = (A(I)+B)*(A(I)+B)/(XM*B)                                     140
      DO 2  N = 1,NE                                                   150
    2 S(I,N) = S(I,N)*F                                                160
C                                                                      170
      RETURN                                                           180
C                                                                      190
      END                                                              200
```

```
      SUBROUTINE PUNK(NGR,NEGR,ABN,NA,NE,NEN,ALFA,NK,NR,ISM,            10
     -                ISMP,ISA,E,R,ALLA)                                20
C                                                                       30
C*****GRUNDPUNKTE INTERVALLWEISE LOGARITHMISCH AEQUIDISTANT************40
C                                                                       50
      REAL*8  C,ED,EX,EP                                                60
      DIMENSION  ABN(NEGR),E(ISM),R(NGR)                                70
C                                                                       80
      JJ = 0                                                            90
      DO 2  N = NA,NE                                                  100
      J = NK+NR                                                        110
      AB = -R(N)/ALLA                                                  120
      IF(AB.LT.1.)   J = AB*NK+1                                       130
    2 JJ = JJ+J                                                        140
      JJ = JJ+NA-NE+1                                                  150
      ISMP = MAX0(0,JJ+NEN-ISM)                                        160
      IF(ISMP.GT.0)   RETURN                                           170
C                                                                      180
      E(1) = ABN(NE+1)                                                 190
      J = 2                                                            200
      DO 10  NN = NA,NE                                                210
      N = NA+NE-NN                                                     220
      AB = -R(N)/ALLA                                                  230
      EX = DBLE(1./(NK-1))                                             240
      IF(AB.LT.1.)   EX = DBLE(1./(AB*NK))                             250
      EC = DBLE(E(J-1))                                                260
      AB = ABN(N)                                                      270
      A = AMIN1(AB,ABN(N+1)/ALFA)                                      280
    4 D = DBLE(A/ABN(N+1))                                             290
      C = C**EX                                                        300
    6 EP = ED*D                                                        310
```

```
      E(J) = SNGL(EP)                                                   320
      IF(E(J).GT.A)   GOTO 8                                            330
      EC = EP                                                           340
      J = J+1                                                           350
      GOTO 6                                                            360
    8 E(J-1) = A                                                        370
      IF(A.GE.AB)   GOTO 7                                              380
      EC = DBLE((AB/A)**(1./NR))                                        390
      IF(ED.GE.D)   C = EC                                              400
      EC = DBLE(A)                                                      410
   11 EP = ED*D                                                         420
      E(J) = SNGL(EP)                                                   430
      IF(E(J).GT.AB)   GOTO 9                                           440
      ED = EP                                                           450
      J = J+1                                                           460
      GOTO 11                                                           470
    9 E(J-1) = AB                                                       480
    7 EM = .99999*E(J-1)                                                490
      IF(J.LE.2)   GOTO 10                                              500
      IF(E(J-2).GE.EM)   GOTO 10                                        510
      E(J) = E(J-1)                                                     520
      E(J-1) = EM                                                       530
      J = J+1                                                           540
   10 CONTINUE                                                          550
      ISN = J-1                                                         560
      ISMP = MAXO(0,ISN-ISM)                                            570
      RETURN                                                            580
C                                                                       590
      END                                                               600
```

```
      SUBROUTINE LOCK0(XMAT,MASSE,COM,*)                                10
C                                                                       20
C*****LESEN DES ATOMGEWICHTS ***************************************** 30
C                                                                       40
      REAL*8  STOFF,F(6),ST                                             50
      INTEGER*2 U/'H '/,V                                               60
      DIMENSION  NWORT(4),NADAT(2)                                      70
      COMMON  STOFF,ISTRUK,ISPA,NOUT                                    80
      EQUIVALENCE(ST,V)                                                 90
      DATA F(2),F(3) /'BEST ','ISOT1'/                                  100
C                                                                       110
      NWORT(1) = 3                                                      120
      F(1) = STOFF                                                      130
      CALL NDFLOC(KP,NWORT,F,NADAT,KC)                                  140
      IF(KP.NE.1)  GO TO 1                                              150
      F(4) = F(4)/1.008665                                              160
      XMAT = F(4)                                                       170
      COM = 2/(3*F(4))                                                  180
      MASSE = XMAT                                                      190
      IF(XMAT-MASSE.GT.0.5)   MASSE = MASSE+1                           200
      RETURN                                                            210
C                                                                       220
    1 ST=STOFF                                                          230
      IF(U.NE.V)  RETURN 1                                              240
      WRITE (NOUT,2)                                                    250
    2 FORMAT(/' WARNING NDF. 3 MAY BE IGNORED IN THE CASE OF HYDROGEN'/) 260
      XMAT=1.                                                           270
      MASSE=1                                                           280
      COM=0.6666667                                                     290
      RETURN                                                            300
      END                                                               310
```

```
      SUBROUTINE LOCK1(ISC,K,E,SGN,EO,EE,NT,ISGT)                       10
C                                                                       20
C*****LESEN DER SGN, MUEL UND SGT VON KEDAK *************************** 30
C                                                                       40
      REAL*8  STOFF,A(5),B(3)                                           50
      DIMENSION E(ISC),SGN(ISC),NWORT(4),NADAT(2)                       60
      COMMON STOFF,ISTRUK,ISPA,NOUT                                     70
      FG(XA,XB,XC,YA,YC) = YA+(YC-YA)/(XC-XA)*(XB-XA)                   80
      DATA A(2),B /'BEST ','SGN  ','MUEL ','SGT  '/                    90
C                                                                       100
      ISGT=0                                                            110
      A(3) = B(NT+1)                                                    120
    1 NWORT(1) = 3                                                      130
      A(1) = STOFF                                                      140
      CALL NDFLOC(KP,NWORT,A,NADAT,KC)                                  150
      IF(KP.NE.1)   GOTO 15                                             160
      K = 1                                                             170
      E(1) = A(4)                                                       180
      SGN(1) = A(5)                                                     190
      IF(E(1)-EO)   5,4,3                                               200
    3 WRITE(NOUT,40)   STOFF,EO,A(3)                                    210
      ISGT=1                                                            220
      RETURN                                                            230
    4 K = K+1                                                           240
    5 CALL NDFNXT(KP,NWORT,A,NADAT,KC)                                  250
      IF(KP.NE.1)   GOTO 14                                             260
      IF(K.GT.1)   GOTO 11                                              270
      IF(A(4)-EO)   8,9,10                                              280
    8 E(1) = A(4)                                                       290
      SGN(1) = A(5)                                                     300
      GOTO 5                                                            310
    9 E(1) = A(4)                                                       320
      SGN(1) = A(5)                                                     330
      GOTO 4                                                            340
   10 K = 2                                                             350
   11 E(K) = A(4)                                                       360
      IF(K.EQ.ISC)   RETURN                                             370
      SGN(K) = A(5)                                                     380
      IF(E(K)-EE)   4,16,12                                             390
   12 Y = FG(E(K-1),EE,E(K),SGN(K-1),SGN(K))                            400
      E(K) = EE                                                         410
      SGN(K) = Y                                                        420
```

```
      GOTO 16                                                          430
   14 E(K) = EE                                                        440
      SGN(K) = SGN(K-1)                                                450
      WRITE(NOUT,42)   A(3),STOFF,E(K-1),A(3),E(K-1)                   460
   16 IF(E(1).EQ.EO)   RETURN                                          470
      Y = FG(E(1),EC,E(2),SGN(1),SGN(2))                               480
      E(1) = EO                                                        490
      SGN(1) = Y                                                       500
      RETURN                                                           510
   15 WRITE(NOUT,41)   STOFF,EO,A(3)                                   520
      ISGT=1                                                           530
      RETURN                                                           540
C                                                                      550
   40 FORMAT(//' ***ERROR 6.2 : FOR  ',A8,' SCATTERING MATRICES CANNOT B 560
     1E CALCULATED'/16X'FOR ENERGIES BELOW',1PE10.3,' EV FOR LACK OF  ', 570
     2A8,' ON KEDAK')                                                  580
   41 FORMAT(//' ***ERROR 6.9 : FOR  ',A8,' SCATTERING MATRICES CANNOT B 590
     1E CALCULATED'/16X'FOR ENERGIES BELOW',1PE10.3,' EV FOR LACK OF  ', 600
     2A8,' ON KEDAK')                                                  610
   42 FORMAT(//' ***WARNING 6.1 : THE  ',A8,' FOR  ',A8,' AT ENERGIES AB 620
     1OVE',1PE10.3,' EV'/18X,'ARE SET EQLAL TO THE  ',A8,' AT',E10.3,' E 630
     2V'//)                                                            640
C                                                                      650
      END                                                              660
```

```
      SUBROUTINE LOOK2(NEN,EA,ICOS,ICOSP,AR,ISM,SGNC)                   10
C                                                                       20
C*****LESEN DER SGNC VOM KERNDATENBAND**********************************  30
C                                                                       40
      REAL*8  STOFF,F(6)                                                50
      DIMENSION EA(ISM),NWORT(4),NADAT(2),SGNC(ICCS,ISM),AR(ICCS)       60
      COMMON STOFF,ISTRUK,ISPA,NOUT                                     70
      DATA F(2),F(3) /'BEST ','SGNC '/                                  80
C                                                                       90
      ICCSP = 0                                                        100
    2 NWORT(1) = 4                                                     110
      F(1) = STOFF                                                     120
      DO 4  NE = 1,NEN                                                 130
      F(4) = EA(NE)                                                    140
      CALL NDFLOC(KP,NWORT,F,NADAT,KC)                                 150
      IF(KP.NE.1)   STOP                                               160
      IP = 1                                                           170
    3 IF(IP.LE.ICOS)  GO TO 5                                          180
    7 ICCSP=ICOSP+1                                                    190
      CALL NDFNXT(KP,NWORT,F,NADAT,KC)                                 200
      IF(KP.EQ.1)  GO TO 7                                             210
      WRITE(NOUT,44) STOFF,ICCS,EA(NE)                                 220
      RETURN                                                           230
    5 AR(IP) = F(5)                                                    240
      SGNC(IP,NE) = F(6)                                               250
      IP = IP+1                                                        260
      CALL NDFNXT(KP,NWORT,F,NADAT,KC)                                 270
      IF(KP.EQ.1)   GOTO 3                                             280
      IF(IP.GT.ICOS)  GO TO 4                                          290
      ICCSP = IP-1-ICOS                                                300
      WRITE(NOUT,44)   STOFF,ICOS,EA(NE)                               310
      RETURN                                                           320
    4 CONTINUE                                                         330
      RETURN                                                           340
C                                                                      350
   44 FORMAT(//' ***WARNING 6.3 : FOR  ',A8,' THE SGNC COSINE MESH HAS M 360
     1ORE'/18X,'THAN ',I3,' MESHPOINTS AT',1PE10.3,' EV')              370
C                                                                      380
      END                                                              390
```

```
      SUBROUTINE LOCK3(NE,EA,ISC,NGR,ABN,ISM,ISMP,LST,NEGR,ISEL,ISGNC)   10
C                                                                        20
C*****LESEN DER SGNC-ENERGIEN VOM KERNDATENBAND**********************    30
C                                                                        40
      REAL*8  STOFF,F(6)                                                 50
      DIMENSION EA(ISM),ABN(NEGR),LST(NEGR),NWORT(4),NADAT(2)            60
      COMMON STOFF,ISTRUK,ISPA,NOUT                                      70
      DATA F(2),F(3) /'BEST ','SGNC '/                                   80
C                                                                        90
      ISGNC=0                                                           100
    2 NWORT(1) = 4                                                      110
      F(1) = STOFF                                                      120
      F(4) = 0.                                                         130
      NE = 1                                                            140
    4 CALL NDFLOC(KP,NWORT,F,NADAT,KC)                                  150
      IF(KP.EQ.1)  GO TO 5                                              160
      CALL NDFLOC(KP,NWORT,F,NADAT,KC)                                  170
      IF(KP.EQ.1)  GO TO 5                                              180
      IF(NE-1)13,13,6                                                   190
    5 EA(NE)=F(4)                                                       200
      F(4) = F(4)+F(4)*(1.E-06)                                         210
      IF(EA(NE).LT.1.    )  GO TO 4                                     220
      NE = NE+1                                                         230
      IF(NE.LE.ISM)   GOTO 4                                            240
      ISMP=50                                                           250
      RETURN                                                            260
    6 WRITE(NOUT,62)                                                    270
      IF(EA(1).GE.ABN(1))  GO TO 12                                     280
C                                                                       290
C*****ANZAHL DER SGNC IN DER N-TEN GRUPPE*****************************  300
      NE=NE-1                                                           310
      DO 10  N = 1,NGR                                                  320
      LST(N) = 0                                                        330
      DO 8  M = 1,NE                                                    340
      IF((ABN(N+1).LE.EA(M)).AND.(EA(M).LT.ABN(N)))   LST(N) = LST(N)+1 350
    8 CONTINUE                                                          360
   10 CONTINUE                                                          370
      IF(ISEL.GT.0)  GO TO 11                                           380
      WRITE(NOUT,52)                                                    390
```

```
      DO 7 N=1,NGR                                                          400
    7 WRITE(NOUT,54) N,LST(N)                                               410
C                                                                           420
C*****ANISOTROPIE-SCHWELLE*************************************************430
   11 DO 14 N = 1,NGR                                                       440
      NN = NGR-N+1                                                          450
      IF(LST(NN).NE.0)   GOTO 16                                            460
   14 CONTINUE                                                              470
   16 ISO = NN+1                                                            480
      RETURN                                                                490
C                                                                           500
   12 IF(ISEL.GT.0)  GO TO 15                                               510
      WRITE (NOUT,52)                                                       520
      WRITE(NOUT,58)                                                        530
   15 EA(1) = ABN(1)                                                        540
      ISC=1                                                                 550
      RETURN                                                                560
C                                                                           570
   13 WRITE(NOUT,60)   STOFF                                                580
      ISGNC=1                                                               590
      RETURN                                                                600
C                                                                           610
   52 FORMAT(///10X,'STUETZSTELLEN FUER SGNC'//                             620
     -       10X,'GRUPPE',11X,'ANZAHL'/)                                    630
   54 FORMAT(9X,I6,11X,I6)                                                  640
   58 FORMAT(5X,'ENERGIEBEREICH LIEGT IM BEREICH ISOTROPER STREUUNG')       650
   60 FORMAT(//' ***ERROR 6.4 : FOR  ',A8,' SCATTERING MATRICES CANNOT B   660
     1E CALCULATED'/16X'FOR LACK OF SGNC ON KEDAK')                         670
   62 FORMAT(//' ***MESSAGE 6.1 : WARNING NOF. 2 MAY BE IGNORED')           680
C                                                                           690
      END                                                                   700
```

```
      SUBROUTINE LECAL(MASSE,XMAT,ALFA,ISOT,LEG,NLE,NANF,NENG,NUEB,IL,       10
     1                 IM,NEGR,ABN,ICOS,AR,ISN,E,SGNC,NST,NSTIS,ISM,ISO,      20
     2                 NECU,ITA,NF,GR,FEKOE,FU,EW,A,F,V,W,F,FEKO)             30
C                                                                            40
C*****BERECHNUNG DER ENERGIEDIFFERENTIELLEN LEGENDRE-KOEFFIZIENTEN******     50
C                                                                            60
      DIMENSION  NST(6),LEG(6),AR(ICOS),FU(ICOS),ABN(NEGR),GR(NEGR),         70
     1           FEKOE(NEGR),A(ISO),H(ISO),E(ISM),EW(ISM),V(ISO),W(ISO),     80
     2           F(ISO),SGNC(ICOS,ISM),FEKO(ISM,NECU)                        90
C                                                                           100
      EP = 0.8                                                              110
      XP = XMAT+1                                                           120
      XM = XMAT-1                                                           130
      IF(MASSE.EQ.1)   XM = 0.                                              140
      NP = NUEB-1                                                           150
      IA = NANF                                                             160
      IC = MINO(NEGR,NENG+NUEB)                                             170
      IB = IC-1                                                             180
      IF(ITA.EQ.0.AND.ISOT.EQ.0)                                            190
     1CALL LEGINT(NLE,NSTIS,XMAT,ITA)                                       200
```

```
      REWIND NF                                                             210
C                                                                           220
C*****ENERGIEDIFF. LEGENDRE-KOEFF. (L-1)-TER ORDNUNG***********************230
      N = 0                                                                 240
      L = 1                                                                 250
      GOTO 2                                                                260
    1 N=N+1                                                                 270
      L=LEG(N)                                                              280
    2 IF(ISOT.EQ.0)   GOTO 3                                                290
      NSB = NSTIS                                                           300
      NSA = NST(L)                                                          310
      CALL LEGPOL(NSA,H,NLE)                                                320
C                                                                           330
    3 DO 28  J = 1,ISN                                                      340
C                                                                           350
C*****GRENZEN FUER WINKELINTEGRATION********************************       360
      GRM = 0.                                                              370
      EL = AMAX1(ABN(IM+1),ALFA*E(J))                                       380
      DO 8  I = IA,IC                                                       390
      IF(EL.LT.ABN(I))   GOTO 6                                             400
      GR(I) = -1.                                                           410
      GOTO 8                                                                420
    6 IF(E(J).GT.ABN(I))   GOTO 7                                           430
      GR(I) = 1.                                                            440
      GOTO 8                                                                450
    7 G = SQRT(ABN(I)/E(J))                                                 460
      GR(I) = 0.5*(XP*G-XM/G)                                               470
      GRA = ABS(GR(I))                                                      480
      IF((GRA.LT.1.).AND.(GRM.LT.GRA))   GRM = GRA                          490
    8 CONTINUE                                                              500
      IF(ISOT.EQ.0)   GOTO 11                                               510
C                                                                           520
C*****MOMENTE BEI ANISOTROPIE IM SP-SYSTEM**************************       530
      IF(GRM.LT.EP)   NSB = NST(L)                                          540
      IF(NSA.EQ.NSB)   GOTO 9                                               550
      NSA = NSB                                                             560
      CALL LEGPOL(NSA,H,NLE)                                                570
    9 DO 10  IP = 1,ICOS                                                    580
   10 FU(IP) = SGNC(IP,J)                                                   590
      CALL IPOLA(ICOS,AR,FU,NSA,H,A,F)                                      600
      CALL LEGANS(L,NSA,A,IA,IB,NEGR,GR,FEKOE,V,W)                          610
      NSB = NSTIS                                                           620
      GOTO 12                                                               630
C                                                                           640
C*****MOMENTE BEI ISOTROPIE IM SP-SYSTEM**************************         650
   11 CALL LEGIST(L,NSTIS,IA,IB,NEGR,GR,FEKOE)                              660
C                                                                           670
C*****VORBEREITUNG ZUM ABSPEICHERN*****************************************680
   12 II = 1                                                                690
      DO 22  I = IA,IB                                                      700
      IF(ABN(I+1).GT.E(J))   GOTO 22                                        710
      FEKO(J,II) = 6.283185*FEKOE(I)                                        720
      II = II+1                                                             730
      IF(II.GE.NUEB)   GOTO 27                                              740
   22 CONTINUE                                                              750
```

```
      DO 26  I = II,NM                                                  760
   26 FEKO(J,I) = 0.                                                    770
   27 FEKO(J,NUEB) = 6.283185*FEKCE(NEGR)                               780
C                                                                       790
   28 CONTINUE                                                          800
C                                                                       810
C*****NORMIERUNG FUER ZWISCHENPUNKTE************************************ 820
      IF(N.GT.0)   GOTO 30                                              830
      DO 29  J = 1,ISN                                                  840
   29 EW(J) = FEKO(J,NUEB)                                              850
      GOTO 1                                                            860
   30 DO 31  J = 1,ISN                                                  870
      DO 31  I = 1,NUEB                                                 880
   31 FEKO(J,I) = FEKO(J,I)/EW(J)                                       890
C                                                                       900
C*****SPEICHERN DER ENERGIEDIFF. LEGENDRE-KOEFF. (L-1)-TER ORDNUNG****** 910
      DO 32  I = 1,NUEB                                                 920
   32 WRITE(NF)   (FEKO(J,I),J = 1,ISN)                                 930
      IF(N.LT.NLE+1)   GOTO 1                                           940
C                                                                       950
      REWIND NF                                                         960
C                                                                       970
      RETURN                                                            980
C                                                                       990
      END                                                              1000
```

```
      SUBROUTINE LEGPOL(NST,A,N,NSTIS)                                  10
C                                                                       20
C*****BERECHNUNG VON LEGENDRE-POLYNOMEN**********************************  30
C                                                                       40
      REAL*8  X(321),F(6,321),D                                         50
      DIMENSION A(NSTIS)                                                60
      COMMON /INTEG/  X,F,D                                             70
C                                                                       80
      NSM = NST-1                                                       90
      NA = -100000                                                     100
      ND = 320/NSM*625                                                 110
      DO 6  I = 1,NST                                                  120
      X(I) = DFLOAT(NA)*1.D-05                                         130
      A(I) = SNGL(X(I))                                                140
    6 NA = NA+ND                                                       150
      E = ND*1.E-05                                                    160
C                                                                      170
      IF(N.GT.0)   GOTO 2                                              180
      DO 1  I = 1,NST                                                  190
    1 F(1,I) = 1.                                                      200
      RETURN                                                           210
C                                                                      220
    2 IF(N.GT.1)   GOTO 4                                              230
      DO 3  I = 1,NST                                                  240
      F(1,I) = 1.                                                      250
    3 F(2,I) = X(I)                                                    260
      RETURN                                                           270
C                                                                      280
    4 NM = N-1                                                         290
      DO 5  I = 1,NST                                                  300
      F(1,I) = 1.                                                      310
      F(2,I) = X(I)                                                    320
      DO 5  J = 1,NM                                                   330
    5 F(J+2,I) = ((2*J+1)*X(I)*F(J+1,I)-J*F(J,I))/(J+1)                340
C                                                                      350
      RETURN                                                           360
C                                                                      370
      END                                                              380
```

```
      SUBROUTINE LEGINT(N,NAK,XMAT,ITA)                                 10
C                                                                       20
C*****BERECHNUNG VON LEGENDRE-INTEGRALEN*********************************  30
C                                                                       40
      REAL*8  H(321),GRAL(6,321),F(6),A,B,C,D,DE,G,P,F0,F1,F2,F3,F4,F5,  50
     1        X,Y                                                       60
      COMMON /INTEG/ H,GRAL,D                                           70
C                                                                       80
      ITA = 1                                                           90
      NST = 321                                                        100
C                                                                      110
      NA = -100000                                                     120
      DO 1  K = 1,NST                                                  130
      H(K) = DFLOAT(NA)*1.D-05                                         140
    1 NA = NA+625                                                      150
      D = 0.00625                                                      160
C                                                                      170
      IF(XMAT.GT.1.5)   GOTO 4                                         180
C*****WASSERSTOFF********************************************************* 190
      DO 2  K = 1,160                                                  200
      DO 2  L = 1,6                                                    210
    2 GRAL(L,K) = 0.                                                   220
      DO 3  K = 161,321                                                230
      A = H(K)*H(K)                                                    240
      B = A*H(K)                                                       250
      GRAL(1,K) = 2*A                                                  260
      GRAL(2,K) = 4*B/3                                                270
      GRAL(3,K) = 0.5*A*(3*A-2)                                        280
      GRAL(4,K) = 2*B*(A-1)                                            290
      GRAL(5,K) = A*(35*(A-1)*(A-2./7)-1)/12                           300
      GRAL(6,K) = 4.5*B*(A-1)*(A-5./9)                                 310
    3 CONTINUE                                                         320
      GOTO 12                                                          330
C                                                                      340
C*****NICHT-WASSERSTOFFE************************************************ 350
    4 A = DBLE(XMAT)                                                   360
      DO 5  L = 1,6                                                    370
    5 GRAL(L,1) = 0                                                    380
      IF(XMAT.GT.30.)   GOTO 8                                         390
```

```
      C = 0.5*DSQRT((A+1)*(A-1))                                          400
      F(1) = C                                                            410
      DO 6  L = 2,5                                                       420
    6 F(L) = F(L-1)*C                                                     430
      P = A-1./A                                                          440
      Y = DSQRT((A-1)/(A+1))                                              450
C                                                                         460
      DO 7  K = 2,NST                                                     470
      X = (H(K)+DSQRT((H(K)+1)*(H(K)-1)+A*A))/(2*C)                       480
      DE = X-Y                                                            490
      FC = 0.5*G(2,X,Y)                                                   500
      F1 = F(1)*(G(3,X,Y)/3-1)                                            510
      F2 = F(2)*(0.25*G(4,X,Y)-G(2,X,Y)+DLOG(X/Y)/DE)                     520
      F3 = F(3)*(0.2*G(5,X,Y)-G(3,X,Y)+3-1./(X*Y))                        530
      F4 = F(4)*(G(6,X,Y)/6-G(4,X,Y)+3*G(2,X,Y)-4*DLOG(X/Y)/DE            540
     1      +0.5/(X*Y)*G(2,1./X,1./Y))                                    550
      F5 = F(5)*(G(7,X,Y)/7-G(5,X,Y)+10*G(3,X,Y)/3-10+5./(X*Y)            560
     1      -G(3,1./X,1./Y)/(3*X*Y))                                      570
      GRAL(1,K) = P*F0*DE                                                 580
      GRAL(2,K) = P*F1*DE                                                 590
      GRAL(3,K) = P*0.5*(3*F2-F0)*DE                                      600
      GRAL(4,K) = P*0.5*(5*F3-3*F1)*DE                                    610
      GRAL(5,K) = P*0.125*(35*F4-30*F2+3*F0)*DE                           620
      GRAL(6,K) = P*0.125*(63*F5-70*F3+15*F1)*DE                          630
    7 CONTINUE                                                            640
      GOTO 11                                                             650
C                                                                         660
    8 B = 1./(A*A)                                                        670
      C = B*B                                                             680
      DO 10  K = 2,NST                                                    690
      X = H(K)                                                            700
      Y = -1.                                                             710
      DO 9  L = 1,6                                                       720
    9 F(L) = -0.125*(5*G(L+4,X,Y)/(L+4)-6*G(L+2,X,Y)/(L+2)+G(L,X,Y)/L)*C  730
     1        +0.5*(3*G(L+2,X,Y)/(L+2)-G(L,X,Y)/L)*B                      740
     2        +2*G(L+1,X,Y)/(A*(L+1))+G(L,X,Y)/L                          750
      DE = X-Y                                                            760
      GRAL(1,K) = F(1)*DE                                                 770
      GRAL(2,K) = F(2)*DE                                                 780
      GRAL(3,K) = 0.5*(3*F(3)-F(1))*DE                                    790
      GRAL(4,K) = 0.5*(5*F(4)-3*F(2))*DE                                  800
      GRAL(5,K) = 0.125*(35*F(5)-30*F(3)+3*F(1))*DE                       810
      GRAL(6,K) = 0.125*(63*F(6)-70*F(4)+15*F(2))*DE                      820
   10 CONTINUE                                                            830
C                                                                         840
   11 GRAL(1,NST) = 2.                                                    850
      GRAL(2,NST) = 4/(3*A)                                               860
      GRAL(4,NST) = 0.                                                    870
      GRAL(6,NST) = 0.                                                    880
C                                                                         890
C*****REDUKTION VON NST AUF NAK ***************************************** 900
   12 NP = N+1                                                            910
   13 IF(NAK.EQ.NST)   RETURN                                             920
      K1 = (NST-1)/(NAK-1)                                                930
      KK = K1+1                                                           940
      DO 15  K = 2,NAK                                                    950
      H(K) = H(KK)                                                        960
      DO 14  L = 1,NP                                                     970
   14 GRAL(L,K) = GRAL(L,KK)                                              980
   15 KK = KK+K1                                                          990
      D = 2./(NAK-1)                                                     1000
C                                                                        1010
      RETURN                                                             1020
C                                                                        1030
      END                                                                1040
```

```
      FUNCTION G(N,X,Y)                                                    10
C                                                                          20
C     BERECHNUNG VON (X**N-Y**N)/(X-Y) DURCH ENTWICKLUNG NACH  POTENZEN    30
C     VON  D = X-Y                                                         40
C                                                                          50
      REAL*8  G,X,Y,D                                                      60
      D = X-Y                                                              70
      GOTO(1,2,3,4,5,6,7,8,9,10),N                                         80
    1 G = 1.                                                               90
      RETURN                                                              100
    2 G = D+2*Y                                                           110
      RETURN                                                              120
    3 G = D*D+3*Y*D+3*Y*Y                                                 130
      RETURN                                                              140
    4 G = D*D*D+4*Y*D*D+6*Y*Y*D+4*Y*Y*Y                                   150
      RETURN                                                              160
    5 G = D**4+5*Y*D*D*D+10*Y*Y*D*D+10*Y*Y*Y*D+5*Y**4                     170
      RETURN                                                              180
    6 G = D**5+6*Y*D**4+15*Y*Y*D*D*D+20*Y*Y*Y*D*D+15*Y**4*D+6*Y**5        190
      RETURN                                                              200
    7 G = D**6+7*Y*D**5+21*Y*Y*D**4+35*Y*Y*Y*D*D*D+35*Y**4*D*D            210
     1     +21*Y**5*D+7*Y**6                                              220
      RETURN                                                              230
    8 G = D**7+8*Y*D**6+28*Y*Y*D**5+56*Y*Y*Y*D**4+70*Y**4*D*D*D           240
     1     +56*Y**5*D*D+28*Y**6*D+8*Y**7                                  250
      RETURN                                                              260
    9 G = D**8+9*D**7*Y+36*D**6*Y*Y+84*D**5*Y*Y*Y+126*D**4*Y**4           270
     1     +126*D*D*D*Y**5+84*D*D*Y**6+36*D*Y**7+9*Y**8                   280
      RETURN                                                              290
   10 G = D**9+10*D**8*Y+45*D**7*Y*Y+120*D**6*Y*Y*Y+210*D**5*Y**4        300
     1     +252*D**4*Y**5+210*D*D*D*Y**6+120*D*D*Y**7+45*D*Y**8+10*Y**9   310
      RETURN                                                              320
      END                                                                 330
```

```
      SUBROUTINE LEGIST(L,NST,IA,IB,NEGR,GR,E)                          10
C                                                                       20
C*****BERECHNUNG VON PARTIELLEN LEGENDRE-KOEFFIZIENTEN BEI ISOTROPIE IM   30
C*****SP-SYSTEM*************************************************       40
C                                                                       50
      REAL*8  X(321),GRAL(6,321),D,A,B                                  60
      DIMENSION GR(NEGR),E(NEGR)                                        70
      COMMON /INTEG/ X,GRAL,D                                           80
C                                                                       90
      DO 7 I=IA,IB                                                     100
      GO = 1.                                                          110
      GL = -1.                                                         120
      IKO = NST                                                        130
      IKU = 1                                                          140
      IF(GR(I+1).GE.1.)   GOTO 5                                       150
      IF(GR(I).LE.-1.)   GOTO 5                                        160
      IF(GR(I).GE.1.)   GOTO 2                                         170
      GO = GR(I)                                                       180
      XIKO = 1.+0.5*(NST-1)*(GO+1.)                                    190
      IKO = XIKO                                                       200
      IF(FLOAT(IKO).LT.XIKO)   IKO = IKO+1                             210
    2 IF(GR(I+1).LE.-1.)   GOTO 3                                      220
      GU = GR(I+1)                                                     230
      XIKU = 1.+0.5*(NST-1)*(GU+1.)                                    240
      IKU = XIKU                                                       250
      IF(FLOAT(IKU).LT.XIKU)   IKU = IKU+1                             260
    3 A = GRAL(L,IKO)                                                  270
      IF(GO.LT.X(IKO))  A = A+(GO-X(IKO))/D*(GRAL(L,IKO)-GRAL(L,IKO-1))  280
      B = GRAL(L,IKU)                                                  290
      IF(GU.LT.X(IKU))  B = B+(GU-X(IKU))/D*(GRAL(L,IKU)-GRAL(L,IKU-1))  300
    4 E(I) = (A-B)*0.7957747E-01                                       310
      GOTO 7                                                           320
    5 E(I) = 0.                                                        330
    7 CONTINUE                                                         340
      E(NEGR ) = GRAL(L,NST)*0.7957747E-01                             350
C                                                                      360
      RETURN                                                           370
C                                                                      380
      END                                                              390
```

```
      SUBROUTINE LEGANS(L,NST,F,IA,IB,NEGR,GR,E,POLY,A)                 10
C                                                                       20
C*****BERECHNUNG VON PARTIELLEN LEGENDRE-KOEFFIZIENTEN BEI ANISOTROPIE    30
C*****IM SP-SYSTEM*********************************************       40
C                                                                       50
      REAL*8  X(321),PCL(6,321),D,B                                     60
      DIMENSION F(NST),GR(NEGR),E(NEGR),POLY(NST),A(NST)                70
      COMMON /INTEG/  X,POL,D                                           80
C                                                                       90
C*****BESTIMMUNG DER ZU INTEGRIERENDEN FUNKTION*********************   100
      DO 2  J = 1,NST                                                  110
      B = DBLE(F(J))                                                   120
    2 POLY(J) = B*POL(L,J)                                             130
C                                                                      140
C*****SUCHEN DER GRENZINDICES MIT KORREKTURINTERVALLEN**************   150
      ES = 0                                                           160
      I=IA-1                                                           170
    3 I = I+1                                                          180
      IF((GR(I+1).GE.1.).OR.(GR(I).LE.-1.))   GOTO 18                  190
      IF(GR(I).LT.1.)   GOTO 4                                         200
      II = I                                                           210
      GOTO 18                                                          220
    4 GO = GR(I)                                                       230
      GU=AMAX1(-1.,GR(I+1))                                            240
      XIKO = 1.+0.5*(NST-1)*(1.+GO)-0.001                              250
      NO = XIKO                                                        260
      XIKU = 1.+0.5*(NST-1)*(1.+GU)+0.001                              270
      NU = XIKU                                                        280
      IF(FLOAT(NO).LT.XIKO)   NO = NO+1                                290
      NUO = NO-NU                                                      300
      IF((NUO/2*2).NE.NUO)   NO =  NO-1                                310
      DL = GU-X(NU)                                                    320
      DO = GO-X(NO)                                                    330
      IF(ABS(DU).LT.1.E-20)   DU = 0                                   340
      IF(ABS(DO).LT.1.E-20)   DO = 0                                   350
C                                                                      360
C*****SIMPSON-INTEGRATION FUER UEBERSTREUUNG UND TOTALES MOMENT*****   370
    5 NO1 = NO-2                                                       380
      NO2 = NO-1                                                       390
      NU1 = NU+2                                                       400
      NU2 = NU+1                                                       410
      IF(NO1.GE.NU1)   GOTO 7                                          420
      E(I) = (POLY(NU)+POLY(NO))*D/2.                                  430
      IF(NO2.LT.NU2)   GOTO 19                                         440
      DO 6  J = NU2,NO2                                                450
    6 E(I) = E(I)+D*POLY(J)                                            460
      GOTO 19                                                          470
    7 DO 12  J = NU2,NO2,2                                             480
      JJ = (J-NU2+2)/2                                                 490
   12 A(JJ) = POLY(J)                                                  500
      CALL SUM(JJ,A,SA)                                                510
      DO 15  J = NU1,NO1,2                                             520
      JJ = (J-NU1+2)/2                                                 530
   15 A(JJ) = POLY(J)                                                  540
      CALL SUM(JJ,A,SO)                                                550
      SE = POLY(NO)+POLY(NU)                                           560
      E(I) = (4*SA+2*SO+SE)*D/3                                        570
C                                                                      580
C*****RANDKORREKTUR DES SIMPSON-INTEGRALS***************************   590
      IF(I.EQ.NEGR)   GOTO 20                                          600
      TU = (POLY(NU2)-POLY(NU))/D                                      610
      TO = (POLY(NO)-POLY(NO2))/D                                      620
      E(I) = (POLY(NO)+0.5*DO*TO)*DO-(POLY(NU)+0.5*DL*TU)*DU+E(I)      630
      GOTO 19                                                          640
   18 E(I) = 0.                                                        650
   19 ES = ES+E(I)                                                     660
      IF(I.LT.IB)    GOTO 3                                           670
```

```
C                                                                       680
C*****INTEGRATIONSBEREICH FUER DAS TOTALE MOMENT************************ 690
      NU = 1                                                            700
      NC = NST                                                          710
      I=NEGR                                                            720
      GOTO 5                                                            730
C                                                                       740
C*****G,G-STREUUNG ****************************************************** 750
   20 E(II) = E(NEGR)-ES                                                760
      RETURN                                                            770
C                                                                       780
      END                                                               790
```

```
      SUBROUTINE GRUPIN(MASSE,XMAT,ALFA,COM,ISCT,PM,LEG,NLE,NANF,NEND,   10
     1                  NUEB,IL,IM,NGR,NEGR,ABN,ISN,EH,K,H,F,M,G,EN,     20
     2                  NTT,ET,ST,MAZ,KSPE,KSPEK,ESP,SPEK,NSPEK,LSPEK,   30
     3                  ISM,ISD,NECU,ISCC,ISEC,NF,E,EW,GR,WA,U,V,W,ISTT, 40
     4                  RSP,ELSIG,NGT,NGG,EG,SG,SGTOT)                   50
C                                                                       60
C*****GEWICHTETE MULTIGRUPPEN-ENERGIEINTEGRATION************************ 70
C                                                                       80
      REAL*8  DXY                                                       90
      DIMENSION  LEG(6),ABN(NEGR),RSP(6,NGR),ESP(NSPEK),SPEK(LSPEK),   100
     1           EH(ISM),EW(ISM),H(ISD),F(ISD),G(ISD),EN(ISD),V(ISD),  110
     2           W(ISD),E(ISD),WA(ISCO),L(ISEC),ET(NTT),ST(NTT),GR(NGR),120
     3           MAZ(2),ELSIG(6,NECU,NGR),EG(ISC),SG(ISD),SGTOT(6,NGR) 130
C                                                                      140
      NF = NLE+1                                                       150
      XP = XMAT+1                                                      160
      XM = XMAT-1                                                      170
      GW = -1.                                                         180
      IF(MASSE.EQ.1)   GW = 0.                                         190
      IF(MASSE.EQ.1)   XM = 0.                                         200
      NM = NUEB-1                                                      210
C                                                                      220
C*****VEREINIGUNG DER ENERGIESTUFTZPUNKTMENGEN************************** 230
      JI = 0                                                           240
      JP = 0                                                           250
      IF(KSPE.EQ.0)   GOTO 3                                           260
      XX = EH(1)                                                       270
      XY = EH(ISN)                                                     280
      DO 1  J = 1,KSPEK                                                290
      IF(JI.EQ.0.AND.XX.LE.ESP(J))   JI = J                            300
      IF(XY.LE.ESP(J))   JP = J-JI                                     310
      IF(JP.GT.0)   GOTO 3                                             320
    1 CONTINUE                                                         330
    3 DO 2  J = 1,ISN                                                  340
    2 E(J) = EH(J)                                                     350
      ISTT = ISN                                                       360
      CALL PUSUM(ISD,K,H,ISTT,F,V)                                     370
      IF(KSPE*JI*JP.NE.0)   CALL PUSUM(ISD,JP,ESP(JI),ISTT,E,V)        380
C                                                                      390
```

```
C*****INTERPOLATION DER TOTALEN ELASTISCHEN QUERSCHNITTE*************** 400
      CALL IPOLIN(K,H,F,ISTT,E,W,U)                                    410
C                                                                      420
C*****INTERPOLATION DER TOTALEN QUERSCHNITTE*************************** 430
      IF(NGT.EQ.0)   GOTO 7                                            440
      CALL IPOLIN(NGG,EG,SG,ISTT,E,F,U)                                450
      NGG = ISTT                                                       460
      DO 5  J = 1,NGG                                                  470
      EG(J) = E(J)                                                     480
    5 SG(J) = F(J)                                                     490
C                                                                      500
C*****INTERPOLATION DER MITTLEREN STREUKOSINUS************************ 510
    7 CALL IPOLIN(M,G,EN,ISTT,E,V,U)                                   520
C                                                                      530
C                                                                      540
    8 DO 66  N = 1,NP                                                  550
      L = LEG(N)                                                       560
C*****LESEN UND INTERPOLATION DER NORMIERTEN ENERGIEDIFF. LEGENDRE-KOEFF 570
      DO 11  I = 1,NUEB                                                580
      JI = (I-1)*ISTT                                                  590
      READ(NF)   (EW(J),J = 1,ISN)                                     600
      IF(ISOT.EQ.0.AND.I.EQ.NUEB)   GOTO 9                             610
      CALL IPOLIN(ISN,EH,EW,ISTT,E,WA(1+JI),U)                         620
      GOTO 11                                                          630
    9 XY = EW(ISN)                                                     640
      DO 10  J = 1,ISTT                                                650
   10 WA(J+JI) = XY                                                    660
   11 CONTINUE                                                         670
C                                                                      680
C*****MUEL-ANGEPASSTE ENERGIEDIFF. LEGENDRE-KOEFF. ******************** 690
      DO 44  J = 1,ISTT                                                700
      DXY = 0.                                                         710
      JP = J+NM*ISTT                                                   720
      IF(L.NE.2)   GOTO 27                                             730
      V(J) = PM*(V(J)-WA(JP))                                          740
      IF(ABS(V(J)).LT.1.E-7)   V(J) = 0.                               750
   27 DO 12  NN = NANF,NEND                                            760
      IF((ABN(NN+1).LE.E(J)).AND.(E(J).LE.ABN(NN)))   GOTO 14          770
   12 CONTINUE                                                         780
      NN = NEND                                                        790
   14 EL = AMAX1(ABN(IM+1),ALFA*E(J))                                  800
      DO 42  I = 1,NUEB                                                810
      JI = J+(I-1)*ISTT                                                820
      NI = MINO(IM,NN+I-1)                                             830
      P = 0.                                                           840
      GU = GW                                                          850
      IF(EL.GE.ABN(NI+1))   GOTO 16                                    860
      GU = SQRT(ABN(NI+1)/E(J))                                        870
      GU = 0.5*(XP*GU-XM/GU)                                           880
   16 GO = 1.                                                          890
      IF(I.EQ.1)   GOTO 18                                             900
      LI = MINO(IM+1,NN+I-1)                                           910
      GO = GW                                                          920
      IF(EL.GE.ABN(LI))   GOTO 18                                      930
      GO = SQRT(ABN(LI)/E(J))                                          940
```

```
      GC = 0.5*(XP*GO-XM/GO)                                            950
   18 IF(GU.LT.GO)    GOTO 20                                           960
      P = 0.                                                            970
      GOTO 36                                                           980
   20 IF(GO-GU.LT.2.)    GOTO 22                                        990
      P = 0.                                                           1000
      IF(L.EQ.2)    P = 1.                                             1010
      GOTO 36                                                          1020
   22 C2 = GO*GO                                                       1030
      U2 = GU*GU                                                       1040
      C3 = O2*GO                                                       1050
      U3 = U2*GU                                                       1060
      IF(MASSE.EQ.1)    GOTO 13                                        1070
      GOTO(24,26,28,30,32,34),L                                        1080
   13 GOTO(15,17,19,21,23,25),L                                        1090
   15 P = 12*(O3-O2)                                                   1100
      P = P-12*(U3-U2)                                                 1110
      GOTO 36                                                          1120
   17 P = O3*(9*GO-8)                                                  1130
      P = P-U3*(9*GU-8)                                                1140
      GOTO 36                                                          1150
   19 P = .6*O2*(12*O3-10*(O2*GO-1))                                   1160
      P = P-.6*U2*(12*U3-10*(U2*GU-1))                                 1170
      GOTO 36                                                          1180
   21 P = 1.5*O3*(10*O3-8*O2-9*GO+8)                                   1190
      P = P-1.5*U3*(10*U3-8*U2-9*GU+8)                                 1200
      GOTO 36                                                          1210
   23 P = .5*O2*(O2*(45*O3-35*O2 -54*GO+45)+9*GO-9)                    1220
      P = P-.5*U2*(U2*(45*U3-35*U2 -54*GU+45)+9*GU-9)                  1230
      GOTO 36                                                          1240
   25 P = .1875*O3*(O2*(189*C3-144*O2-280*GC+224)+90*GO-80)            1250
      P = P-.1875*U3*(U2*(189*U3-144*U2-280*GU+224)+90*GU-80)          1260
      GOTO 36                                                          1270
   24 P = 0.75*(O2-U2)                                                 1280
      GOTO 36                                                          1290
   26 P = 0.5*(O3-U3)                                                  1300
      GOTO 36                                                          1310
   28 P = 0.1875*(O2*(3*O2-2)-U2*(3*U2-2))                             1320
      GOTO 36                                                          1330
   30 P = 0.75*(O3*(O2-1)-U3*(U2-1))                                   1340
      GOTO 36                                                          1350
   32 P = 0.03125*(O2*((O2-1)*(35*O2-10)-1)-L2*((U2-1)*(35*U2-10)-1))  1360
      GOTO 36                                                          1370
   34 P = 0.1875*(O3*(O2-1)*(9*O2-5)-U3*(U2-1)*(9*U2-5))               1380
   36 IF(ABS(P).LT.1.E-16)    P = 0.                                   1390
      IF(EL.LT.ABN(NI+1).AND.I.LT.NUEB)    GOTO 40                     1400
      WA(JI) = WA(JP)-SNGL(DXY)                                        1410
      IF(I.EQ.NUEB)    GOTO 42                                         1420
      IA = I+1                                                         1430
      DO 38  II = IA,NUEB                                              1440
   38 WA(J+(II-1)*ISTT) = 0.                                           1450
      WA(JI) = WA(JI)+P*V(J)                                           1460
      GOTO 44                                                          1470
   40 DXY = DXY+DBLE(WA(JI))                                           1480
   42 WA(JI) = WA(JI)+P*V(J)                                           1490

   44 CONTINUE                                                         1500
C                                                                      1510
C*****AUSSORTIEREN ZUR GEWICHTETEN INTEGRATION************************ 1520
      DO 64  NR = 1,NUEB                                               1530
      NI = (NR-1)*ISTT                                                 1540
      JA = 1                                                           1550
      DO 58  NT = NANF,NEND                                            1560
      NN = NANF+NEND-NT                                                1570
C     NN-TE GRUPPE = AUSSTREUGRUPPE                                    1580
C     (NN+NR-1)-TE GRUPPE = EINSTREUGRUPPE                             1590
      AM = ABN(NN)                                                     1600
      DO 46  J = JA,ISTT                                               1610
      IF(E(J).GT.AM)    GOTO 48                                        1620
      JI = J-JA+1                                                      1630
      EN(JI) = E(J)                                                    1640
   46 F(JI) = WA(J+NI)*W(J)                                            1650
      J = ISTT+1                                                       1660
   48 IKK = J-JA                                                       1670
      JA = J-1                                                         1680
      IF(NN+NR-1.GT.IM)    GOTO 58                                     1690
      IF(IKK.GE.3)    GOTO 52                                          1700
      IKK = 2                                                          1710
      EN(2) = AM                                                       1720
      F(2) = F(1)                                                      1730
      GOTO 56                                                          1740
   52 EN(IKK) = AM                                                     1750
      T = (F(IKK-2)-F(IKK-1))/(EN(IKK-2)-EN(IKK-1))                    1760
      F(IKK) = F(IKK-1)+T*(AM-EN(IKK-1))                               1770
C                                                                      1780
C*****SPEKTRUMSGEWICHTETE ENERGIEINTEGRATION************************** 1790
   56 CALL SPRAL(KSPE,KSPEK,MAZ,ESP,SPEK,NTT,ET,ST,L,IKK,EN,F,G,       1800
     1             ELSIG(L,NR,NN),NSPEK,LSPEK,NLE)                     1810
   58 CONTINUE                                                         1820
   64 CONTINUE                                                         1830
   66 CONTINUE                                                         1840
C                                                                      1850
C*****NORMIERUNG****************************************************** 1860
      JA = 1                                                           1870
      DO 70  NT = NANF,NEND                                            1880
      NN = NANF+NEND-NT                                                1890
      AM = ABN(NN)                                                     1900
      DO 67  J = JA,ISTT                                               1910
      IF(E(J).GT.AM)    GOTO 68                                        1920
      I = J-JA+1                                                       1930
      EN(I) = E(J)                                                     1940
   67 F(I) = 1.                                                        1950
      J = ISTT+1                                                       1960
   68 IKK = J-JA                                                       1970
      JA = J-1                                                         1980
      EN(IKK) = AM                                                     1990
      F(IKK) = 1.                                                      2000
      DO 70  L = 1,NP                                                  2010
      CALL SPRAL(KSPE,KSPEK,MAZ,ESP,SPEK,NTT,ET,ST,L,IKK,EN,F,G,       2020
     1             RSP(L,NN),NSPEK,LSPEK,NLE)                          2030
      II = MINO(NUEB,IM-NN+1)                                          2040
```

```
      DO 69  I = 1,II                                                   2050
   69 ELSIG(L,I,NN) = ELSIG(L,I,NN)/RSP(L,NN)                           2060
   70 CONTINUE                                                          2070
C                                                                       2080
C***** L-GEWICHTETE TOTALE QUERSCHNITTE ********************************2090
      IF(NGT.EQ.0)   RETURN                                             2100
      JA = 2                                                            2110
      DO 82  NT = NANF,NEND                                             2120
      NN = NANF+NEND-NT                                                 2130
      AM = ABN(NN)                                                      2140
      DO 72  J = JA,NGG                                                 2150
      IF(EG(J).GT.AM)   GOTO 74                                         2160
      I = J-JA+2                                                        2170
      E(I) = EG(J)                                                      2180
   72 F(I) = SG(J)                                                      2190
      J = NGG+1                                                         2200
   74 IKK = J-JA+1                                                      2210
      T = (SG(JA)-SG(JA-1))/(EG(JA)-EG(JA-1))                           2220
      E(1) = ABN(NN+1)                                                  2230
      F(1) = SG(JA-1)+T*(E(1)-EG(JA-1))                                 2240
      IF(IKK.GT.1)   GOTO 76                                            2250
      E(2) = AM                                                         2260
      F(2) = SG(JA-1)+T*(E(2)-EG(JA-1))                                 2270
      IKK = 2                                                           2280
      GOTO 78                                                           2290
   76 IF(J.EQ.NGG+1)   GOTO 78                                          2300
      T = (SG(J)-SG(J-1))/(EG(J)-EG(J-1))                               2310
      F(IKK) = F(IKK)+T*(AM-EG(J-1))                                    2320
      E(IKK) = AM                                                       2330
   78 DO 80  L = 1,NP                                                   2340
      CALL SPRAL(KSPE,KSPEK,MAZ,ESP,SPEK,NTT,ET,ST,L,IKK,F,F,G,VAL,     2350
     1           NSPEK,LSPEK,NLE)                                       2360
   80 SGTOT(L,NN) = VAL/RSP(L,NN)                                       2370
   82 JA = J                                                            2380
C                                                                       2390
      RETURN                                                            2400
C                                                                       2410
      END                                                               2420
```

```
      SUBROUTINE IPOLIN(M,A,B,N,X,Y,HR)                                  10
C                                                                        20
C*****LINEARE INTERPOLATION*************************************************30
C                                                                        40
      DIMENSION A(M),B(M),X(N),Y(N),HR(M)                                50
C                                                                        60
      NM = N-1                                                           70
C                                                                        80
C*****KOEFFIZIENTEN HR ******************************************************90
      MM = M-1                                                          100
      DO 6  I = 1,MM                                                    110
    6 HR(I) = (B(I+1)-B(I))/(A(I+1)-A(I))                               120
C                                                                       130
```

```
C*****INTERPOLATION*********************************************************140
      Y(1) = B(1)                                                       150
      Y(N) = B(M)                                                       160
      I = 1                                                             170
      DO 14  J = 2,NM                                                   180
    8 IF(A(I+1)-X(J))   9,10,11                                         190
    9 I = I+1                                                           200
      GOTO 8                                                            210
   10 Y(J) = B(I+1)                                                     220
      GOTO 14                                                           230
   11 Y(J) = B(I)+HR(I)*(X(J)-A(I))                                     240
   14 CONTINUE                                                          250
C                                                                       260
      RETURN                                                            270
C                                                                       280
      END                                                               290
```

```
      SUBROUTINE SPRAL(KS,NS,MZ,E,S,NTT,ET,ST,L,IKK,EN,H,G,VAL,NP,NL,    10
     1NLE)                                                               20
C                                                                        30
C***** GEWICHTETE INTEGRATION                                            40
C                                                                        50
      REAL*8  W,WER                                                      60
      DIMENSION E(NP),S(NL),EN(IKK),G(IKK),H(IKK),ET(NTT),ST(NTT),MZ(2)  70
C                                                                        80
      WW(D1,D2,D3,S1,S2,S3) = (S1*D2*D3+D1*S2*D3+D1*D2*S3)/3.+S1*S2*S3    90
C                                                                       100
C***** MAKROSPEKTRUM  1/E                                               110
      IF(KS.NE.0)   GOTO 16                                             120
      DO 2  I = 1,IKK                                                   130
    2 G(I) = PHI(EN(I))                                                 140
      GOTO 24                                                           150
C                                                                       160
C***** MAKROSPEKTRUM AUS PUNKTWEISER EINGABE                            170
   16 NN = 2                                                            180
      DO 22  I = 1,IKK                                                  190
      DO 18  N = NN,NS                                                  200
      M = N                                                             210
      IF(MZ(1).NE.0)   M = M+(L-1)*NL/(NLE+1)                           220
      IF(E(N)-EN(I))   18,19,20                                         230
   18 CONTINUE                                                          240
      N = NS                                                            250
   19 G(I) = S(M)                                                       260
      NN = N                                                            270
      GOTO 22                                                           280
   20 G(I) = S(M-1)+(S(M)-S(M-1))/(E(N)-E(N-1))*(EN(I)-E(N-1))          290
      IF(N.GT.2)   NN = N-1                                             300
   22 CONTINUE                                                          310
C                                                                       320
C***** INTERVALLINTEGRALE OHNE MIKROWICHTUNG                            330
   24 WER = 0.                                                          340
      IF(NTT.GT.1)   GOTO 28                                            350
```

```
      IK = IKK-1                                                        360
      DO 26  I = 1,IK                                                   370
      D1 = H(I+1)-H(I)                                                  380
      S1 = H(I+1)+H(I)                                                  390
      D2 = G(I+1)-G(I)                                                  400
      S2 = G(I+1)+G(I)                                                  410
      DE = EN(I+1)-EN(I)                                                420
   26 WER = WER+(D1*D2/3.+S1*S2)*DE                                     430
      VAL = .25*WER                                                     440
      RETURN                                                            450
C                                                                       460
C***** INTERVALLINTEGRALE MIT  MIKROWICHTUNG                           470
   28 DO 27  M = 2,NTT                                                  480
      IF(ET(M)-EN(1))   27,27,29                                        490
   27 CONTINUE                                                          500
      M = NTT                                                           510
   29 IK = IKK-1                                                        520
      DO 54  I = 1,IK                                                   530
      N = M                                                             540
      IF(I.GT.1)   GOTO 32                                              550
      STE = ST(N)+(EN(I)-ET(N))*(ST(N)-ST(N-1))/(ET(N)-ET(N-1))         560
      IF(NTT.EQ.2)   GOTO 35                                            570
      DO 30  N = 2,NTT                                                  580
      IF(ET(N)-EN(I))   30,30,32                                        590
   30 CONTINUE                                                          600
      N = NTT                                                           610
   32 DO 34  M = N,NTT                                                  620
      IF(ET(M)-EN(I+1))   34,35,35                                      630
   34 CONTINUE                                                          640
      M = NTT                                                           650
   35 STA = STE                                                         660
      STE = ST(M)+(EN(I+1)-ET(M))*(ST(M-1)-ST(M))/(ET(M-1)-ET(M))       670
      DE = EN(I+1)-EN(I)                                                680
      TH = (H(I+1)-H(I))/DE                                             690
      AH = H(I)-TH*EN(I)                                                700
      TG = (G(I+1)-G(I))/DE                                             710
      AG = G(I)-TG*EN(I)                                                720
      IF(MZ(2).EQ.0)   GOTO 36                                          730
      IF(L.GT.2)   GOTO 48                                              740
      GOTO(36,42),L                                                     750
C***** 0. MOMENT                                                       760
   36 IF(M.GT.N)   GOTO 38                                              770
      D1 = H(I+1)-H(I)                                                  780
      S1 = H(I+1)+H(I)                                                  790
      D2 = G(I+1)-G(I)                                                  800
      S2 = G(I+1)+G(I)                                                  810
      U = 1./STA                                                        820
      V = 1./STE                                                        830
      D3 = V-U                                                          840
      S3 = V+U                                                          850
      W = WW(D1,D2,D3,S1,S2,S3)*DE                                      860
      GOTO 54                                                           870
   38 U = H(I)                                                          880
      V = TH*ET(N)+AH                                                   890
      D1 = V-U                                                          900
      S1 = V+U                                                          910
      U = G(I)                                                          920
      V = TG*ET(N)+AG                                                   930
      D2 = V-U                                                          940
      S2 = V+U                                                          950
      U = 1./STA                                                        960
      V = 1./ST(N)                                                      970
      D3 = V-U                                                          980
      S3 = V+U                                                          990
      DE = ET(N)-EN(I)                                                 1000
      W = WW(D1,D2,D3,S1,S2,S3)*DE                                     1010
      MM = M-1                                                         1020
      U = TH*ET(MM)+AH                                                 1030
      V = H(I+1)                                                       1040
      D1 = V-U                                                         1050
      S1 = V+U                                                         1060
      U = TG*ET(MM)+AG                                                 1070
      V = G(I+1)                                                       1080
      D2 = V-U                                                         1090
      S2 = V+U                                                         1100
      U = 1./ST(MM)                                                    1110
      V = 1./STE                                                       1120
      D3 = V-U                                                         1130
      S3 = V+U                                                         1140
      DE = EN(I+1)-ET(MM)                                              1150
      W = W+WW(D1,D2,D3,S1,S2,S3)*DE                                   1160
      IF(N.EQ.MM)   GOTO 54                                            1170
      MM = M-2                                                         1180
      VH = TH*ET(N)+AH                                                 1190
      VG = TG*ET(N)+AG                                                 1200
      VS = 1./ST(N)                                                    1210
      DO 40  J = N,MM                                                  1220
      JP = J+1                                                         1230
      UH = VH                                                          1240
      UG = VG                                                          1250
      US = VS                                                          1260
      VH = TH*ET(JP)+AH                                                1270
      VG = TG*ET(JP)+AG                                                1280
      VS = 1./ST(JP)                                                   1290
      D1 = VH-UH                                                       1300
      S1 = VH+UH                                                       1310
      D2 = VG-UG                                                       1320
      S2 = VG+UG                                                       1330
      D3 = VS-US                                                       1340
      S3 = VS+US                                                       1350
      DE = ET(JP)-ET(J)                                                1360
   40 W = W+WW(D1,D2,D3,S1,S2,S3)*DE                                   1370
      GOTO 54                                                          1380
C***** 1. MOMENT                                                       1390
   42 IF(M.GT.N)   GOTO 44                                             1400
      D1 = H(I+1)-H(I)                                                 1410
      S1 = H(I+1)+H(I)                                                 1420
      D2 = G(I+1)-G(I)                                                 1430
      S2 = G(I+1)+G(I)                                                 1440
      U = 1./(STA*STA)                                                 1450
```

```
      V = 1./(STE*STE)                                                  1460
      D3 = V-U                                                          1470
      S3 = V+U                                                          1480
      W = WW(D1,D2,D3,S1,S2,S3)*DE                                      1490
      GOTO 54                                                           1500
   44 U = H(I)                                                          1510
      V = TH*ET(N)+AH                                                   1520
      D1 = V-U                                                          1530
      S1 = V+U                                                          1540
      L = G(I)                                                          1550
      V = TG*ET(N)+AG                                                   1560
      D2 = V-U                                                          1570
      S2 = V+U                                                          1580
      U = 1./(STA*STA)                                                  1590
      V = 1./(ST(N)*ST(N))                                              1600
      D3 = V-U                                                          1610
      S3 = V+U                                                          1620
      DE = ET(N)-EN(I)                                                  1630
      W = WW(D1,D2,D3,S1,S2,S3)*DE                                      1640
      MM = M-1                                                          1650
      U = TH*ET(MM)+AH                                                  1660
      V = H(I+1)                                                        1670
      D1 = V-U                                                          1680
      S1 = V+U                                                          1690
      U = TG*ET(MM)+AG                                                  1700
      V = G(I+1)                                                        1710
      D2 = V-U                                                          1720
      S2 = V+U                                                          1730
      U = 1./(ST(MM)*ST(MM))                                            1740
      V = 1./(STE*STE)                                                  1750
      D3 = V-U                                                          1760
      S3 = V+U                                                          1770
      DE = EN(I+1)-ET(MM)                                               1780
      W = W+WW(D1,D2,D3,S1,S2,S3)*DE                                    1790
      IF(N.EQ.MM)    GOTO 54                                            1800
      MM = M-2                                                          1810
      VH = TH*ET(N)+AH                                                  1820
      VG = TG*ET(N)+AG                                                  1830
      VS = 1./(ST(N)*ST(N))                                             1840
      DO 46  J = N,MM                                                   1850
      JP = J+1                                                          1860
      UH = VH                                                           1870
      UG = VG                                                           1880
      US = VS                                                           1890
      VH = TH*ET(JP)+AH                                                 1900
      VG = TG*ET(JP)+AG                                                 1910
      VS = 1./(ST(N)*ST(N))                                             1920
      D1 = VH-UH                                                        1930
      S1 = VH+UH                                                        1940
      D2 = VG-UG                                                        1950
      S2 = VG+UG                                                        1960
      D3 = VS-US                                                        1970
      S3 = VS+US                                                        1980
      DE = ET(JP)-ET(J)                                                 1990
   46 W = W+WW(D1,D2,D3,S1,S2,S3)*DE                                    2000
      GOTO 54                                                           2010
C***** 2. UND HOEHERE MOMENTE                                           2020
   48 IF(M.GT.N)   GOTO 50                                              2030
      D1 = H(I+1)-H(I)                                                  2040
      S1 = H(I+1)+H(I)                                                  2050
      D2 = G(I+1)-G(I)                                                  2060
      S2 = G(I+1)+G(I)                                                  2070
      U = 1./STA**L                                                     2080
      V = 1./STE**L                                                     2090
      D3 = V-U                                                          2100
      S3 = V+U                                                          2110
      W = WW(D1,D2,D3,S1,S2,S3)*DE                                      2120
      GOTO 54                                                           2130
   50 U = H(I)                                                          2140
      V = TH*ET(N)+AH                                                   2150
      D1 = V-U                                                          2160
      S1 = V+U                                                          2170
      U = G(I)                                                          2180
      V = TG*ET(N)+AG                                                   2190
      D2 = V-U                                                          2200
      S2 = V+U                                                          2210
      U = 1./STA**L                                                     2220
      V = 1./ST(N)**L                                                   2230
      D3 = V-U                                                          2240
      S3 = V+U                                                          2250
      DE = ET(N)-EN(I)                                                  2260
      W = WW(D1,D2,D3,S1,S2,S3)*DE                                      2270
      MM = M-1                                                          2280
      U = TH*ET(MM)+AH                                                  2290
      V = H(I+1)                                                        2300
      D1 = V-U                                                          2310
      S1 = V+U                                                          2320
      U = TG*ET(MM)+AG                                                  2330
      V = G(I+1)                                                        2340
      D2 = V-U                                                          2350
      S2 = V+U                                                          2360
      U = 1./ST(MM)**L                                                  2370
      V = 1./STE**L                                                     2380
      D3 = V-U                                                          2390
      S3 = V+U                                                          2400
      DE = EN(I+1)-ET(MM)                                               2410
      W = W+WW(D1,D2,D3,S1,S2,S3)*DE                                    2420
      IF(N.EQ.MM)    GOTO 54                                            2430
      MM = M-2                                                          2440
      VH = TH*ET(N)+AH                                                  2450
      VG = TG*ET(N)+AG                                                  2460
      VS = 1./ST(N)**L                                                  2470
      DO 52  J = N,MM                                                   2480
      JP = J+1                                                          2490
      UH = VH                                                           2500
      UG = VG                                                           2510
      US = VS                                                           2520
      VH = TH*ET(JP)+AH                                                 2530
      VG = TG*ET(JP)+AG                                                 2540
      VS = 1./ST(JP)**L                                                 2550
```

```
      D1 = VH-UH                                                        2560
      S1 = VH+UH                                                        2570
      D2 = VG-UG                                                        2580
      S2 = VG+UG                                                        2590
      D3 = VS-US                                                        2600
      S3 = VS+US                                                        2610
      DE = ET(JP)-ET(J)                                                 2620
   52 W = W+WW(D1,D2,D3,S1,S2,S3)*DE                                    2630
   54 WER = WER+W                                                       2640
      VAL = .125*WER                                                    2650
C                                                                       2660
      RETURN                                                            2670
C                                                                       2680
      END                                                               2690
```

```
      SUBROUTINE MUKON(ELSIG,ELTOT,NLE,NECU,NUEB,IL,IM,NGR,MASSE)        10
C                                                                        20
C*****MULTIGRUPPENKONSTANTEN*************************************       30
C                                                                        40
      DIMENSION ELSIG(6,NECU,NGR),ELTOT(2,NGR)                           50
C                                                                        60
      NP = NLE+1                                                         70
C*****TOTALER STREUQUERSSCHNITT**********************************       80
      DO 14  NN = IL,IM                                                  90
      STO = 0.                                                          100
      DO 12  NS = 1,NUEB                                                110
      NT = NS+NN-1                                                      120
      STO = STO+ELSIG(1,NS,NN)                                          130
      IF(NT.EQ.IM)   GOTO 14                                            140
   12 CONTINUE                                                          150
   14 ELTOT(1,NN) = STO                                                 160
C                                                                       170
C*****NORMIERUNG AUF DEN TOTALEN STREUQUERSCHNITT*********************  180
   22 DO 26  L = 1,NP                                                   190
      DO 26 NN=IL,IM                                                    200
      DO 24  I = 1,NUEB                                                 210
      NT=I+NN-1                                                         220
      ELSIG(L,I,NN) = ELSIG(L,I,NN)/ELTOT(1,NN)                         230
      IF(NT.EQ.IM)  GO TO 26                                            240
   24 CONTINUE                                                          250
   26 CONTINUE                                                          260
C                                                                       270
C*****MITTLERER STREUKOSINUS*************************************       280
   15 DO  20  NN = IL,IM                                                290
      STO = 0.                                                          300
      DO 18  NS = 1,NUEB                                                310
      NT = NS+NN-1                                                      320
      STO = STO+ELSIG(2,NS,NN)                                          330
      IF(NT.EQ.IM)   GOTO 20                                            340
   18 CONTINUE                                                          350
   20 ELTOT(2,NN) = STO                                                 360
C                                                                       370
```

```
C*****ABSCHNEIDEN (NULLSETZEN) VON GROESSEN KLEINER 1.E-6 **********  380
      IF(MASSE.EQ.1)   RETURN                                           390
      DO 40  L = 1,NP                                                   400
      DO 40 NN=IL,IM                                                    410
      DO 38  I = 1,NUEB                                                 420
      NT=I+NN-1                                                         430
      ELSIG(L,I,NN) = AINT(ELSIG(L,I,NN)*1.E+5)*1.E-5                   440
      IF(NT.EQ.IM)  GO TO 40                                            450
   38 CONTINUE                                                          460
   40 CONTINUE                                                          470
C                                                                       480
      RETURN                                                            490
C                                                                       500
      END                                                               510
```

```
      SUBROUTINE PRINT(ELSIG,ELTOT,NLA,NLE,NECU,NUEB,ISEL,NGR,KSPEK,     10
     -                 MAZ,NTK,KIM,NGT,SGTOT,RSP,MASSE,NGS)              20
C                                                                        30
C*****SUBROUTINE ZUM AUSDRUCKEN DER STREUMATRIX,DER STREUKOSINUSMATRIX**  40
C                                                                        50
      REAL*8 STOFF,MMM                                                   60
      DIMENSION  ELSIG(6,NECU,NGR),ELTOT(2,NGR),MAZ(2),SGTOT(6,NGR),     70
     -           RSP(6,NGR)                                              80
      COMMON STOFF,ISTRUK,ISPA,NOUT,KPR,NEND,NANF                        90
C                                                                       100
      NP = NLE+1                                                        110
C                                                                       120
C*****AUSDRUCKEN DER STREUMATRIZEN*******************************       130
      DO 3  L = 1,NP                                                    140
      LM = L-1                                                          150
      WRITE(NOUT,21) LM,LM,STOFF                                        160
      IF(IABS(ISEL).EQ.1)   WRITE(NOUT,28) NGS                          170
      I1 = NANF                                                         180
    1 I2 = I1+MIN0(9,NEND-I1)                                           190
      WRITE(NOUT,24)   (I,I = I1,I2)                                    200
      WRITE(NOUT,19)                                                    210
      DO 2  I = 1,NUEB                                                  220
      I3=MIN0(I2,NEND+KIM-I+1)                                          230
      IF(I3.LT.I1)  GO TO 2                                             240
      WRITE(NOUT,22) (ELSIG(L,I,NN    ),NN=I1,I3)                       250
    2 CONTINUE                                                          260
      WRITE(NOUT,20)                                                    270
      IF(I2.GE.NEND)  GOTO 3                                            280
      I1 = I2+1                                                         290
      GOTO 1                                                            300
    3 CONTINUE                                                          310
      WRITE(NOUT,52)                                                    320
C                                                                       330
C*****INFORMATIONEN UEBER DIE WICHTUNG***************************       340
      WRITE(NOUT,30)                                                    350
      IF(KSPEK.GT.0.AND.MAZ(1).EQ.0)WRITE(NOUT,32)                      360
      IF(KSPEK.GT.0.AND.MAZ(1).EQ.1)WRITE(NOUT,34)   NLE                370
```

```
      IF(KSPEK.EQ.0.AND.MAZ(1).EQ.C)WRITE(NOUT,36)                      380
      IF(KSPEK.EQ.0.AND.MAZ(1).EQ.1)WRITE(NOUT,38)                      390
      WRITE(NOUT,40)                                                    400
      IF(NTK.EQ.1.AND.MAZ(2).EQ.0)WRITE(NOUT,42)                        410
      IF(NTK.EQ.1.AND.MAZ(2).EQ.1)WRITE(NOUT,44)   NLE                  420
      IF(NTK.EQ.0)  WRITE(NOUT,46)                                      430
      WRITE(NOUT,47)                                                    440
C                                                                       450
C*****AUSDRUCKEN DER TOTALEN ELAST. QUERSCHNITTE UND STREUKOSINUS        460
      WRITE(NOUT,27)   STOFF                                            470
      IF(MASSE.EQ.1)   WRITE(NOUT,29)                                   480
      IF(IABS(ISEL).EQ.1)   WRITE(NOUT,28) NGS                          490
      I1 = NANF                                                         500
    9 I2 = I1+MINO(9,NEND-I1)                                           510
      WRITE(NOUT,24)   (I,I = I1,I2)                                    520
      WRITE(NOUT,19)                                                    530
      DO 10  I = 1,2                                                    540
   10 WRITE(NOUT,25)   (ELTOT(I,NN),NN = I1,I2)                         550
      WRITE(NOUT,20)                                                    560
      IF(I2.GE.NEND)   GOTO 11                                          570
      I1 = I2+1                                                         580
      GOTO 9                                                            590
   11 WRITE(NOUT,54)                                                    600
C                                                                       610
C*****AUSDRUCKEN DER TOTALEN QUERSCHNITTE*******************************620
      IF(NGT.EQ.0)   GOTO 15                                            630
      WRITE(NOUT,48)   STOFF                                            640
      IF(IABS(ISEL).EQ.1)   WRITE(NOUT,28) NGS                          650
      I1 = NANF                                                         660
   12 I2 = I1+MINO(9,NEND-I1)                                           670
      WRITE(NOUT,24)   (I,I=I1,I2)                                      680
      WRITE(NOUT,19)                                                    690
      DO 13  L = 1,NP                                                   700
   13 WRITE(NOUT,25)   (SGTOT(L,NN),NN=I1,I2)                           710
      WRITE(NOUT,20)                                                    720
      IF(I2.GE.NEND)   GOTO 14                                          730
      I1 = I2+1                                                         740
      GOTO 12                                                           750
   14 WRITE(NOUT,50)                                                    760
C                                                                       770
C*****ALSDRUCKEN DER NORMIERUNGSINTEGRALE*******************************780
   15 WRITE(NOUT,66)   NLE                                              790
      I1 = NANF                                                         800
   16 I2 = I1+MINO(9,NEND-I1)                                           810
      WRITE(NOUT,24)   (I,I=I1,I2)                                      820
      WRITE(NOUT,19)                                                    830
      DO 17  L = 1,NP                                                   840
   17 WRITE(NOUT,25)   (RSP(L,NN),NN=I1,I2)                             850
      WRITE(NOUT,20)                                                    860
      IF(I2.GE.NEND)   GOTO 23                                          870
      I1 = I2+1                                                         880
      GOTO 16                                                           890
   23 WRITE(NOUT,68)                                                    900
C                                                                       910
C*****RESERVIEREN DER RESULTATE*****************************************920
```

```
      CALL DOPW(8HFLUM    ,MMM)                                         930
      I=C                                                               940
      WRITE (KPR) I,MMM                                                 950
      I1=NANF                                                           960
      I2=NEND                                                           970
      I=4                                                               980
      L=NLE-NLA+1                                                       990
      NN=I2-I1+1                                                       1000
      WRITE (KPR)I,STOFF,NN,L                                          1010
      I=3+L                                                            1020
      DO 31 NN=I1,I2                                                   1030
      WRITE (KPR) I,NN,ELTOT(1,NN),ELTOT(2,NN),(SGTOT(K,NN),K=1,L)     1040
   31 CONTINUE                                                         1050
      DO 33  L = 1,NP                                                  1060
      LM=L-1                                                           1070
      DO 33 NN=I1,I2                                                   1080
      LL=MINO(NUEB,I2+KIM-NN+1)                                        1090
      I=LL+2                                                           1100
      WRITE (KPR)     I,LM,NN,(ELSIG(L,K,NN ),K=1,LL)                  1110
   33 CONTINUE                                                         1120
C                                                                      1130
      RETURN                                                           1140
C                                                                      1150
   19 FORMAT(1H )                                                      1160
   20 FORMAT(1HO)                                                      1170
   21 FORMAT(1HO//29X,'SGNC',I1,8X,'ELASTISCHE STREUMATRIX  ',I1,'. ORDN 1180
     1UNG FUER  ',A8//)                                               1190
   22 FORMAT(1X,10E13.5)                                               1200
   24 FORMAT(1X,10(I6,'.GRUPPE'))                                      1210
   25 FORMAT(1X,1P10E13.5)                                             1220
   27 FORMAT(1HO//20X,'TOTALE ELASTISCHE GRUPPENSTREUQUERSCHNITTE SGN UN 1230
     1D GRUPPENSTREUKOSINUS MUEL FUER ',A8//)                         1240
   28 FORMAT(42X,'SGN(E) = SGT(E) = 1  GESETZT AB GRUPPE',I4//)        1250
   29 FORMAT(20X,'** BEI WASSERSTOFF WIRD UNTERHALB 10 EV DIE STREUUNG I 1260
     1M SCHWERPUNKTSYSTEM ISOTROP ANGENOMMEN'/20X,'** UND FS WIRD DER MI 1270
     3TTLERE STREUKOSINUS IM LABORSYSTEM GLEICH 0.6667GESETZT **'//)   1280
   30 FORMAT(////42X,'M A K R O W I C H T U N G  F'/)                  1290
   32 FORMAT(42X,'ALLE MOMENTE WIE DAS 0. MOMENT MIT DEM'/             1300
     1       42X,'EINGELESENEN PUNKTSPEKTRUM F(E,1)')                 1310
   34 FORMAT(42X,'DAS L-TE MOMENT MIT DEM (L+1)-TEN EINGE-'/           1320
     1       42X,'LESENEN PUNKTSPEKTRUM F(E,L+1), L = 0,1,...',I2)    1330
   36 FORMAT(42X,'ALLE MOMENTE WIE DAS 0. MOMENT MIT'/                 1340
     1       42X,'F(E,1)   (STANDARD F(E,1) = 1/E)')                  1350
   38 FORMAT(42X,'DAS L-TE MOMENT MIT F(E,1)'/                         1360
     1       42X,'(STANDARD F(E,1) = 1/E)')                           1370
   40 FORMAT(///42X,'M I K R O W I C H T U N G  FS  (FEINSTRUKTUR)'/)  1380
   42 FORMAT(42X,'ALLE MOMENTE WIE DAS 0. MOMENT MIT FS(E,1)=1/SGT(E)'/ 1390
     1       42X,'SGT(E)=TOTALER QUERSCHNITT DER EINGELESENEN MISCHUNG') 1400
   44 FORMAT(42X,'DAS L-TE MOMENT MIT FS(E,L+1), L = 0,1,...',I2/      1410
     1       42X,'(STANDARD FS(E,L)=1/SGT(E)**L )'/                   1420
     2       42X,'SGT(E)=TOTALER QUERSCHNITT DER EINGELESENEN MISCHUNG') 1430
   46 FORMAT(42X,'ALLE MOMENTE MIT FS(E,1) = 1'/                       1440
     1       42X,'(KEINE FEINSTRUKTURWICHTUNG)')                      1450
   47 FORMAT(///42X,'G E S A M T W I C H T U N G   F * FS')            1460
   48 FORMAT(1HO//44X,'TOTALE GRUPPENQUERSCHNITTE SGT FUER ',A8//)     1470
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```
   50 FORMAT(//29X,'ERLAEUTERUNG'/29X,'G-TE GRUPPE, L-TE ZEILE: TOTALER  1480
     -QUERSCHNITT DER G-TEN GRUPPE,'/29X,'GEWICHTET MIE DAS (L-1)-TE MOM 1490
     -ENT DER STREUMATRIX')                                              1500
   52 FORMAT(//29X,'ERLAEUTERUNG'/29X,'L-TE ORDNUNG, G-TE GRUPPE, I-TE Z 1510
     1EILE: MATRIXELEMENT L-TER ORDNUNG'/29X,'FUER STREUUNG AUS DER G-TE 1520
     2N GRUPPE IN DIE (G+I-1)-TE GRUPPE, BEZOGEN'/29X,'AUF DEN TOTALEN E 1530
     3LASTISCHEN QUERSCHNITT (TOTALES C.MOMENT) DER'/29X,'G-TEN GRUPPE') 1540
   54 FORMAT(//29X,'ERLAEUTERUNG'/29X,'G-TE GRUPPE, I. ZEILE: TOTALER EL 1550
     1ASTISCHER QUERSCHNITT DER G-TEN'/29X,'GRUPPE'/29X,'G-TE GRUPPE, 2. 1560
     2 ZEILE: MITTLERER STREUKOSINUS DER G-TEN GRUPPE')                  1570
   66 FORMAT(////42X,'NORMIERUNGSINTEGRALE BIS ZUM',I3,'. MOMENT'//)     1580
   68 FORMAT(//29X,'ERLAEUTERUNG'/29X,'G-TE GRUPPE, L-TE ZEILE: (L-1)-TE 1590
     -S MOMENT DES WICHTUNGSSPEKTRUMS'/29X,'INTEGRIERT UEBER DIE G-TE GR 1600
     -UPPE')                                                             1610
C                                                                        1620
      END                                                                1630
```

```
      SUBROUTINE INFORM(ALFA,NEGR,ABN,R,IL,IM,INTT,IAT,NST,NSTIS,          10
     1                  IR,ISTT,K,NTK,NTT,NOUT)                            20
C                                                                         30
C*****INFORMATIONEN************************************************       40
C                                                                         50
      DIMENSION  ABN(NEGR),R(NEGR),INT(NEGR),NST(6),NA(6),NB(6)           60
C                                                                         70
      IF(IR.GT.1)   GOTO 6                                                80
      WRITE(NOUT,919)                                                     90
      WRITE(NOUT,935)   ALFA                                             100
    3 DO 5  I = 1,6                                                      110
      NA(I) = I-1                                                        120
    5 NB(I) = NSTIS                                                      130
      WRITE(NOUT,936)   (NA(I),I = 1,6),(NB(I),I = 1,6),                 140
     1                  (NST(I),I = 1,6)                                 150
    6 IF(IR+1.LT.INTT)   GOTO 7                                          160
      WRITE(NOUT,932)                                                    170
      DO 4  I = IL, IM                                                   180
    4 WRITE(NOUT,933)   I,ABN(I),ABN(I+1),R(I)                           190
      WRITE(NOUT,934)                                                    200
    7 I1 = INT(IR+1)+1                                                   210
      I2 = INT(IR)+1                                                     220
      IF(IR.EQ.1)   I2 = I2-1                                            230
      WRITE(NOUT,909)                                                    240
      EFIN = AMAX1(ALFA*ABN(I1),ABN(IM+1))                               250
      WRITE(NOUT,920)   IR,IR,ABN(I1),ABN(I2)                            260
      WRITE(NOUT,921)   IR,EFIN,ABN(I2)                                  270
      WRITE(NOUT,922)   IR,ISTT                                          280
      WRITE(NOUT,925)   K                                                290
      IF(NTK.EQ.1)  WRITE(NOUT,126) NTT                                  300
      RETURN                                                             310
C                                                                        320
  909 FORMAT(1HO)                                                        330
  919 FORMAT(1HO//24X,'I N F O R M A T I O N E N'//)                     340
  920 FORMAT(1HO,I2,'. AUSSTREUINTERVALL = ',I2,'. MAKROGRUPPE', 5X,E10. 350
     14,' EV',' - ',E10.4,' EV')                                         360
  921 FORMAT(1HO,I2,'. EINSTREUINTERVALL',23X,E10.4,' EV',' - ',E10.4,   370
     1' EV')                                                             380
  922 FORMAT(1HO,'ZAHL DER ENERGIESTUETZPUNKTE IM ',I2,'. AUSSTREUINTERV 390
     1ALL',18X,I4)                                                       400
  925 FORMAT(1HO,'ZAHL DER GELESENEN SCA IM AUSSTREUINTERVALL',28X,I4)    410
  932 FORMAT(////16X,'F E I N G R U P P E N E I N T E I L U N G'///)     420
  933 FORMAT(1X,I3,'.GRUPPE',1X,1PE10.3,' EV  -',1PE10.3,' EV',1X,'DU =  430
     -',E9.2)                                                            440
  934 FORMAT(////18X,'DU = LETHARGIEDIFFERENZ')                          450
  935 FORMAT(1HO,'ALFA = ',F8.5)                                         460
  936 FORMAT(1HO,'WINKELSTUETZSTELLEN'//12X,'MOMENT',5X,6(3X,I3)/12X,'IS 470
     1OTROPIE',3X,6(3X,I3)/12X,'ANISOTROPIE',1X,6(3X,I3))                480
  126 FORMAT(1HO,'ZAHL DER SGT FUER FEINSTRUKTURWICHTUNG IM AUSSTREUINTE 490
     1RVALL',11X,I5)                                                     500
C                                                                        510
      END                                                                520
```

```
C     BESTIMMUNG DER 1/V - WERTE                                          10
C                                                                         20
      SUBROUTINE EDV (NE,ENG,NSP,E,F,EPS,V,NEF,ST,FI,IW)                  30
      REAL*8 MAT,MMM                                                      40
      DIMENSION ENG(NE),E(NSP),F(NSP),V(NE),ST(NEF),FI(NEF)               50
      COMMON MAT,ISTRUK,ISPA,NOUTP,JA,NANF,NEND,KL                        60
      DATA MMM/'SI/V    '/                                                70
      WRITE (NOUTP,1)                                                     80
    1 FORMAT(1HO/1HO/' EDV - A PROGRAM FOR THE CALCULATION OF THE 1/V AV  90
     1ERAGE GROUP VALUES'/)                                             100
      IW=0                                                               110
      JF=0                                                               120
      C=7.229286E-7                                                      130
      L=NE-1                                                             140
      IF(NSP.GT.1)  GO TO 9                                              150
C                                                                        160
C     WICHTUNGSFUNKTION E(E) IST ALS FUNCTION GEGEBEN                    170
C                                                                        180
      NN=1                                                               190
      LI=L                                                               200
   36 DO 2 II=NN,LI                                                      210
      K=10                                                               220
      ER1=ENG(II)                                                        230
      ER2=ENG(II+1)                                                      240
    4 M=1                                                                250
      ST(M)=ER1                                                          260
      DO 3 J=1,K                                                         270
      M=M+1                                                              280
      IF(M.LE.NEF)  GO TO 31                                             290
      NEF=K+1                                                            300
      IW=1                                                               310
      GO TO 30                                                           320
   31 ST(M)=ER1+FLOAT(J)*(ER2-ER1)/FLOAT(K)                              330
    3 CONTINUE                                                           340
```

```
      Z1=0.                                                              350
      XN1=0.                                                             360
      N=1                                                                370
    7 FI1=PHI(ST(1))                                                     380
      DO 5 J=1,K                                                         390
      FI2=PHI(ST(J+1))                                                   400
      Z1=Z1+0.5*(FI1*C/SQRT(ST(J))+FI2*C/SQRT(ST(J+1)))*(ST(J+1)-ST(J))  410
      XN1=XN1+0.5*(FI1+FI2)*(ST(J+1)-ST(J))                              420
    5 FI1=FI2                                                            430
      IF(N.EQ.2)  GO TO 6                                                440
      Z2=Z1                                                              450
      XN2=XN1                                                            460
      Z1=0.                                                              470
      XN1=0.                                                             480
      N=2                                                                490
      GO TO 7                                                            500
    6 ABWZ=ABS(Z2-Z1)/Z1                                                 510
      ABWN=ABS(XN2-XN1)/XN1                                              520
      IF(ABWZ.LE.EPS.AND.ABWN.LE.EPS)  GO TO 8                           530
      K=K+K                                                              540
      GO TO 4                                                            550
    8 V(II+1)=Z1/XN1                                                     560
    2 CONTINUE                                                           570
      IF(JF.EQ.1)  GO TO 37                                              580
      V(1)=0.8862269*C/SQRT(0.0253)                                      590
      GO TO 26                                                           600
C                                                                        610
C     WICHTUNGSFUNKTION IST PUNKTWEISE GEGEBEN                           620
C                                                                        630
    9 DO 10 I=1,L                                                        640
      JF=0                                                               650
      ST(1)=ENG(I)                                                       660
      DO 16 J=1,NSP                                                      670
      IF(E(J).LT.ST(1)) GO TO 16                                         680
      IF(E(J).EQ.ST(1)) GO TO 17                                         690
      IF(J.EQ.1)  GO TO 38                                               700
      FI(1)=F(J-1)+(F(J)-F(J-1))/(E(J)-E(J-1))*(ST(1)-E(J-1))            710
      GO TO 18                                                           720
   16 CONTINUE                                                           730
   38 JF=1                                                               740
      NN=I                                                               750
      II=I                                                               760
      GO TO 36                                                           770
   37 J=NE-I                                                             780
      WRITE (NOUTP,35) J                                                 790
   35 FORMAT(1HO/' ***WARNING : IN ENERGYGROUP ',I5,' THE 1/V VALUE IS C 800
     1ALCULATED WITH THE FUNCTION PHI(E)'/14X,                           810
     1'BECAUSE NO POINT OF SPECTRUM IS GIVEN IN THIS GROUP')             820
      GO TO 10                                                           830
   17 FI(1)=F(J)                                                         840
   18 N=J-1                                                              850
      M=1                                                                860
      DO 11 J=N,NSP                                                      870
      IF(E(J).LT.ENG(I))  GO TO 11                                       880
      IF(E(J).LE.ENG(I+1))  GO TO 12                                     890
      GO TO 13                                                           900
   12 M=M+1                                                              910
      IF(M.LE.NEF)  GO TO 32                                             920
      NEF=NSP                                                            930
      IW=1                                                               940
      GO TO 30                                                           950
   32 ST(M)=E(J)                                                         960
      FI(M)=F(J)                                                         970
      GO TO 11                                                           980
   13 N=J-1                                                              990
      GO TO 14                                                          1000
   11 CONTINUE                                                          1010
      GO TO 38                                                          1020
   14 IF(ST(M).EQ.ENG(I+1))  GO TO 15                                   1030
      M=M+1                                                             1040
      IF(M.LE.NEF) GO TO 33                                             1050
      NEF=NEF+1                                                         1060
      IW=1                                                              1070
      GO TO 30                                                          1080
   33 ST(M)=ENG(I+1)                                                    1090
      FI(M)=F(J-1)+(F(J)-F(J-1))/(E(J)-E(J-1))*(ST(M)-E(J-1))           1100
   15 Z1=0.                                                             1110
      XN1=0                                                             1120
      K=1                                                               1130
   23 MM=M-1                                                            1140
      DO 19 J=1,MM                                                      1150
      Z1=Z1+     (C/SQRT(ST(J))*FI(J)+C/SQRT(ST(J+1))*FI(J+1))*(ST(J+1)-1160
     1ST(J))                                                            1170
   19 XN1=XN1+(FI(J)+   FI(J+1))*(ST(J+1)-ST(J))                        1180
      IF(K.EQ.2)  GO TO 20                                              1190
   25 Z2=Z1                                                             1200
      XN2=XN1                                                           1210
      Z1=0.                                                             1220
      XN1=0.                                                            1230
      K=2                                                               1240
      IF(2*M-1.LE.NEF)  GO TO 34                                        1250
      NEF=M                                                             1260
      IW=1                                                              1270
      GO TO 30                                                          1280
   34 DO 21 J=1,M                                                       1290
      MM=M-J                                                            1300
      ST(MM*2+1)=ST(MM+1)                                               1310
   21 FI(MM*2+1)=FI(MM+1)                                               1320
      M=2*M-1                                                           1330

      DO 22 J=2,M,2                                                     1340
      ST(J)=0.5*(ST(J-1)+ST(J+1))                                       1350
   22 FI(J)=0.5*(FI(J-1)+FI(J+1))                                       1360
      GO TO 23                                                          1370
   20 ABWZ=ABS(Z2-Z1)/Z1                                                1380
      ABWN=ABS(XN2-XN1)/XN1                                             1390
      IF(ABWZ.LE.EPS.AND.ABWN.LE.EPS)  GO TO 24                         1400
      GO TO 25                                                          1410
   24 V(I+1)=Z1/XN1                                                     1420
   10 CONTINUE                                                          1430
      V(1)=0.8862269*C/SQRT(C.0253)                                     1440
```

```
C                                                                       1450
C     AUSGABE DER ERGEBNISSE                                            1460
C                                                                       1470
   26 I=0                                                               1480
      WRITE(JA)I,MMM                                                    1490
      WRITE (NOUTP,27)                                                  1500
   27 FORMAT(/' GRUPPE',7X,'1/V')                                       1510
      L=NE                                                              1520
      WRITE (JA) L,(V(I),I=1,L)                                         1530
      DO 28 I=1,L                                                       1540
      K=L-I+1                                                           1550
   28 WRITE (NOUTP,29)I,V(K)                                            1560
   29 FORMAT(I5,E17.8)                                                  1570
      KL=KL+1                                                           1580
   30 RETURN                                                            1590
      END                                                               1600
```

```
      SUBROUTINE CHIINM(E1,E2,TETA,X2)                                    10
      WPI=1.772454                                                        20
      XX1=E1/TETA                                                         30
      XX2=E2/TETA                                                         40
      XR1=SQRT(XX1)                                                       50
      XR2=SQRT(XX2)                                                       60
      IF(XX1.LT.1.0E-03.AND.XX2.LT.1.0E-03) GO TO 3                       70
      IF(XX1.LT.1.317.AND.XX2.LT.1.317) GO TO 1                           80
      ERFSUM=ERFC(XR1)-ERFC(XR2)                                          90
      GO TO 2                                                            100
    1 ERFSUM=ERF(XR2)-ERF(XR1)                                           110
    2 EXPSUM=XR2*EXP(-XX2)-XR1*EXP(-XX1)                                 120
      X2=ERFSUM-EXPSUM*2.0/WPI                                           130
      GO TO 4                                                            140
    3 S1=(XR2*XX2-XR1*XX1)*2.0/3.0                                       150
      S2=(XR2*XX2**2-XR1*XX1**2)*2.0/5.0                                 160
      S3=(XR2*XX2**3-XR1*XX1**3)*2.0/7.0                                 170
      S4=(XR2*XX2**4-XR1*XX1**4)*2.0/9.0                                 180
      X2=(-S4+S3-S2+S1)*2.0/WPI                                          190
    4 RETURN                                                             200
      END                                                                210
```

```
      SUBROUTINE SPALT(NE,ENG,X)                                          10
C                                                                         20
C     BERECHNUNG DES SPALTSPEKTRUMS                                       30
      REAL*8 MAT,FEST(10),NFEST(10),MMM,MNAME                             40
      REAL*8 E,B,C,T,EF,EW,EG,EG1,XG,XG1,YG,YG1,XG2,YG2,XG12,YG12         50
      DIMENSION ENG(NE),NADAT(2),NSATZ(4),X(NE)                           60
      COMMON MAT,ISTRUK,ISPA,NOUTP,JA,NANF,NEND,KL                        70
      EQUIVALENCE(FEST(1),NFEST(1))                                       80
      DATA MNAME/'        '/                                              90
      WRITE (NOUTP,9000)                                                 100
```

```
9000 FORMAT(1HO/1HC/' PROGRAMM KENNZIFFER 7')                            110
     WRITE (NOUTP,9001)                                                  120
9001 FORMAT(' PROGRAMM ZUR BERECHNUNG DES SPALTSPEKTRUMS'/)              130
     IF(ENG(NE).LT.10.E6)  GO TO 35                                      140
     Z=ENG(NE)                                                           150
     ENG(NE)=20.E6                                                       160
     WRITE(NOUTP,36)                                                     170
  36 FORMAT(/' IN THIS MODULE THE HIGHEST ENERGY GROUP BOUNDARY IS SET    180
    1EQUAL TO 20.E6 EV'/)                                                190
  35 N=1                                                                 200
     I=0                                                                 210
     L=NE-NANF                                                           220
     IGRUP=NE-NEND                                                       230
     CALL DOPW (8HBEST    ,NFEST(2))                                     240
     CALL DOPW (8HCHICR   ,NFEST(3))                                     250
     CALL DOPW (8HSPALT   ,MMM)                                          260
     NSATZ(1)=3                                                          270
     NFEST(1)=MAT                                                        280
     CALL NDFLOC (NSUCH,NSATZ,FEST,NUDAT,NC)                             290
     IF(NSUCH)6,6,7                                                      300
   6 IF(MAT.NE.MNAME)  GO TO 19                                          310
     TETA=9.999999SE-40                                                  320
     E=9.9999999E-40                                                     330
     GO TO 20                                                            340
  19 CALL DOPW (8HSEDF    ,NFEST(3))                                     350
     NSATZ(1)=4                                                          360
     FEST(4)=0.                                                          370
     IT=0                                                                380
  45 CALL NDFLOC (NSUCH,NSATZ,FEST,NUDAT,NC)                             390
     IF(NSUCH)38,38,16                                                   400
  38 CALL NDFLOC (NSUCH,NSATZ,FEST,NUDAT,NC)                             410
     IF(NSUCH)15,15,16                                                   420
  15 WRITE (NOUTP,8) FEST(1)                                             430
   8 FORMAT(' FUER DAS MATERIAL',A9,' GIBT ES KEIN SPALTSPEKTRUM')       440
     GO TO 5                                                             450
   7 E=FEST(4)                                                           460
     B=FEST(6)                                                           470
     C=FEST(7)                                                           480
     T=1./B                                                              490
     EF=  C/(4.*B*B)                                                     500
     EW=DSQRT(EF/T)                                                      510
     DO 9 K=L,IGRUP                                                      520
     EG=DSQRT(ENG(K)/T)                                                  530
     EG1=DSQRT(ENG(K+1)/T)                                               540
     XG=EG1-EW                                                           550
     XG1=EG-EW                                                           560
     YG=EG1+EW                                                           570
     YG1=EG+EW                                                           580
     XG2=XG*XG                                                           590
     YG2=YG*YG                                                           600
     XG12=XG1*XG1                                                        610
     YG12=YG1*YG1                                                        620
     X(K)=0.2820947917738/EW*(DEXP(-XG12)-DEXP(-XG2)-DEXP(-YG12)         630
    1+DEXP(-YG2))-0.5*(DERF(XG1)-DERF(XG)+DERF(YG1)-DERF(YG))            640
   9 CONTINUE                                                            650
```

```
      IF(N.EQ.2) GO TO 10                                                660
      N=2                                                                670
      IJ=0                                                               680
      WRITE (JA) IJ,MMM                                                  690
   10 IJ=6                                                               700
      K=NE-L                                                             710
      J=NE-IGRUP                                                         720
      WRITE (JA) IJ,MAT,E,K,J                                            730
      NNN=IGRUP+1-L                                                      740
      WRITE(JA) NNN,(X(IJ),IJ=L,IGRUP)                                   750
      WRITE (NOUTP,29)                                                   760
   29 FORMAT(//' WATT - CRANBERG SPEKTRUM')                              770
      WRITE (NOUTP,12) MAT,E,K,J                                         780
   12 FORMAT(1HO,A9,'  EINFALLSENERGIE =',E16.8,'  VON GRUPPE',I3,' BIS'  790
     1,I3)                                                               800
      WRITE(NOUTP,14) I                                                  810
   14 FORMAT(' CHI ',I1)                                                 820
      I=I+1                                                              830
      WRITE (NOUTP,13) (X(IJ),IJ=L,IGRUP)                               840
   13 FORMAT(1H ,7E16.8/(1X,7E16.8))                                     850
      CALL NDFNXT(NSUCH,NSATZ,FEST,NUDAT,NC)                             860
      IF(NSUCH) 5,5,7                                                    870
   16 F=FEST(5)*1.0001                                                   880
      G=FEST(6)*1.0001                                                   890
      IF(IT.EQ.0)  E=FEST(4)                                             900
      IF(IFIX(F).EQ.2.AND.IFIX(G).EQ.1)  GO TO 17                        910
      CALL NDFNXT (NSUCH,NSATZ,FEST,NUDAT,NC)                            920
      IF (NSUCH)39,39,16                                                 930
   39 IF(FEST(4).GT.E)  GO TO 38                                         940
      WRITE (NOUTP,37) FEST(1)                                           950
   37 FORMAT(' MATERIAL ',A10,' : DIE BEDINGUNGEN ZUR BERECHNUNG EINES S  960
     1PALTSPEKTRUMS (K=2, P=1) SIND NICHT ERFUELLT')                     970
      GO TO 5                                                            980
   17 IF(FEST(4)-1.65D5)22,22,23                                         990
   23 IF(IT.EQ.0)  GO TO 22                                             1000
      TETA2=FEST(7)                                                     1010
      TETA=TETA1+(TETA2-TETA1)/(FEST(4)-E)*(1.65D5-E)                   1020
      E=1.65D5                                                          1030
      GO TO 20                                                          1040
   22 TETA1=FEST(7)                                                     1050
      E=FEST(4)                                                         1060
      IT=1                                                              1070
      IF(E-1.65D5)21,18,18                                              1080
   21 FEST(4)=FEST(4)*1.0001                                            1090
      GO TO 45                                                          1100
   18 TETA=TETA1                                                        1110
   20 DO 28 K=L,IGRUP                                                   1120
   28 CALL CHIINM (ENG(K),ENG(K+1),TETA,X(K))                           1130
      IJ=0                                                              1140
      WRITE (JA) IJ,MMM                                                 1150
      IJ=6                                                              1160
      K=NE-L                                                            1170
      J=NE-IGRUP                                                        1180
      WRITE (JA) IJ,MAT,E,K,J                                           1190
      NNN=IGRUP+1-L                                                     1200
      WRITE (JA) NNN,(X(IJ),IJ=L,IGRUP)                                 1210
      WRITE (NOUTP,30)                                                  1220
   30 FORMAT(//' MAXWELL SPEKTRUM')                                     1230
      WRITE (NOUTP,31) MAT,E,TETA,K,J                                   1240
   31 FORMAT(1HO,A9,'  EINFALLSENERGIE =',E16.8,'  TETA =',E16.8,       1250
     1'  VON GRUPPE',I3,' BIS',I3)                                      1260
      WRITE (NOUTP,14) I                                                1270
      WRITE (NOUTP,13) (X(IJ),IJ=L,IGRUP)                               1280
    5 KL=KL+1                                                           1290
      ENG(NE)=Z                                                         1300
      RETURN                                                            1310
      END                                                               1320
```

```
      SUBROUTINE REMO(NG,ABN,NSP,F,E,ERR,NLA,NLE,NGRE,NFG,NFI,NJM,NUJM,
     1ISEL,IWORK,WORK,L)
C
C   SUBROUTINE MODIFIED BY BROEDERS,INR   JUNE,1975
C
C   CONTROL VARIABLES IN THE FIRST 36 WORDS OF THE WORKING FIELD
C   WORD                 MEANING
C     1     ADRESS OF ENERGY POINTS OF ANGULAR DISTRIBUTION          (EA)
C     2     ADRESS OF ANGLE MESH POINTS OF ANGULAR DISTRIBUTION      (XL)
C     3     ADRESS OF ANGULAR DISTRIBUTIONS                          (SGNC)
C     4     IG NUMBER OF THE ACTUALLY CALCULATED GROUP
C
C----------------EXTENSION BY BROEDERS--------------------------------
C
C   THE LENGTH OF THE WORKING AREAS OF WORD (5-7) IS ENLARGED
C   IN ORDER TO CALCULATE FROM KEDAK-DATA WITH DIFFERENT ENERGY-POINTS
C   FOR DIFFERENT DATA-TYPES.
C   NOW THE LENGTH OF THESE ARRAYS IS 3*NMAX OF WORD 36
C     5     ADRESS OF ELASTIC SCATTERING OR TOTAL CROSS-SECTIONS     (SGN)
C     6     ADRESS OF AVEREGE COSINES                                (AMU)
C     7     ADRESS OF ENERGIE MESH POINTS FOR CROSS-SECTIONS         (ES)
C
C----------------------------------------------------------------------
C
C     8     ISEL (SEE INPUT DESC.) OR  E THE  ACTUAL ENERGY
C     9     ADRESS OF AN ACTUAL ANGULAR DISTRIBUTION                 (SG)
C    10     ADRESS OF AUX. ARRAY IN WAHRS FOR ROMBERG INTEGRATION    (TF)
C    11     ADRESS OF AUX. ARRAY IN LMI   FOR ROMBERG INTEGRATION    (PER)
C    12     ADRESS OF RESULT STORAGE                                 (SP)
C    13     ADRESS OF A BUFFER STORAGE                               (BUF)
C    14     NG NUMBER OF GROUPS
C    15     NSP  NUMBER OF SPECTRUM POINTS
C    16     NLA  THE LOWEST LEGENDRE MOMENT
C    17     NLE  THE HIGHEST LEGENDRE MOMENT
C    18     IMAX MAXIMUM GROUPCHANGE+1
C    19     NJM+1  (SEE INPUT DESC.)
C    20     NUJM   (SEE INPUT DESC.)
C    21     ICOS  NUMBER OF MESHPOINTS OF ANGULAR DISTRIBUTION
C    22     ADRESS OF ACTUALLY FREE PLACE FOR RESULTS
C    23     KJ  CONTROL NUMBER FOR ANISOTROPIE
C    24     NJ  CONTROL NUMBER IN ANGLE INTEGRATION
C    25     NDAT  NUMBER OF CROSS-SECTION POINTS IN AN ENERGY INTERVAL
C    26     NIV   NUMBER OF ANGULAR DISTRIBUTION
C    27     ERR ERROR FOR ROMBERG INTEGRATION
C    28     AM    ATOMIC MASS
C    29     QM=((AM+1)/(AM-1))**2
C    30     XM=(AM+1)**2/2/AM
C    31     QMX=ALOG(QM)
C    32     Q=-0.1
C    34     ADRESS OF A WORKING FIELD FOR ANGLE INTEGRATION
C
C----------------EXTENSION BY BROEDERS--------------------------------
C
C    33     FIRST FREE WORD IN IWORK. FOR THIS VERSION ENLARGED TO 37.
C    35     ADDRESS OF DOUBLE PRECISSION ARRAY FOR COARSE-GROUP-WISE
C           ENERGY-INTERVAL-BOUNDARIES.
C    36     NMAX, THE MAXIMUM NUMBER OF DATAPOINTS PRO COARSE ENERGY GROUP
C           FOR ONE OF THE FOLLOWING DATA-TYPES
C           SGT,SGN OR MUEL.
C
C----------------------------------------------------------------------
C
      DIMENSION IWORK(1),WORK(1),KDAT(3)
      REAL*8 FNEV(4)
      REAL*8 NHID/'H   H1'/
      REAL*8 REM/'REMO '/
      DATA N2KBY/2048/
      REAL*8 MATN
      DIMENSION ABN(1),F(1),E(1),NFG(1),NFI(1)
      COMMON MATN,IQQ(2),NOUT,LI,M1,M2,KLL
      EQUIVALENCE(N7,N8)
      EQUIVALENCE(N3,N4)
      DATA FNEV/'SGNC ','SGT  ','SGN  ','MUEL   '/
      KLL=KLL+1
      WRITE (NOUT ,9000)
 9000 FORMAT('1HO/1HO/' PROGRAMM KENNZIFFER 9')
      WRITE (NOUT ,9001)
 9001 FORMAT(' PROGRAMM ZUR BERECHNUNG DER ELASTISCHEN STREUMATRIZEN FUE
     1R DIE REMO-KORREKTUR'/)
      DO 1 I=1,L
    1 IWORK(I)=0
      IWORK(33)=37
      MC=IWORK(33)+2+2*NJM
      MM=MO+NG+1
      IF(MM-(MM/2)*2.EQ.0) MM=MM+1
      IWORK(34)=MM
      IWORK(8)=ISEL
      IWORK(14)=NG
      IWORK(15)=NSP
      IWORK(16)=NLA
      IWORK(17)=NLE
      IWORK(19)=NJM+1
      IWORK(20)=NUJM
      WORK(27)=ERR
      WORK(32)=-0.1
      DO 30 I=1,NG
      I1=NG-I+1
   30 WORK(MO+I1-1)=ABN(I)
      WORK(MO+NG)=0.
      CALL MASSIN(WORK,WORK(MO))
      IMAX=IWORK(18)
      MM=MM+(NLE+1)*IMAX*2
      IWORK(35)=MM
      NFIM=NFI(M2)
      NFGM=NFG(M2)
      DO 31 I=M2,M1
      IG=M1+M2-I
      NFIM=MAXO(NFI(IG),NFIM)
   31 NFGM=MAXO(NFG(IG),NFGM)
      NC=IWORK(35)+2*(NFIM*NFGM+1)
      IWORK(1)=NO
```

```
      IF(MATN.EQ.NHID)GOTO 3                                                1120
      CALL NIVNUM(MATN,FNEV(1),NIV,WORK(MO+M2-1),WORK(MO+M1),FNW,           1130
     1&3,&3,&3)                                                             1140
      NIV=NIV+2                                                             1150
      GOTO 4                                                                1160
    3 NIV=0                                                                 1170
      ICOS=0                                                                1180
      N2=NO                                                                 1190
      N3=NO                                                                 1200
      N4=NO                                                                 1210
      IS=M2-1                                                               1220
      LMA=NO                                                                1230
      WRITE(NOUT,74)MATN,FNEV(1)                                            1240
   74 FORMAT(///' FOR MATERIAL',A10,' , TYPE=',A10,' NO KEDAK-DATA HAS B    1250
     *EEN USED.')                                                           1260
    4 IWORK(26)=NIV                                                         1270
      N1=NO+NIV                                                             1280
      IWORK(2)=N1                                                           1290
      IF(NIV.EQ.0)GOTO 5                                                    1300
      NW=1                                                                  1310
      CALL DATNUM(MATN,FNEV(1),ICOS,NW,1.0,-1.0,&3,&3,&3)                   1320
      LM=N1+ICOS                                                            1330
      IF(LM.GT.L)GOTO 20                                                    1340
      IF(FNW.GE.WORK(MO+M2-1))GOTO 3                                        1350
      IS=ICSOP(FNW,WORK(MO))                                                1360
      IF(FNW.EQ.WORK(MO+IS-1))IS=IS-1                                       1370
      N2=N1+ICOS*2                                                          1380
      N3=N2+ICOS*NIV                                                        1390
      L1=N3+NIV                                                             1400
      L2=L1+ICOS                                                            1410
      LM=L2+ICOS*NIV                                                        1420
      LMA=LM                                                                1430
      IF(M1.LT.IS)IS=M1                                                     1440
      IF(LM.GT.L)GOTO 20                                                    1450
      CALL KEDLEC(MATN,FNEV(1),NIV,WORK(NO),IWORK(N3),WORK(MO+M2-1),        1460
     1WORK(MO+IS),                                                          1470
     1WORK(N1),WORK(L1),WORK(L2),WORK(N2),1.0,-1.0,&3,&3,&3)                1480
      IWORK(26)=NIV                                                         1490
      WRITE(NOUT,73)MATN,FNEV(1),NIV,ICOS,IS                                1500
   73 FORMAT(///' FOR MATERIAL',A10,' , TYPE',A10,'  THERE ARE',I6,         1510
     *' ANGULAR DISTRIBUTIONS WITH',I6,' ANGLE POINTS RETRIEVED FOR TH      1520
     *IS TASK.',/' THE LOWEST CALCULATED ENERGY GROUP NUMBER WITH SGNC I     1530
     *S',I3,'.')                                                            1540
    5 CONTINUE                                                              1550
      IWORK(21)=ICOS                                                        1560
      IWORK(3)=N2                                                           1570
      IWORK(5)=N4                                                           1580
      KDAT(1)=1                                                             1590
      KDAT(2)=1                                                             1600
      KDAT(3)=1                                                             1610
      DO 6 I=M2,M1                                                          1620
      IGR=MO+I-1                                                            1630
      DO 6 J=1,3                                                            1640
      CALL DATNUM(MATN,FNEV(J+1),NDAT,NW,WORK(IGR),WORK(IGR+1),             1650
     1&10,&10,&10)                                                          1660
      IF(KDAT(J).LT.NDAT)KDAT(J)=NDAT                                       1670
      GOTO 6                                                                1680
   10 WRITE(NOUT,71)MATN,FNEV(J+1)                                          1690
   71 FORMAT('  ***ERROR  9.5  :  FOR  ',A8,'  THERE IS NO  ',A8)           1700
    6 CONTINUE                                                              1710
      NMAX=MAXO(KDAT(1),KDAT(2),KDAT(3))*3                                  1720
      IWORK(36)=NMAX/3                                                      1730
      NTOT=KDAT(1)+KDAT(2)+KDAT(3)                                          1740
      N5=N4+2*NMAX                                                          1750
      N6=N5+2*NMAX                                                          1760
      IMAX=IWORK(18)                                                        1770
    7 N7=N6+NMAX                                                            1780
      N9=N8+ICOS                                                            1790
      N10=N9+IMAX*NUJM*(NLE+1)                                              1800
      N11=IMAX*(NLE+1)+N10                                                  1810
      N11=N11+1+IMAX                                                        1820
      IWORK(6)=N5                                                           1830
      IWORK(7)=N6                                                           1840
      IWORK(9)=N8                                                           1850
      IWORK(10)=N9                                                          1860
      IWORK(11)=N10                                                         1870
      IWORK(12)=N11                                                         1880
      NZM=1                                                                 1890
      DO 9 I=M2,M1                                                          1900
      NZ=NFG(I)*NFI(I)                                                      1910
      NZM=MAXO(NZM,NZ)                                                      1920
    9 CONTINUE                                                              1930
      IZV=IMAX*(NLE+1)                                                      1940
      IZV=MAXO(4,IZV)                                                       1950
      IWORK(13)=N11+NZM*IZV                                                 1960
      JJ=2+IMAX*NZM                                                         1970
      JJ=MAXO(JJ,NTOT)                                                      1980
      LM=IWORK(13)+JJ                                                       1990
   20 CONTINUE                                                              2000
      LREST=L-MAXO(LM,LMA)                                                  2010
      LRESTA=4*IABS(LREST)/N2KBY*2                                          2020
      IF(LREST.GE.0)GOTO 21                                                 2030
      LRESTA=LRESTA+2                                                       2040
      WRITE(NOUT,70)LM,L,LRESTA                                             2050
   70 FORMAT(' ***ERROR 9.1 : REGION.G TOO SMALL',/                         2060
     *' *** REQUIRED NUMBER OF WORDS',I10,/                                 2070
     *' *** AVAILABLE NUMBER OF WORDS',I9,/                                 2080
     *' *** PLEASE INCREASE REGION.G WITH AT LEAST',I10,'  K BYTES.')       2090
      RETURN                                                                2100
   21 WRITE(NOUT,72)LRESTA                                                  2110
   72 FORMAT(///' IN MODULE  9',I10,'  K BYTES OF REGION.G NOT USED.',//    2120
     */)                                                                    2130
      NG=0                                                                  2140
      WRITE(LI)NQ,REM                                                       2150
      NQ=4                                                                  2160
      NM1=NLE-NLA+1                                                         2170
      WRITE(LI)NQ,MATN,NG,NM1                                               2180
      CALL REMP(WORK(MO),NFG,NFI,F,F,WORK,IWORK,IS)                         2190
      RETURN                                                                2200
      END                                                                   2210
```

```
      SUBROUTINE ENERG(NFG,NFI,EM,EP,E)                                 10
C                                                                       20
C  SUBROUTINE ADDED BY BROEDERS,INR    JUNE,1975                        30
C                                                                       40
      REAL*8 E(1),DE,DDE,ER1,ER2,EF1,EF2,EDE1                           50
      IP=0                                                              60
      DE=DLOG(DBLE(EP/EM))/DFLOAT(NFG)                                  70
      EDE1=DEXP(DE)                                                     80
      ER1=DBLE(EM)                                                      90
      DO 2 I=1,NFG                                                     100
      ER2=ER1*EDE1                                                     110
      DDE=(ER2-ER1)/DFLOAT(NFI)                                        120
      EF1=ER1                                                          130
      DO 1 J=1,NFI                                                     140
C     EF2=EF1*DEXP(DDE)                                                150
      EF2=EF1+DDE                                                      160
      E(IP+1)=EF1                                                      170
      IP=IP+1                                                          180
    1 EF1=EF2                                                          190
    2 ER1=ER2                                                          200
      E(IP+1)=ER2                                                      210
      RETURN                                                           220
      END                                                              230
      SUBROUTINE KEDDAT(NAMIZ,NAMTYP,NW,NW1,ENW,NDAT,FA,FF,EP,EM,*,*,*)  10
C                                                                       20
C  SUBROUTINE MODIFIED BY BROEDERS,INR    JUNE,1975                     30
C                                                                       40
      REAL*8 FM(6),NAMIZ,NAMTYP,NGNC,NGIZ,NISO                          50
      DIMENSION EA(1),IEA(1),FA(1),FF(1),FAW(1),FFW(1),NWORT(4),NDT(2)  60
      COMMON MATN(4),NCUT                                               70
      DATA FM(2)/'BEST '/,KERST/0/ ,NGNC/'SGNC '/,NGIZ/'SGIZ '/         80
     1,NISO/'ISOT1'/                                                    90
      KK=1                                                             100
      IF(NAMTYP.EQ.NGNC.OR.NAMTYP.EQ.NGIZ)KK=2                         110
      GOTO 1                                                           120
      ENTRY DATNUM(NAMIZ,NAMTYP,NDAT,NW,EP,EM,*,*,*)                   130
      KK=3                                                             140
      IF(NAMTYP.EQ.NGNC.OR.NAMTYP.EQ.NGIZ)KK=4                         150
      GOTO 1                                                           160
      ENTRY KEDLEC(NAMIZ,NAMTYP,NW1,EA,IEA,EPW,EMW,FA,FF,FAW,FFW,EP,EM,  170
     1*,*,*)                                                           180
      KK=5                                                             190
      NW=0                                                             200
      GOTO 1                                                           210
      ENTRY NIVNUM(NAMIZ,NAMTYP,NW1,EPW,EMW,EFR,*,*,*)                 220
      NW=0                                                             230
      KK=6                                                             240
    1 CONTINUE                                                         250
      IF(KERST.NE.0)GOTO 20                                            260
      L=1                                                              270
      KERST=1                                                          280
   20 FM(1)=NAMIZ                                                      290
      FM(3)=NAMTYP                                                     300
      GOTO (2,3,2,3,3,3),KK                                            310
    2 CONTINUE                                                         320
      NWORT(1)=3                                                       330
      LL=0                                                             340
      CALL NDFLOC(NT,NWORT,FM,N1,N2)                                   350
      IF(NT.EQ.0)RETURN 1                                              360
   22 NDAT=1                                                           370
      IF(FM(4+LL).LE.EM)GOTO 21                                        380
      IF(KK.EQ.3)GOTO 40                                               390
      FA(1)=EM                                                         400
      FF(1)=FM(5+LL)                                                   410
   40 CONTINUE                                                         420
      NDAT=2                                                           430
   21 CONTINUE                                                         440
      IF(KK.EQ.3)GOTO 8                                                450
      FA(NDAT)=FM(4+LL)                                                460
      FF(NDAT)=FM(5+LL)                                                470
    8 NDAT=NDAT+1                                                      480
      CALL NDFNXT(NT,NWORT,FM,N1,N2)                                   490
      IF(NT.EQ.0)GOTO 9                                                500
      IF(FM(4+LL ).LE.EM)NDAT=1                                        510
      IF(KK.EQ.3)GOTO 41                                               520
      FA(NDAT)=FM(4+LL)                                                530
      FF(NDAT)=FM(5+LL)                                                540
   41 CONTINUE                                                         550
      IF(FM(4+LL).GE.EP)GOTO 30                                        560
      GOTO 8                                                           570
   30 CONTINUE                                                         580
      IF(KK.EQ.1.AND.NAMTYP.NE.NISO.AND.NAMTYP.NE.NGIZ) GO TO 92       590
      GO TO 93                                                         600
   92 CALL AUSGL(NDAT,EM,EP,FA,FF)                                     610
   93 IF(LL.EQ.0)RETURN                                                620
      IF(KK.EQ.1.OR.KK.EQ.3)RETURN                                     630
      GOTO 10                                                          640
    9 CONTINUE                                                         650
      IF(KK.EQ.3)GOTO 42                                               660
      IF(NAMTYP.NE.NISO.AND.NAMTYP.NE.NGIZ)                            670
     *WRITE(NOUT,100)FM(1),FM(3),FA(NDAT-1),FF(NDAT-1)                 680
  100 FORMAT(/' ***WARNING 9.4 MATERIAL',A10,'  TYPE',A10,/             690
     *' ***LAST ENERGY POINT ON KEDAK IS',1PE14.6,                     700
     *' EV WITH THE CROSS-SECTION VALUE',1PE14.6,' BARN.'/             710
     *' *** EXTRAPOLATION IS CARRIED OUT WITH THE CONSTANT VALUE OF THE  720
     *CROSS-SECTION.')                                                 730
      FA(NDAT)=EP                                                      740
      FF(NDAT)=FF(NDAT-1)                                              750
      IF(NAMTYP.EQ.NGIZ)FF(NDAT)=0.                                    760
   42 CONTINUE                                                         770
      GOTO 30                                                          780
    3 CONTINUE                                                         790
      NWORT(1)=4                                                       800
      LL=1                                                             810
      NW1=0                                                            820
      FM(4)=1.0                                                        830
```

```
 23  CALL NDFLOC(NT,NWORT,FM,N1,N2)                                    840
     CALL NDFLOC(NT,NWORT,FM,N1,N2)                                    850
     IF(NT.EQ.0.AND.NW1.EQ.0)RETURN 1                                  860
     IF(NT.EQ.0)GOTO 18                                                870
     IF(KK.EQ.6.AND.NW1.EQ.0)EFR=FM(4)                                 880
     NW1=NW1+1                                                         890
      IF(NW.EQ.0.AND.FM(4).GE.EMW)GOTO 24                              900
     IF(NW.EQ.NW1)GOTO 24                                              910
      FM(4)=(1+1.E-6)*FM(4)                                            920
     GOTO 23                                                           930
 24  CONTINUE                                                          940
     IF(KK.GE.7)GOTO 26                                                950
     IF(KK.GE.5)GOTO 25                                                960
     FNW=FM(4)                                                         970
     KK=KK-1                                                           980
     GOTO 22                                                           990
 25  NW=NW1-1                                                         1000
     IF(EMW.EQ.FM(4))NW=NW1                                           1010
     LZ=0                                                             1020
     IF(NW.EQ.0)LZ=1                                                  1030
     IF(NW.EQ.0)NW=1                                                  1040
     NPN=0                                                            1050
     KK=KK+2                                                          1060
     GOTO 3                                                           1070
  26 FNW=FM(4)                                                        1080
     IF(KK.EQ.7)GOTO 22                                               1090
      IF(FM(4).GE.EPW)RETURN                                          1100
      FM(4)=(1+1.E-6)*FM(4)                                           1110

     NW=NW+1                                                          1120
     GOTO 23                                                          1130
 10  IF(LZ.NE.0)GOTO 88                                               1140
     DO 90 I=1,NDAT                                                   1150
      FAW(I)=FA(I)                                                    1160
 90  FFW(I)=FF(I)                                                     1170
     IEA(1)=NDAT                                                      1180
     EA(1)=EMW                                                        1190
     LZ=2                                                             1200
     NPN=NDAT                                                         1210
 88  CONTINUE                                                         1220
     DO 91 I=1,NDAT                                                   1230
     FAW(I+NPN)=FA(I)                                                 1240
 91  FFW(I+NPN)=FF(I)                                                 1250
     EA(LZ)=FNW                                                       1260
     IEA(LZ)=NDAT                                                     1270
     NPN=NPN+NDAT                                                     1280
     LZ=LZ+1                                                          1290
      IF(FNW.GE.EPW)GOTO 89                                           1300
     NW=NW+1                                                          1310
     FM(4)=(1+1.E-6)*FNW                                              1320
     GOTO 23                                                          1330
 18  FNW=EPW                                                          1340
     IF(KK.EQ.7)GOTO 88                                               1350
     NW1=NW1+1                                                        1360
     RETURN                                                           1370
 89  NW1=LZ-1                                                         1380
```

```
     94 RETURN                                                        1390
        END                                                           1400




        SUBROUTINE LININT(N,X1,Y1,M,X2,Y2)                              10
C                                                                       20
C  SUBROUTINE ADDED BY BRCEDERS, INR   JUNE, 1975                       30
C                                                                       40
        COMMON MATN(4),NOUT                                             50
        DIMENSION X1(N),Y1(N),X2(M),Y2(M)                               60
        JA=1                                                            70
        JN=1                                                            80
        DO 3 I=1,M                                                      90
        NN=1                                                           100
        IF(X2(I).GE.X1(1))GOTO 4                                       110
        Y2(I)=Y1(1)                                                    120
        GOTO 5                                                         130
      4 NN=N                                                           140
        IF(X2(I).LE.X1(N ))GOTO 6                                      150
        Y2(I)=Y1(N)                                                    160
      5 WRITE(NOUT,100)X2(I),X1(1),X1(N),Y2(I)                         170
        GOTO 9                                                         180
      6 CONTINUE                                                       190
        DO 1 J=JA,N                                                    200
        JN=J                                                           210
        IF(X2(I).LE.X1(J))GOTO 2                                       220
      1 CONTINUE                                                       230
      2 IF(X1(JN).EQ.X1(JN-1))GOTO 7                                   240
        Y2(I)=FIPOL(X1(JN-1),X2(I),X1(JN),Y1(JN-1),Y1(JN))             250
        GOTO 8                                                         260
      7 NN=JN                                                          270
      9 Y2(I)=Y1(NN)                                                   280
      8 CONTINUE                                                       290
        JA=MAXO(1,(JN-2))                                              300
      3 CONTINUE                                                       310
     10 RETURN                                                         320
    100 FORMAT(/' ***WARNING 9.6 INTERPOLATION ERROR.',/               330
       *' ***DESIRED ENERGY',1PE14.6,'  NOT IN RANGE (',1PE14.6,' ,',  340
       *1PE14.6,'). CONSTANT BOUNDARY VALUE',1PE14.6,'  TAKEN.',/      350
       *' ***PROBABLY PROGRAM-ERROR.')                                 360
        END                                                            370




        SUBROUTINE AUSGL(NDAT,EM,EP,FA,FF)                              10
C                                                                       20
C  SUBROUTINE ADDED BY BRCEDERS, INR   JUNE, 1975                       30
C                                                                       40
        COMMON MATN(4),NOUT                                             50
        DATA EPS/1.E-6/                                                 60
        DIMENSION FA(1),FF(1)                                           70
        DO 1 I=1,2                                                      80
```

```
      IM=I                                                              50
      IF(ABS((FA(I)-EM)/EM).LT.EPS)GOTO 2                              100
    1 CONTINUE                                                         110
      IM=1                                                             120
    2 CONTINUE                                                         130
      FF(1)=FIPOL(FA(1),EM,FA(2),FF(1),FF(2))                          140
      FA(1)=EM                                                         150
      IF(IM.EQ.1)GOTO 4                                                160
      NDAT=NDAT-1                                                      170

      DO 3 I=2,NDAT                                                    180
      FA(I)=FA(I+1)                                                    190
    3 FF(I)=FF(I+1)                                                    200
    4 CONTINUE                                                         210
      IA=NDAT-1                                                        220
      DO 5 I=IA,NDAT                                                   230
      IM=I                                                             240
      IF(ABS((FA(I)-EP)/EP).LT.EPS)GOTO 6                              250
    5 CONTINUE                                                         260
    6 CONTINUE                                                         270
      FF(NDAT)=FIPOL(FA(NDAT-1),EP,FA(NDAT),FF(NDAT-1),FF(NDAT))       280
      FA(NDAT)=EP                                                      290
      NDAT=IM                                                          300
    7 CONTINUE                                                         310
      RETURN                                                           320
      END                                                              330
```

```
      SUBROUTINE ORDN1(KMAX,FELD)                                       10
C                                                                       20
C  SUBROUTINE ADDED BY BROEDERS,INR   JUNE,1975                         30
C                                                                       40
      DIMENSION FELD(2)                                                 50
C                                                                       60
C  ORDNEN ORDNET FELD NACH WACHSENDEN WERTEN                            70
C                                                                       80
      IF(KMAX.LT.2) GOTO 100                                            90
      DO 99 K=2,KMAX                                                   100
      M=K-1                                                            110
      IF(FELD(K).GE.FELD(M)) GOTO 99                                   120
      R=FELD(K)                                                        130
   10 M=M-1                                                            140
      IF(M.EQ.0) GOTO 20                                               150
      IF(R.LT.FELD(M)) GOTO 10                                         160
   20 IA=M+1                                                           170
      IE=K-1                                                           180
      J=IE                                                             190
      DO 30 I=IA,IE                                                    200
      FELD(J+1)=FELD(J)                                                210
   30 J=J-1                                                            220
      FELD(IA)=R                                                       230
   99 CONTINUE                                                         240
      KMAXX=KMAX                                                       250
      DO 500 K=2,KMAX                                                  260
  502 IF(K   .GT.KMAXX) GO TO 501                                      270
      M=K-1                                                            280
      IF(FELD(K).EQ.FELD(M))GOTO 600                                   290
      GO TO 500                                                        300
  600 KMAXX=KMAXX-1                                                    310
      KMAXS= MAXO(K,KMAXX)                                             320
      DO 700 KK=K,KMAXS                                                330
  700 FELD(KK)=FELD(KK+1)                                              340
      GO TO 502                                                        350
  500 CONTINUE                                                         360
  501 KMAX=KMAXX                                                       370
  100 RETURN                                                           380
      END                                                              390
```

```
      FUNCTION BCM(EI,EO,WORK)                                          10
      DIMENSION WORK(1)                                                 20
      AM=WORK(28)                                                       30
      Q=WORK(32)                                                        40
      IF(EO.EQ.0.0)GOTO 1                                               50
      IF(Q.LT.0)Q=0.0                                                   60
      U=0.5*((AM+1)*EO-(AM-1)*EI+AM*Q)/SQRT(EI*EO)                      70
      IF(U.LT.-1)GOTO 1                                                 80
      IF(U.GT.1)U=1.0                                                   90
      Z=U*U-1                                                          100
      F=1.0/AM                                                         110
      IF(Q.NE.0.0)F=F*SQRT(EI/(EI-(AM+1)/AM*Q))                        120
      BCM=F*(Z+U*SQRT(Z+AM*AM-AM*(AM+1)/EI*Q))                         130
      RETURN                                                           140
    1 BCM=-1                                                           150
      RETURN                                                           160
      END                                                              170
```

```
      FUNCTION ICSOP(E,ABN)                                             10
      DIMENSION ABN(1)                                                  20
      J=0                                                               30
    1 J=J+1                                                             40
      IF(E.LE.ABN(J).AND.ABN(J).GT.0.)GOTO 1                            50
      ICSOP=J-1                                                         60
      RETURN                                                            70
      END                                                               80
```

```
      DOUBLE PRECISION FUNCTION PTL(N,XX)                               10
      REAL*8 XX                                                         20
      GOTO (1,2,3,4,5,6),N                                              30
    1 PTL=1.0                                                           40
      RETURN                                                            50
```

```
    2   PTL=XX                                                          60
        RETURN                                                          70
     3  PTL=0.5*(3*(XX**2)-1.0)                                         80
        RETURN                                                          90
     4  PTL=0.5*(5*(XX**3)-3*XX)                                        100
        RETURN                                                          110
    5   PTL=0.125*(35*(XX**4)-30*(XX**2)+3)                             120
        RETURN                                                          130
      6 PTL=0.125*(63*(XX**5)-70*(XX**3)+15*XX)                         140
        RETURN                                                          150
        END                                                             160
```

```
        SUBROUTINE ZWIN(KL,EP,EM,ES,J2,J1)                              10
        DIMENSION ES(KL)                                                20
        J1=KL                                                           30
        J2=1                                                            40
        KL1=KL-1                                                        50
        DO 1 I=1,KL1                                                    60
        IF(ES(I).EQ.ES(I+1))GOTO 1                                      70
        IF(EP.GE.ES(I).AND.EP.LT.ES(I+1))GOTO 2                         80
        GOTO 1                                                          90
     2  J1=I+1                                                          100
        GOTO 11                                                         110
     1  CONTINUE                                                        120
    11  CONTINUE                                                        130
        DO 12 I=2,KL                                                    140
        IF(ES(I).EQ.ES(I+1).AND.I.LT.KL)GOTO 12                         150
        IF(EM.LE.ES(I).AND.EM.GT.ES(I-1))GOTO 13                        160
        GOTO 12                                                         170
     13  J2=I-1                                                         180
        GOTO 14                                                         190
    12   CONTINUE                                                       200
    14  CONTINUE                                                        210
        RETURN                                                          220
        END                                                             230
```

```
        FUNCTION FIPOL(XA,XB,XC,YA,YC)                                  10
C                                                                       20
C   FUNCTION ADDED BY BROEDERS,INR JUNE,1975                            30
C                                                                       40
        DX=XC-XA                                                        50
        IF(DX.NE.0.)GOTO 1                                              60
        FIPOL=0.5*(YA+YC)                                               70
        GOTO 2                                                          80
     1  CONTINUE                                                        90
        DX1=XB-XA                                                       100
        DX2=XC-XB                                                       110
        FIPOL=(YA*DX2+YC*DX1)/DX                                        120
     2  RETURN                                                          130
        END                                                             140
```

```
        SUBROUTINE IPOL(M,A,B,X,Y,T)                                    10
C                                                                       20
C   SUBROUTINE IPOLA BY H. WIESE,INR                                    30
C                                                                       40
C   MODIFIED BY BROEDERS,INR  JUNE,1975                                 50
C                                                                       60
C                                                                       70
C       KUBISCH-QUADRATISCH-LINEARE INTERPOLATION                       80
C       OHNE ERZEUGUNG ZUSAETZLICHER EXTREMWERTE                        90
C                                                                       100
        DIMENSION  A(M),B(M),T(M)                                       110
        DATA AA1/0./,AAH/0./,AAM/0./,BB1/0./,BBH/0./,BBM/0./            120
        NH=M/2                                                          130
C                                                                       140
        IF(BB1.NE.B(1).OR.BBH.NE.B(NH).OR.BBM.NE.B(M))GOTO 20           150
        IF(AA1.NE.A(1).OR.AAH.NE.A(NH).OR.AAM.NE.A(M))GOTO 20           160
        GOTO 21                                                         170
C                                                                       180
C       TANGENTEN                                                       190
   20 CONTINUE                                                          200
        T(1) = (B(2)-B(1))/(A(2)-A(1))                                  210
        T(M) = (B(M)-B(M-1))/(A(M)-A(M-1))                              220
        MN = M-1                                                        230
        DO 2  J = 2,MN                                                  240
        JP = J+1                                                        250
        JM = J-1                                                        260
        T(J) = 0.                                                       270
        IF(B(JP).GT.B(J).AND.B(J).GT.B(JM))                             280
       -T(J) = (B(JP)-B(JM))/(A(JP)-A(JM))                              290
        IF(B(JP).LT.B(J).AND.B(J).LT.B(JM))                             300
       -T(J) = (B(JP)-B(JM))/(A(JP)-A(JM))                              310
     2 CONTINUE                                                         320
        AA1=A(1)                                                        330
        AAH=A(NH)                                                       340
        AAM=A(M)                                                        350
        BB1=B(1)                                                        360
        BBH=B(NH)                                                       370
        BBM=B(M)                                                        380
   21 CONTINUE                                                          390
C                                                                       400
C       INTERPOLATION                                                   410
        J = 1                                                           420
     4 IF(X   -A(J))   6,8,10                                           430
     6 S = X   -A(K)                                                    440
        Y     = A0+(A1+(A2+A3*S)*S)*S                                   450
        GOTO 16                                                         460
     8 Y     = B(J)                                                     470
        GOTO 16                                                         480
    10 K = J                                                            490
        J = J+1                                                         500
        U = A(J)-A(K)                                                   510
```

```
      V = B(J)-B(K)                                                     520
      R = V-T(K)*U                                                      530
      W = U*(T(J)-T(K))                                                 540
      A0 = B(K)                                                         550
      A1 = T(K)                                                         560
      A2 = (3*R-W)/(U*U)                                                570
      A3 = (W-2*R)/(U*U*U)                                              580
      IF(T(K).EQ.0..AND.T(J).EQ.0.)   GOTO 4                            590
      IF(ABS(A3).LT.1.E-30)   GOTO 4                                    600
      XW = -A2/(3*A3)                                                   610
      IF(XW.LE.0..OR.XW.GE.U)   GOTO 4                                  620
      A3 = 0.                                                           630
      IF(T(J).EQ.0.)   GOTO 12                                          640
      IF(T(K).EQ.0.)   GOTO 14                                          650
      A2 = R/(U*U)                                                      660
      T(J) = 2*V/U-T(K)                                                 670
      IF(ABS(A2).LT.1.E-30)   GOTO 4                                    680
      XW = -A1/(2*A2)                                                   690
      IF(XW.LE.0..OR.XW.GE.U)   GOTO 4                                  700
      A1 = V/U                                                          710
      A2 = 0.                                                           720
      T(J) = A1                                                         730
      GOTO 4                                                            740
   12 A1 = 2*V/U                                                        750
      A2 = -V/(U*U)                                                     760
      GOTO 4                                                            770
   14 A1 = 0.                                                           780
      A2 = V/(U*U)                                                      790
      GOTO 4                                                            800
   16 CONTINUE                                                          810
      RETURN                                                            820
C                                                                       830
      END                                                               840
```

```
      SUBROUTINE MASSIN(WORK,ABN)                                       10
C                                                                       20
C  SUBROUTINE MODIFIED BY BROEDERS,INR   JUNE,1975                      30
C                                                                       40
      REAL*8 MATN                                                       50
      REAL*8 HID                                                        60
      DIMENSION WORK(1),ABN(1),A(6),AC(13)                              70
      DIMENSION FF(6),FA(6)                                             80
      COMMON MATN,IS(2),NCUT,LI,IR(2)                                   90
      DATA A/0.57735,0.774596,0.33998,0.86114,0.53847,0.90618/         100
      DATA HID/'H   H1'/                                               110
      IF(MATN.EQ.HID)GOTO 40                                           120
      CALL KEDDAT(MATN,'ISOT1    ',C,NW1,FNW,NDAT,FA,FF,3C0.0,1.C,     130
     1&40,&40,&40)                                                     140
      AME=FA(2)                                                        150
      GOTC 41                                                          160
   4C CONTINUE                                                         170
      AME=1.008665                                                     180
   41 CONTINUE                                                         190
      AME=AME/1.008665                                                 200
      DO 10 I=1,6                                                      210
      XA=A(I)**2-1                                                     220
      AC(I+6)=(XA-A(I)*SQRT(XA+AME**2))/AME                            230
   10 AC(I)=(XA+A(I)*SQRT(XA+AME**2))/AME                              240
      AC(13)=-1/AME                                                    250
      XM=(AME+1)**2/2/AME                                              260
      IF(AME.EQ.1.)GOTO 1                                              270
      QM=((AME+1.)/(AME-1.))**2                                        280
      GOTO 2                                                           290
    1 QM=2.E8                                                          300
    2 CONTINUE                                                         310
      QMX=ALOG(QM)                                                     320
      WORK(28)=AME                                                     330
      WORK(29)=QM                                                      340
      WORK(30)=XM                                                      350
      WORK(31)=QMX                                                     360
      CALL IROMES(AC)                                                  370
      I1=IR(1)                                                         380
      I2=IR(2)                                                         390
      IMAX=2                                                           400
      DO 11 I=I2,I1                                                    410
      E=ABN(I+1)/QM                                                    420
      IM=ICSOP(E,ABN(I))                                               430
      IF(IM.GT.IMAX)IMAX=IM                                            440
   11 CONTINUE                                                         450
      CALL IWIN(18,IMAX,WORK)                                          460
      RETURN                                                           470
      END                                                              480
```

```
      SUBROUTINE INTFN(E,SG,SGNC,EA,ICCS)                               10
C                                                                       20
C  SUBROUTINE MODIFIED BY BROEDERS,INR   JUNE,1975                      30
C                                                                       40
      DIMENSION SG(1),SGNC(ICCS,1),EA(1)                                50
      NE=0                                                              60
    3 NE=NE+1                                                           70
      IF(E.GT.EA(NE)+EA(NE)*1.0E-4)GOTC 3                               80
      IF(NE.EQ.1)GOTO 5                                                 90
      DO 4 I=1,ICOS                                                    100
    4 SG(I)=FIPOL(EA(NE-1),E,EA(NE),SGNC(I,NE-1),SGNC(I,NE))           110
      RETURN                                                           120
    5 DO 6 I=1,ICOS                                                    130
      SG(I)=0.5                                                        140
    6 CONTINUE                                                         150
      RETURN                                                           160
      END                                                              170
```

```
      FUNCTION FXINT(EP,EM,SGN,ES,FLUX,EFLUX,NSP,NDAT)                  10
C                                                                       20
C  FUNCTION MODIFIED BY BROEDERS,INR   JUNE,1975                        30
C                                                                       40
      DIMENSION FLUX(1),EFLUX(1)                                        50
      DIMENSION SGN(1),ES(1)                                            60
      CALL ZWIN(NDAT,EP,EM,ES,J2,J1)                                    70
      Y=0.                                                              80
C                                                                       90
C  SAVE BOUNDARY VALUES                                                100
C                                                                       110
      SGN1=SGN(J1)                                                      120
      SGN2=SGN(J2)                                                      130
      ES1=ES(J1)                                                        140
      ES2=ES(J2)                                                        150
      SGN(J1)=FIPOL(ES(J1),EP,ES(J1-1),SGN(J1),SGN(J1-1))               160
      SGN(J2)=FIPOL(ES(J2),EM,ES(J2+1),SGN(J2),SGN(J2+1))               170
      ES(J1)=EP                                                         180
      ES(J2)=EM                                                         190
      J11=J1-1                                                          200
      IF(NSP.EQ.1)GOTO 1                                                210
      CALL ZWIN(NSP,EP,EM,EFLUX,JF2,JF1)                                220
      FF1=FIPOL(EFLUX(JF2),EM,EFLUX(JF2+1),FLUX(JF2),FLUX(JF2+1))       230
      GOTO 2                                                            240
    1 FF1=PHI(EM)                                                       250
    2 CONTINUE                                                          260
      IF(J2.GT.J11)GOTO 17                                              270
      DO 16 I=J2,J11                                                    280
      DX=ES(I+1)-ES(I)                                                  290
      IF(NSP.EQ.1)GOTO   3                                              300
      CALL ZWIN(NSP,ES(I+1),ES(I+1),EFLUX,ISG,ISF)                      310
      FF2=FIPOL(EFLUX(ISG),ES(I+1),EFLUX(ISG+1),FLUX(ISG),FLUX(ISG+1))  320
      GOTO 4                                                            330
    3  CONTINUE                                                         340
      FF2=PHI(ES(I+1))                                                  350
    4  Y=Y+DX*(SGN(I)*FF1+SGN(I+1)*FF2)                                 360
      FF1=FF2                                                           370
   16 CONTINUE                                                          380
      FXINT=Y*0.5                                                       390
C                                                                       400
C  RESTORE BOUNDARY VALUES                                              410
C                                                                       420
   17 ES(J1)=ES1                                                        430
      ES(J2)=ES2                                                        440
      SGN(J1)=SGN1                                                      450
      SGN(J2)=SGN2                                                      460
      RETURN                                                            470
      END                                                               480
```

```
      SUBROUTINE SMCRN(PI,N,IM,WORK)                                    10
      DIMENSION PI(N,IM),WORK(1)                                        20
      Q=WORK(32)                                                        30
      JM=1                                                              40
      IF(Q.GT.0)JM=IWO(26,WORK)                                         50
      AS=0                                                              60
      DO 1 I=JM,IM                                                      70
    1 AS=PI(1,I)+AS                                                     80
      IF(AS.EQ.0)RETURN                                                 90
      DO 2 I=JM,IM                                                      100
      DO 2 J=1,N                                                        110
    2 PI(J,I)=PI(J,I)/AS                                                120
      RETURN                                                            130
C                                                                       140
      END                                                               150
```

```
      SUBROUTINE SEARCH(NFG,NFI,WORK,IWORK,FLUX,EFLUX,ENERG)            10
C  SUBROUTINE MODIFIED BY BROEDERS,INR    JUNE,1975                     20
C                                                                       30
      DIMENSION WORK(1),IWORK(1),FLUX(1),EFLUX(1),SGS(4)                40
      REAL*8 MATN,ENERG(1)                                              50
      COMMON MATN,MAY(2),NOUT,LI                                        60
      DATA SGS/'SGT ','SGN ','MUEL', 'FLUX'/                            70
      NDAT=IWORK(25)                                                    80
      N9=IWORK(13)                                                      90
      DO 3 I=1,NDAT                                                     100
    3 WORK(N9+I-1)=1.0                                                  110
      N4=IWORK(7)                                                       120
      NZ=NFG*NFI                                                        130
      N11=IWORK(12)                                                     140
      IW=N11+3*NZ                                                       150
      IG=IWORK(4)                                                       160
      NSP=IWORK(15)                                                     170
      DO 20 I=1,NFG                                                     180
      IP=(I-1)*NFI+1                                                    190
      E1=SNGL(ENERG(IP))                                                200
      E2=SNGL(ENERG(IP+NFI))                                            210
      FF=FXINT(E2,E1,WORK(N9),WORK(N4),FLUX,EFLUX,NSP,NDAT)             220
      DO 21 J=1,NFI                                                     230
      IP=NFI*(I-1)+J                                                    240
      EM=SNGL(ENERG(IP))                                                250
      EP=SNGL(ENERG(IP+1))                                              260
      WORK(IW)=FXINT(EP,EM,WORK(N9),WORK(N4),FLUX,EFLUX,NSP,NDAT)/FF    270
      IW=IW+1                                                           280
   21 CONTINUE                                                          290
   20 CONTINUE                                                          300
      IWORK(22)=N11                                                     310
      NQ=4*NZ+3                                                         320
      J=4*NZ                                                            330
      WRITE(LI)NQ,IG,NFG,NFI,(WORK(N11+I-1),I=1,J)                      340
      WRITE(NOUT,70)IG,NZ,MATN                                          350
      NZ1=NZ+1                                                          360
```

```
      WRITE(NOUT,73)                                                    370
      WRITE(NOUT,74)(ENERG(I),I=1,NZ1)                                  380
      DO 1 M=1,4                                                        390
      WRITE(NOUT,71)SGS(M)                                              400
      IW=N11+(M-1)*NZ-1                                                 410
    1 WRITE(NOUT,72)(WORK(IW+I),I=1,NZ)                                 420
   70 FORMAT(/'_GROUP=',I3,' NUMBER OF FINE INTERVALS=',I5,             430
     1' MATERIAL',2X,A8)                                                440
   71 FORMAT('0THE VALUES OF ',A4)                                      450
   72 FORMAT(' ',1P10E12.4)                                             460
   73 FORMAT('0THE INTERVAL-BOUNDARIES ARE',/)                          470
   74 FORMAT(' ',1P6D20.10)                                             480
   75 FORMAT('1')                                                       490
      RETURN                                                            500
      END                                                               510


      SUBROUTINE REMP(ABN,IGR,NFI,FLUX,EFLUX,WORK,IWORK,IS)              10
C                                                                        20
C  SUBROUTINE MODIFIED BY BROEDERS,INR   JUNE,1975                       30
C                                                                        40
      DIMENSION ABN(1),IGR(1),NFI(1),FLUX(1),EFLUX(1),WORK(1),IWORK(1)   50
      REAL*8 MATN                                                        60
      REAL*8 FNEV(4)                                                     70
      COMMON MATN,IIZ(2),NOUT,LI,IL,IM                                   80
      DATA FNEV/'SGNC ','SGT  ','SGN  ','MUEL '/,EPS/0.15/,ERMTOL/0.5/   90
      REAL*8 WITHP,WITH/'  WITH'/,WITHO/' WITHOUT'/                     100
      NC=IWORK(1)                                                       110
      N2=IWORK(3)                                                       120
      N4=IWORK(5)                                                       130
      N5=IWORK(6)                                                       140
      N6=IWORK(7)                                                       150
      NENERG=IWORK(35)                                                  160
      NMAX=IWORK(36)                                                    170
      NESGT=N4+NMAX*3                                                   180
      NFSGN=NESGT+NMAX                                                  190
      NEMUE=NESGN+NMAX                                                  200
      NWSGT=N5+3*NMAX                                                   210
      NWSGN=NWSGT+NMAX                                                  220
      NWMUE=NWSGN+NMAX                                                  230
      NE=IWORK(26)                                                      240
      NLA=IWORK(16)                                                     250
      NLE=IWORK(17)                                                     260
      N11=IWORK(12)                                                     270
      IMAX=IWORK(18)                                                    280
      AM=WORK(28)                                                       290
      DO 10 IG1=IM,IL                                                   300
      IREAD=0                                                           310
      IG=IM+IL-IG1                                                      320
      WRITE(NOUT,93) IG                                                 330
      CALL ENERG(IGR(IG),NFI(IG),ABN(IG+1),ABN(IG),WORK(NENERG))        340
      IWORK(4)=IG                                                       350
      IF(IG-IS)20,20,21                                                 360
   20 CONTINUE                                                          370
      WITHP=WITH                                                        380
      IWORK(23)=1                                                       390
      CALL ZWIN(NE,ABN(IG),ABN(IG+1),WORK(NO),JW2,JW1)                  400
      CALL NORM(JW2,JW1,WORK(N2),WORK)                                  410
      GOTO 22                                                           420
   21 IWORK(23)=0                                                       430
      WITHP=WITHO                                                       440
   22  CONTINUE                                                        450
      WRITE(NOUT,95)WITHP                                               460
      IWORK(22)=N11                                                     470
      JN=2                                                              480
      CALL KEDDAT(MATN,FNEV(JN),NW,NW1,FNW,NDATT,                       490
     *WORK(NESGT),WORK(NWSGT),                                          500
     1ABN(IG),ABN(IG+1),&2,&3,&4)                                       510
      JN=3                                                              520
      CALL KEDDAT(MATN,FNEV(JN),NW,NW1,FNW,NDATS,                       530
     $WORK(NESGN),WORK(NWSGN),                                          540
     1ABN(IG),ABN(IG+1),&2,&3,&4)                                       550
      JN=4                                                              560
      CALL KEDDAT(MATN,FNEV(JN),NW,NW1,FNW,NDATM,                       570
     *WORK(NEMUE),WORK(NWMUE),                                          580
     1ABN(IG),ABN(IG+1),&5,&3,&4)                                       590
      IF(IWORK(23).NE.0)GOTO 24                                         600
      AMUI=2./3./AM                                                     610
      ERMAX=0.                                                          620
      DO 23 I=1,NDATM                                                   630
      ERM=ABS((WORK(NWMUE-1+I)-AMUI)/AMUI)                              640
      IF(ERM.LE.EPS)GOTO 23                                             650
      WRITE(NOUT,96)FNEV(4),FNEV(1),WORK(NEMUE-1+I),WORK(NWMUE-1+I),    660
     *AMUI,ERM,EPS                                                      670
      ERMAX=AMAX1(ERMAX,ERM)                                            680
   23 CONTINUE                                                          690
      IF(ERMAX.LE.ERMTOL)GOTO 24                                        700
      WRITE(NOUT,97)ERMAX,ERMTOL                                        710
      GOTO 10                                                           720
   24 CONTINUE                                                          730
      DO 30 I=1,NDATS                                                   740
   30 WORK(N6+I-1)=WORK(NESGN+I-1)                                      750
      DO 31 I=1,NDATM                                                   760
   31 WORK(N6+NDATS+I-1)=WORK(NEMUE+I-1)                                770
      DO 32 I=1,NDATT                                                   780
   32 WORK(N6+NDATS+NDATM+I-1)=WORK(NESGT+I-1)                          790
      NDAT=NDATS+NDATM+NDATT                                            800
      CALL CRDN1(NDAT,WORK(N6))                                         810
      WRITE(NOUT,92)MATN,ABN(IG+1),ABN(IG),FNEV(2),NDATT,FNEV(3),NDATS, 820
     *FNEV(4),NDATM,NDAT                                                830
      IWORK(25)=NDAT                                                    840
      CALL LININT(NDATT,WORK(NESGT),WORK(NWSGT),NDAT,WORK(N6),WORK(N4)) 850
      CALL SINT(IGR(IG),NFI(IG),FLUX,EFLUX,WORK,N4,N6,WORK(NENERG))     860
      CALL LININT(NDATS,WORK(NFSGN),WORK(NWSGN),NDAT,WORK(N6),WORK(N4)) 870
      CALL LININT(NDATM,WORK(NEMUE),WORK(NWMUE),NDAT,WORK(N6),WORK(N5)) 880
    7 CONTINUE                                                          890
      N4=-N4                                                            900
      CALL SINT(IGR(IG),NFI(IG),FLUX,EFLUX,WORK,N4,N6,WORK(NENERG))     910
      IF(IREAD.EQ.1)GOTO 6                                              920
      CALL LININT(NDATM,WORK(NEMUE),WORK(NWMUE),NDAT,WORK(N6),WORK(N5)) 930
    8 CONTINUE                                                          940
      CALL SEARCH(IGR(IG),NFI(IG),WORK,IWORK,FLUX,EFLUX,WORK(NENERG))   950
      CALL ISOFAL(ABN(IG),IGR(IG),NFI(IG),FLUX,EFLUX,WORK,WORK(NENERG)) 960
      WRITE(NOUT,94)                                                    970
      DO 16 IQ=NLA,NLE                                                  980
   16 CALL SUCHM(IGR(IG),NFI(IG),WORK,IWORK,IQ,ABN)                     990
      GOTO 10                                                          1000
    5 ASSIGN  7 TO NNN                                                 1010
      IREAD=1                                                          1020
      GOTO 9
```

```
      ASSIGN 8 TO NNN                                                   1030
6     W=2.0/3.0/AM                                                      1040
9     DO 15 J=1,NDAT                                                    1050
      WORK(N5+J-1)=W                                                    1060
15    GOTO NNN,(7,8)                                                    1070
      CONTINUE                                                          1080
10    RETURN                                                            1090
      WRITE(NOUT,80)MATN                                                1100
2     RETURN                                                            1110
      WRITE(NOUT,90)MATN,ENEV(JN)                                       1120
3     RETURN                                                            1130
      WRITE(NOUT,91)MATN,ENEV(JN)                                       1140
4     RETURN                                                            1150
      FORMAT(' ***ERROR 9.2 : MATERIAL ',A8,' IS NOT FOUND')            1160
80    FORMAT(' ***ERROR 9.3   MATERIAL ',A8,'  TYP  ',A8,               1170
90    1'  ARE NOT FOUND')                                               1180
      FORMAT(' ***ERROR 9.4   MATERIAL ',A8,'  TYP  ',A8,               1190
91    1'  ARE NOT FOUND IN LIST')                                       1200
      FORMAT(/' NUMBER OF ENERGY POINTS RETRIEVED FOR MATERIAL',A10,    1210
92    *'  IN THE ENERGY-RANGE',1PE14.6,' ,',1PE14.6,' EV.',/            1220
      *3(/' ',A10,0PI10),/'0TOTAL NUMBER OF DIFFERENT POINTS',I10)      1230
      FORMAT('1CALCULATION FOR GROUP',I4,/' ',25('*'))                  1240
93    FORMAT('1')                                                       1250
94    FORMAT(/' FOR THIS ENERGY GROUP CALCULATION',A10,'  ANGULAR DISTRI 1260
95    *BUTIONS.')                                                       1270
      FORMAT(' ***WARNING 9.5 : DISCREPANCY FOR',A10,' WITHOUT',A10,'.', 1280
96    */      ' ***             : E=',1PE14.6,' MUEL=',E14.6,' 2/(3A)=',1290
      *E14.6,' ERR=',E14.6,' .G.T.',E14.6)                              1300
      FORMAT(' ***ERROR 9.7 : MAXIMUM DISCREPANCY IN NUEL(SEE WARNING 9. 1310
97    *5)=',1PE14.6,' .G.T.',E14.6,/                                    1320
      *'              : NO CALCULATION FOR THIS GROUP.')                1330
      END                                                               1340
                                                                        1350
```

```
      SUBROUTINE NORM(J2,J1,SC,WORK)                                    10
      COMMON A(4),NOUT                                                  20
      REAL*8 ANINT                                                      30
      DIMENSION SC(1),WORK(1)                                           40
      NN=IWO(33,WORK)                                                   50
      NJM=IWO(19,WORK)                                                  60
      NPL=IWO(17,WORK)                                                  70
      NEA=IWO(1,WORK)                                                   80
      KJJ=1                                                             90
      KJJT=1                                                           100
      N5=IWO(2,WORK)                                                   110
      ICOS=IWO(21,WORK)                                                120
      BL=WORK(N5)                                                      130
      BU=WORK(N5+ICOS-1)                                               140
      NJ=0                                                             150
      CALL IWIN(24,NJ,WORK)                                            160
      DO 1 I=J2,J1                                                     170
      IW=(I-1)*ICOS                                                    180
      ASG=ANINT(BU,BL,1,SC(IW+1),WORK(N5),0.0,ICOS,WORK,WORK(NN),NJM)  190
      NJ=IWO(24,WORK)                                                  200
      IF(NJ.LT.(NJM-1))GOTO 3                                          210
      KJJ=2                                                            220
      NJM1=NJM-1                                                       230
      WRITE(NOUT,100)I,WORK(NEA-1+I),NJM1,ASG                          240
    3 CONTINUE                                                         250
      KJJT=MAXO(KJJT,KJJ)                                              260
      NJ=0                                                             270
      CALL IWIN(24,NJ,WORK)                                            280
      DO 2 J=1,ICOS                                                    290
    2 SC(IW+J)=SC(IW+J)/ASG                                            300
    1 CONTINUE                                                         310
      CALL IWIN(23,KJJT,WORK)                                          320
      RETURN                                                           330
  100 FORMAT(                                                          340
     *' ***WARNING 9.8 : FOR ANGLE DISTR. NR.',I3,' AT THE ENERGY',    350
     *1PE11.3,' INTEGRATION PROBLEMS OCCUR WITH NJM=',I3,'. INTEGRAL=', 360
     *E11.3,/' ***',14X,'THE ANGLE MESHPOINTS FROM ANINT WILL BE REPLACE 370
     *D BY THE KEDAK-VALUES. INCREASING OF NJM MAY AVOID THIS POSSIBLY.' 380
     *)                                                                390
      END                                                              400
```

```
      SUBROUTINE SINT(NG,NI,FLUX,EFLUX,WORK,N,N4,ENERG)                 10
C                                                                       20
C  SUBROUTINE MODIFIED BY BROEDERS,INR   JUNE,1975                      30
C                                                                       40
      REAL*8 ENERG(1)                                                   50
      DIMENSION FLUX(1),EFLUX(1),WORK(1)                                60
      N2=IWO(5,WORK)                                                    70
      N3=IWO(6,WORK)                                                    80
      N7=IWO(22,WORK)                                                   90
      N9=IWO(13,WORK)                                                  100
      NSP=IWO(15,WORK)                                                 110
      NDAT=IWO(25,WORK)                                                120
      IC=1                                                             130
      L=N                                                              140
      N=IABS(N)                                                        150
      N2=IABS(N2)                                                      160
      NZ=NI*NG                                                         170
      DO 3 I=1,NDAT                                                    180
      IF(L.LT.0)WORK(N3+I-1)=WORK(N3+I-1)*WORK(N2+I-1)                 190
    3 WORK(N9+I-1)=1.0                                                 200
      IW=N7                                                            210
      DO 1 IP=1,NZ                                                     220
      EM=SNGL(ENERG(IP))                                               230
      EP=SNGL(ENERG(IP+1))                                             240
      WORK(IW)=FXINT(EP,EM,WORK(N),WORK(N4),FLUX,EFLUX,NSP,NDAT)       250
      FF=FXINT(EP,EM,WORK(N9),WORK(N4),FLUX,EFLUX,NSP,NDAT)            260
      IF(L.GT.0)GOTO 4                                                 270
      WORK(IW+NZ)=FXINT(EP,EM,WORK(N3),WORK(N4),FLUX,EFLUX,NSP,NDAT)   280
     1/WORK(IW)                                                        290
    4 WORK(IW)=WORK(IW)/FF                                             300
      IW=IW+1                                                          310
    1 CONTINUE                                                         320
      IF(L.LT.0)IW=IW+NZ                                               330
      CALL IWIN(22,IW,WORK)                                            340
      RETURN                                                           350
      END                                                              360
```

```
      SUBROUTINE ISOFAL(ABN,IGR2,NFI1,FLUX,EFLUX,WORK,ENERG)                10
C                                                                           20
C  SUBROUTINE MODIFIED BY BREEDERS,INR   JUNE,1975                          30
C                                                                           40
      REAL*8 ENERG(1)                                                       50
      DIMENSION ABN(1),FLUX(1),EFLUX(1),WORK(1)                             60
      IG=1                                                                  70
      NS=IWO(10,WORK)                                                       80
      QQ=WORK(32)                                                           90
      IG=IG                                                                100
      IGI=IWO(4,WORK)                                                      110
      IF(QQ.GT.0)CALL EGRENZ(ABN(1),ABN,IG,IV,WORK)                        120
      IFI=IGI+IG-1                                                         130
      CALL IWIN(4,IFI,WORK)                                                140
      NM1=IWO(17,WORK)+1                                                   150
      NJM=IWO(19,WORK)                                                     160
      NUJM=IWO(20,WORK)                                                    170
      AME=WORK(28)                                                         180
      IMAX=IWO(18,WORK)                                                    190
      IX=IWO(11,WORK)                                                      200
      N7=IWO(22,WORK)                                                      210
      NZ=IGR2*NFI1                                                         220
      IGI=IG+1                                                             230
      DO 15 IP=1,NZ                                                        240
      EM=SNGL(ENERG(IP))                                                   250
      EP=SNGL(ENERG(IP+1))                                                 260
      FNW=0.                                                               270
      IF(QQ.GT.0.)FNW=QQ*AME/(AME-1.)                                      280
      NU=NM1*IMAX                                                          290
      DO 9I=1,NU                                                           300
    9 WORK(N7+I-1)=0.0                                                     310
      IF(EP.LE.FNW)GOTO 7                                                  320
      IF(QQ.LE.0)GOTO 6                                                    330
      IF(EM.LE.FNW)EM=FNW                                                  340
    6 CALL WAHRS(EP,EM,IMAX,WORK(N7),ABN(IG),NM1,NUJM,FLUX,EFLUX,          350
     1WORK(N9),WORK,WORK(IX))                                              360
      CALL SMORN(WORK(N7),NM1,IMAX,WORK)                                   370
    7 CONTINUE                                                             380
      N7=N7+NM1*IMAX                                                       390
   15 CONTINUE                                                             400
      CALL IWIN(22,N7,WORK)                                                410
      RETURN                                                               420
      END                                                                  430
```

```
      SUBROUTINE WAHRS(EP,EM,IMAX,PI,ABN,NM1,NUJM,FLLX,EFLUX,TE,WORK,EZ)    10
      DIMENSION FLUX(1),EFLUX(1),WORK(1)                                    20
      DIMENSION TE(NM1,IMAX,NUJM)                                           30
      DIMENSION ABN(IMAX),PI(NM1,IMAX)                                      40
      DIMENSION EZ(1)                                                       50
      COMMON MATN(4),NOUT                                                   60
      QM=WORK(29)                                                           70
      NJM=IWO(19,WORK)-1                                                    80
      NN=IWO(34,WORK)                                                       90
      IG=1                                                                 100
      AM=WORK(28)                                                          110
      Q=WORK(32)                                                           120
      KL=IWO(25,WORK)                                                      130
      N2=IWO(5,WORK)                                                       140
      KJ=IWO(23,WORK)                                                      150
      N3=IWO(6,WORK)                                                       160
      N4=IWO(7,WORK)                                                       170
      N10=IWO(11,WORK)                                                     180
      N1C=N10+ 1+IMAX                                                      190
      EZ(1)=EM                                                             200
      IJ=1                                                                 210
      JM=1                                                                 220
      E=EM/QM                                                              230
      IMAX1=ICSOP(E,ABN)                                                   240
      IF(E.EQ.ABN(IMAX1))IMAX1=IMAX1-1                                     250
      IF(Q.GT.0)CALL EGRENZ(EM,ABN,IK,IMAX1,WORK)                          260
      IMAX1=IMAX1+1                                                        270
      IG=IWO(4,WORK)                                                       280
      NG=IWO(14,WORK)                                                      290
      IT=NG-IG                                                             300
      IT=MINO(IMAX,IT)                                                     310
      IF(Q.GT.0)GOTO 45                                                    320
      DO 42 I=1,IT                                                         330
      EP1=QM*ABN(IT-I+2)                                                   340
      IF(EP1.GE.EP.OR.EP1.LE.EM)GOTO 42                                    350
      IJ=IJ+1                                                              360
      EZ(IJ)=EP1                                                           370
   42 CONTINUE                                                             380
   45 CONTINUE                                                             390
      DO 44 LJ=1,IJ                                                        400
      EZ(IJ+1)=EP                                                          410
      IMAX1=IMAX1-1                                                        420
      CALL ZWIN(KL,EZ(LJ+1),EZ(LJ),WORK(N4),J2,J1)                         430
       J11=J1-1                                                            440
       EM1=EZ(LJ)                                                          450
      DO 44  IK=J2,J11                                                     460
       EP1=WORK(N4+IK)                                                     470
      IF(IK.EQ.J11)EP1=EZ(LJ+1)                                            480
      CALL LMI(EP1,EM1,WORK(N4+IK),WORK(N4+IK-1),WORK(N2+IK),              490
     1WORK(N2+IK-1),WORK(N3+IK),WORK(N3+IK-1),IMAX1,ABN,TE,NM1,NUJ,NUJM,   500
     2FLUX,EFLUX,WORK,WORK(N1C),IMAX,WORK(NN))                             510
       IF(Q.GT.0)JM=IWO(26,WORK)                                           520
      IF(IMAX1.GT.1.OR.KJ.GT.0)GOTO 3                                      530
      IF(NM1.LT.3)GOTO 3                                                   540
      TE(3,JM,NUJ)=TE(1,JM,NUJ)/AM/AM/5                                    550
      IF(NM1.LT.5)GOTO 3                                                   560

      TE(5,JM,NUJ)=-TE(1,JM,NUJ)/AM/AM/AM/AM/63                            570
    3 CONTINUE                                                             580
      NJ=IWO(24,WORK)                                                      590
      IF(NJ.GT.0)WRITE(NOUT,70)EP1,EM1,NJM,WORK(27)                        600
   70 FORMAT(' ***WARNING 9.2 : NO CONVERGENCE FOR RC*BERG ANGLE INTEGRA   610
     *TION IN THE RANGE',1P2E12.4,' EV. NJM=',I3,' ERR=',1PE12.4)          620
      NJ=0                                                                 630
```

```
      CALL IWIN(24,NJ,WORK)                                              640
      EM1=EP1                                                            650
      DO 43 J=JM,IMAX1                                                   660
      DO 43 K=1,NM1                                                      670
   43 PI(K,J)=PI(K,J)+TE(K,J,NUJ)                                        680
   44 CONTINUE                                                           690
      RETURN                                                             700
      END                                                                710
      SUBROUTINE LMI(EP,EM,E1,E2,SG1,SG2,AMU1,AMU2, IMAX,ABN,TE,          10
     1NM1,NUJ,NUJM,FLUX,EFLUX,WORK,PER, IMAM,PL)                          20
C                                                                         30
C  SUBROUTINE MODIFIED BY BROEDERS,INR  JUNE,1975                         40
C                                                                         50
      REAL*8 PLK,PL(NM1,IMAM)                                             60
      REAL*8 ANINT                                                        70
      DIMENSION ABN(IMAX),WORK(1)                                         80
      DIMENSION EFLUX(1),FLUX(1)                                          90
      DIMENSION PER(NM1,IMAM),TE(NM1,IMAM,NUJM)                          100
      COMMON MATN(4),NOUT                                                110
      EQUIVALENCE(JM,JMI)                                                120
      NJM=IWO(19,WORK)                                                   130
      AM=WORK(28)                                                        140
      CM=WORK(29)                                                        150
      KJ=IWO(23,WORK)                                                    160
      XM=WORK(30)                                                        170
      Q=WORK(32)                                                         180
      NSP=IWO(15,WORK)                                                   190
      ERR=WORK(27)                                                       200
      NLA=IWO(16,WORK)                                                   210
      NLE=IWO(17,WORK)                                                   220
      JM=1                                                               230
      IF(Q.GT.0)FNW=Q/AM/(AM+1.)                                         240
      IF(Q.GT.0)CALL EGRENZ(EP,ABN,JM,II,WORK)                           250
      ICOS=IWO(21,WORK)                                                  260
      NNE=IWO(26,WORK)                                                   270
      N1=IWO(3,WORK)                                                     280
      N5=IWO(2,WORK)                                                     290
      NR=IWO(33,WORK)                                                    300
      N8=IWO(9,WORK)                                                     310
      NG=IWO(14,WORK)                                                    320
      N6=IWO(4,WORK)                                                     330
      NL1=1                                                              340
      NL2=NLE+1                                                          350
      IF(NSP.GT.1)CALL ZWIN(NSP,EP,EM,EFLUX,JF2,JF1)                     360
      IF(Q.GT.0)GOTO 9                                                   370
      NO=IWO(1,WORK)                                                     380
      IF(KJ.EQ.0)GOTO 9                                                  390
      CALL ZWIN(NNE,EP,EM,WORK(NO),JW2,JW1)                              400
      JW=JW2+NO-1                                                        410
      IW=(JW2-1)*ICOS+N1                                                 420
    9 CONTINUE                                                           430
      DO 31 I=1,NM1                                                      440
      DO 31 J=1,IMAX                                                     450
      PER(I,J)=1.0                                                       460
      PL(I,J)=0                                                          470
   31 CONTINUE                                                           480
      DU =EP-EM                                                          490
      M1=1                                                               500
      NUJ=0                                                              510
      M2=1                                                               520
      ANS=1.0                                                            530
      SE=1                                                               540
      ISEL=IWO(8,WORK)                                                   550
      JZZ=0                                                              560
   41 NU1=2**NUJ+1                                                       570
      DX=DU/(NU1-1)                                                      580
      DO 21 I=M1,NU1,M2                                                  590
      E=EM+(I-1)*DX                                                      600
      IF(Q.GT.0)WORK(8)=E                                                610
      IF(ISEL.EQ.1)SE=FIPOL(E1,E,E2,SG1,SG2)                             620
      ASE=FIPOL(E1,E,E2,AMU1,AMU2)                                       630
      AZ=(ASE-2.0/3.0/AM)*3/(1.0-3.0/5.0/(AM**2))                        640
      IF(NSP.GT.1)GOTO 2                                                 650
      FF=PHI(E)                                                          660
      GOTO 3                                                             670
    2 DO 22 J=JF2,JF1                                                    680
      ISG=J-1                                                            690
      IF(EFLUX(J).GT.E)GOTO 23                                           700
   22 CONTINUE                                                           710
   23 CONTINUE                                                           720
      FF=FIPOL(EFLUX(ISG),E,EFLUX(ISG+1),FLUX(ISG),FLUX(ISG+1))          730
    3 CONTINUE                                                           740
      ANS=0.0                                                            750
      BU=1.0                                                             760
      J=JM-1                                                             770
      IF(KJ.EQ.0)GOTO 62                                                 780
      CALL INTEN(E,WORK(N8),WORK(IW),WORK(JW),ICOS)                      790
      BL=-1.0                                                            800
      ANS=ANINT(BU,BL,2,WORK(N8),WORK(N5),AZ,ICOS,WORK,WORK(NR),NJM)     810
      ANS=ASE-ANS                                                        820
   62 J=J+1                                                              830
      BL=-1.0                                                            840
      IF(J.GE.NG-N6+1)GOTO 30                                            850
      IF(IMAX.EQ.1)GOTO 30                                               860
       BL=BCM(E,ABN(J+1),WORK)                                           870
      IF(BL.LE.-1.0)BL=-1.0                                              880
   30 CONTINUE                                                           890
      DO 8 K=NL1,NL2                                                     900
      IF(PER(K,J).LT.ERR)GOTO 8                                          910
      IF(BL.EQ.BU)GOTO 4                                                 920
      IF(BL.LT.BU)GOTO 6                                                 930
      JZZ=1                                                              940
      BL1=BL                                                             950
      BU1=BU                                                             960
      BL=BU                                                              970
      BU=BL1                                                             980
    6 CONTINUE                                                           990
      IF(BL.GE.1)GOTO 4                                                 1000
      PLK=ANINT(BJ,BL,K,WORK(N8),WORK(N5),AZ,ICOS,WORK,WORK(NR),NJM)    1010
      IF(ANS.NE.0.)PLK=PLK+AKCR(BU,BL,K,AM)*ANS                         1020
```

```
      IF(K.GT.1.OR.PLK.GE.0.)GOTO 5                                     1030
      WRITE(NOUT,1000)E,BL,BU,PLK,ANS                                   1040
 1000 FORMAT(' ***ERROR 9.8 : NEGATIVE RESULT OF ANIAT FOR L=0.',       1050
     */       ' ***           : E=',                                    1060
     *1PE14.6,' BL=',E14.6,' BU=',E14.6,' PLK=',E14.6,' ANS=',E14.6,    1070
     */       ' ***           : PLK=0. TAKEN.')                         1080
    4 PLK=0.0                                                           1090
    5 CONTINUE                                                          1100
      IF(JZZ.EQ.0)GOTO 66                                               1110
      JZZ=0                                                             1120
      BL=BL1                                                            1130
       BL=BU1                                                           1140
   66 CONTINUE                                                          1150
      PLK=PLK*FF                                                        1160
      IF(I.EQ.1)PL(K,J)=0.5*PLK*DX*SE                                   1170
      IF(I.EQ.NU1)PL(K,J)=PL(K,J)+0.5*PLK*DX*SE                         1180
      IF(I.EQ.1.OR.I.EQ.NU1)GOTO 8                                      1190
      PL(K,J)=PL(K,J)+PLK*DX*SE                                         1200
    8 CONTINUE                                                          1210
      BU=BL                                                             1220
      IF(BU.EQ.-1.0)GOTO 20                                             1230
      GOTO 62                                                           1240
   20 CONTINUE                                                          1250
   21 CONTINUE                                                          1260
      IF(NU1.GT.2)GOTO 27                                               1270
      DO 50 J=JM,IMAX                                                   1280
      DO 50 K=NL1,NL2                                                   1290
      TE(K,J,1)=PL(K,J)                                                 1300
   50 PL(K,J)=0                                                         1310
      NUJ=NUJ+1                                                         1320
      M1=2                                                              1330
      M2=2                                                              1340
      IF(IMAX.GT.JM.OR.KJ.GT.0)GOTO 41                                  1350
      IF(NL2.LT.3)GOTO 41                                               1360
      DO 25 J=3,NL2                                                     1370
      PER(J,JM)=0.                                                      1380
      IF(J.NE.5)TE(J,JM,1)=0.                                           1390
   25 CONTINUE                                                          1400
      GOTO 41                                                           1410
   27 LX=0                                                              1420
      DO 26 J=JM,IMAX                                                   1430
      DO 7 K=NL1,NL2                                                    1440
      IF(PER(K,J).LT.ERR)TE(K,J,NUJ+1)=TE(K,J,NUJ)                      1450
      IF(PER(K,J).LT.ERR)GOTO 7                                         1460
      AJ=0.5*TE(K,J,1)+PL(K,J)                                          1470
      AL=TE(K,J,NUJ)                                                    1480
      ZC=1                                                              1490
      DO 52 IB=1,NUJ                                                    1500
      ZC=4*ZC                                                           1510
      AP=(ZC*AJ-TE(K,J,IB))/(ZC-1)                                      1520
      TE(K,J,IB)=AJ                                                     1530
   52 AJ=AP                                                             1540
      TE(K,J,NUJ+1)=AP                                                  1550
      PER(K,J)=ABS(AP)                                                  1560
      IF(ABS(AP).GT.1.E-10)PER(K,J)=ABS((AP-AL)/AP)                     1570
      IF(PER(K,J).GT.ERR)LX=1                                           1580
      PL(K,J)=0                                                         1590
    7 CONTINUE                                                          1600
   26 CONTINUE                                                          1610
      NUJ=NUJ+1                                                         1620
      IF(NUJ.GE.NUJM.AND.LX.EQ.1)GOTO 100                               1630
      IF(LX.EQ.1)GOTO 41                                                1640
       IF(Q.GT.0)CALL IWIN(26,JMI,WORK)                                 1650
      CALL IWIN(8,ISEL,WORK)                                            1660
      RETURN                                                            1670
  100 CONTINUE                                                          1680
       IF(Q.GT.0)CALL IWIN(26,JMI,WORK)                                 1690
      WRITE(NOUT,71)EP,EM,NUJM,ERR                                      1700
      DO 10 J=JM,IMAX                                                   1710
      DO 10  K=1,NM1                                                    1720
      IF(PER(K,J).LE.ERR)GOTO 10                                        1730
      WRITE(NOUT,70)K,J,TE(K,J,NUJ),PER(K,J)                            1740
      IF(ABS((EP-EM)/EM) .LT.1.E-7) TE(K,J,NUJ)=0.                      1750
   10 CONTINUE                                                          1760
   70 FORMAT(10X,'SCATTERING MATRIX_',2I4, 3X,1PE12.4,  ' ERROR ',      1770
     11PE12.4)                                                          1780
   71 FORMAT(' ***WARNING 9.3 : NO CONVERGENCE FOR ROMBERG ENERGY INTEGR 1790
     *ATION IN THE RANGE',1P2E12.4,' EV. NUJM=',I3,' ERR=',1PE12.4)     1800
      CALL IWIN(8,ISEL,WORK)                                            1810
      RETURN                                                            1820
      END                                                               1830
```

```
      FUNCTION IWO(L,IWORK)                                              10
      DIMENSION IWORK(1)                                                 20
      IWO=IWORK(L)                                                       30
      RETURN                                                             40
      END                                                                50
```

```
      SUBROUTINE IWIN(L,N,IWORK)                                         10
      DIMENSION IWORK(1)                                                 20
      IWORK(L)=N                                                         30
      RETURN                                                             40
      END                                                                50
```

```
      SUBROUTINE SUCHM(NFG,NFI,IWORK,WORK,MOM,ABN)                       10
      DIMENSION ABN(1)                                                   20
      DIMENSION WORK(1),IWORK(1)                                         30
      REAL*8 MATN                                                        40
      COMMON MATN,MAY(2),NOUT,LI      ,IL,IMI                            50
      IG=IWORK(4)                                                        60
      Q=WORK(32)                                                         70
      MK=2                                                               80
```

```
      IK=IG                                                             90
      IF(Q.LT.0)GOTO 15                                                100
      CALL EGRENZ(ABN(IG),ABN,IK,IV,WORK)                              110
      AM=WORK(28)                                                      120
      FNW=Q*AM/(AM-1.)                                                 130
      EE=AMAX1(FNW,ABN(IG+1))                                          140
      CALL EGRENZ(EE,ABN,I,IV,WORK)                                    150
      MK=4                                                             160
   15 CONTINUE                                                         170
      N9=IWORK(13)                                                     180
      N11=IWORK(12)                                                    190
      NLE=IWORK(17)                                                    200
      IM=IWORK(18)                                                     210
      IW=N11                                                           220
      NZ=NFG*NFI                                                       230
      DO 11 J=1,NZ                                                     240
      DO 12 K=1,IM                                                     250
      L=(K-1)*NZ+MK+N9                                                 260
      LL=IW+(K-1)*(NLE+1)+MOM                                          270
      WORK(L+J)=WORK(LL)                                               280
   12 CONTINUE                                                         290
   11 IW=IW+(NLE+1)*IM                                                 300
      IWORK(N9)=IM*NZ+MK                                               310
      L=IWORK(N9)+N9                                                   320
      IWORK(N9+1)=MOM                                                  330
      IWORK(N9+2)=IG                                                   340
      IF(Q.LT.0)GOTO 5                                                 350
      IWORK(N9+3)=IK                                                   360
      IWORK(N9+4)=IV                                                   370
    5 CONTINUE                                                         380
      WRITE(LI)(WORK(I),I=N9,L)                                        390
      NGR=IWORK(14)                                                    400
      WRITE(NOUT,70)MOM,MATA,IG                                        410
      DO 2 I=1,IM                                                      420
      IZ=IK+I-1                                                        430
      IF(IZ.GT.NGR)RETURN                                              440
      WRITE(NOUT,71)IG,IZ                                              450
      IW=N9+MK+(I-1)*NZ                                                460
    2 WRITE(NOUT,72)(WORK(IW+J),J=1,NZ)                                470
   70 FORMAT(/' ELASTIC SCATTERING MATRIX   SGNC',I1,'  FOR ',A8,      480
     1' GROUP=',I4)                                                    490
   71 FORMAT(' FROM GROUP ',I4,' TO GROUP  ',I4)                       500
   72 FORMAT(' ',1P10E12.4)                                            510
      RETURN                                                           520
      END                                                              530
```

```
      SUBROUTINE AMESH(B1,B2,Z,J2,NX,NL)                                10
      DIMENSION Z(6),ZA(6),ZF(6)                                        20
      DIMENSION A(13),AC(1)                                             30
      DATA NW/10/                                                       40
      GOTO (1,2,3,4,5,6),NL                                             50
    1 NX=1                                                              60
      J1=0                                                              70
      J2=1                                                              80
      Z(1)=B1                                                           90
      RETURN                                                           100
    2 N=1                                                              110
      Z(1)=A(13)                                                       120
      GOTO 7                                                           130
    3 N=2                                                              140
      Z(1)=A(7)                                                        150
      Z(2)=A(1)                                                        160
      GOTO 7                                                           170
    4 N=3                                                              180
      Z(1)=A(8)                                                        190
      Z(2)=A(13)                                                       200
      Z(3)=A(2)                                                        210
      GOTO 7                                                           220
    5 N=4                                                              230
      Z(1)=A(10)                                                       240
      Z(2)=A(9)                                                        250
      Z(3)=A(3)                                                        260
      Z(4)=A(4)                                                        270
      GOTO 7                                                           280
    6 Z(1)=A(12)                                                       290
      Z(2)=A(11)                                                       300
      Z(3)=A(13)                                                       310
      Z(4)=A(5)                                                        320
      Z(5)=A(6)                                                        330
      N=5                                                              340
    7 CONTINUE                                                         350
      IF(AC(13).GT.-1+1.0/NW)GOTO 11                                   360
      M=N                                                              370
      N=N/2                                                            380
      IF(N.EQ.0)GOTO 1                                                 390
      DO 12 I=1,N                                                      400
   12 Z(I)=Z(M-N+I)                                                    410
   11 CONTINUE                                                         420
      J1=N                                                             430
      J2=1                                                             440
      ZA(J2)=Z(J2)-(Z(J2)+1)/NW                                        450
      ZF(J1)=Z(J1)+(1-Z(J1))/NW                                        460
      IF(J1.EQ.1)GOTO 9                                                470
      J11=J1-1                                                         480
      DO 8 I=J2,J11                                                    490
      SW=Z(I+1)-Z(I)                                                   500
      SW=SW/NW                                                         510
      ZA(I+1)=Z(I+1)-SW                                                520
      ZF(I)=Z(I)+SW                                                    530
    8 CONTINUE                                                         540
    9 CONTINUE                                                         550
      DO 10 I=1,N                                                      560
      IF(ZA(I).LE.B2)J2=J2+1                                           570
      IF(ZF(I).GE.B1)J1=J1-1                                           580
   10 CONTINUE                                                         590
      NX=J1-J2+2                                                       600
      Z(J1+1)=B1                                                       610
```

```
      RETURN                                                            620
      ENTRY IRDMES(AC)                                                  630
      DO 20 I=1,13                                                      640
   20 A(I)=AC(I)                                                        650
      RETURN                                                            660
      END                                                               670
```

```
      DOUBLE PRECISION FUNCTION ANG(XX,GAM)                              10
      REAL*8 XX,GAM                                                      20
      ANG    =(XX+GAM)/DSQRT(GAM**2+2*XX*GAM+1.0)                        30
      RETURN                                                             40
      END                                                                50
```

```
      DOUBLE PRECISION FUNCTION ANINT(BU,BL,K,SG,XL,AZ,ICOS,WORK,T,NJM)  10
      REAL*8 YA,YB                                                       20
      REAL *8 MATN                                                       30
      REAL*8 T(NJM)                                                      40
      REAL*8 ANG,XX,GAM                                                  50
      REAL *8        XA,XB,XA1,YA1,AJ,AI,AK,AL,AP,AXX                    60
      REAL*8 PTL                                                         70
      DIMENSION SG(1),XL(1),Z(7) ,WORK(1)                                80
      COMMON MAT(4),NOUT                                                 90
      EQUIVALENCE(MATN,MAT(1))                                          100
C     DATA NHD/'H   H1'/                                                110
C     ANG(XX)=(XX+GAM)/DSQRT(GAM**2+2*XX*GAM+1.0)                       120
      ERR=WORK(27)                                                      130
      AM=WORK(28)                                                       140
      GAM=1/AM                                                          150
      Q=WORK(32)                                                        160
      IF(Q.LT.0)GOTO 56                                                 170
      EI=WORK(8)                                                        180
      GAM=GAM*SQRT(EI/(EI-(AM+1)/AM*Q))                                 190
   56 CONTINUE                                                          200
      IF(AM.LT.1.1)CALL HIDR(BU,BL,K,AXX,&50)                           210
      IF(AM.LT.1.1)GOTO 50                                              220
      XP=WORK(30)                                                       230
      KJ=IWO(23,WORK)                                                   240
      CALL AMESH(BU,BL,Z,L2,NX,K)                                       250
       NU=1                                                             260
      XA=BL                                                             270
      YA=ANG(XA,GAM)                                                    280
      YA=PTL(K,YA)                                                      290
      YA=YA*WINK(XL,SG,KJ,ICOS,AZ,XA)                                   300
      AXX=0                                                             310
      IL=1                                                              320
   18 CONTINUE                                                          330
      XA1=XA                                                            340
      XB=Z(IL+L2-1)                                                     350
      IF(KJ.NE.2)GOTO 20                                                360
      DO 21 I=1,ICOS                                                    370
      J=I                                                               380
      IF(XL(I).GT.XA+ERR.AND.XL(I).LT.XB-ERR)GOTO 22                    390
   21 CONTINUE                                                          400
      GOTO 20                                                           410
   22 XB=XL(J)                                                          420
      IL=IL-1                                                           430
   20 CONTINUE                                                          440
      YB=ANG(XB,GAM)                                                    450
      IF(YB.EQ.0.AND.(K-2*(K/2)).EQ.0)GOTO 57                           460
      YB=PTL(K,YB)                                                      470
      GOTO 58                                                           480
   57 YB=0.0                                                            490
   58 CONTINUE                                                          500
      YB=YB*WINK(XL,SG,KJ,ICOS,AZ,XB)                                   510
      NJ=0                                                              520
      AJ=0.5*(YA+YB)*(XB-XA)                                            530
      XA1=XA                                                            540
      YA1=YA                                                            550
       T(1)=AJ                                                          560
   10 NJ=NJ+1                                                           570
      XA=XA1                                                            580
      YA=YA1                                                            590
      AI=AJ                                                             600
      NP=2**NJ+1                                                        610
      DM=(XB-XA)/(NP-1)                                                 620
      AJ=0.5*AI                                                         630
      DO 40 IZ=2,NP,2                                                   640
      XA=XA+DM                                                          650
      YA=ANG(XA,GAM)                                                    660
      YA=PTL(K,YA)                                                      670
      YA=YA*WINK(XL,SG,KJ,ICOS,AZ,XA)                                   680
      XA=XA+DM                                                          690
   40 AJ=AJ+YA*DM                                                       700
      AK=AJ                                                             710
      AL=T(NJ)                                                          720
      ZC=1                                                              730
      DO 51  IB=1,NJ                                                    740
      ZC=ZC*4                                                           750
      AP=(ZC*AK-T(IB))/(ZC-1)                                           760
      T(IB)=AK                                                          770
   51 AK=AP                                                             780
      T(NJ+1)=AP                                                        790
      EPS=(AP-AL)/AP                                                    800
         EPS=10.0*EPS                                                   810
      IF(NJ.GE.NJM-1.AND.ABS(EPS).GT.ERR)GOTO 28                        820
      IF(ABS(EPS).GT.ERR)GOTO 10                                        830
      GOTO 29                                                           840
   28 CONTINUE                                                          850
      NJM1=NJM-1                                                        860
      WRITE(NOUT,70)BL,BU,NJM1,ERR,EPS,KJ                               870
   70 FORMAT(' ***WARNING 9.7 : NO CONVERG. FOR ROMBERG ANGLE INTEGR. IN  880
     * THE RANGE',1P2E10.2,'. NJM=',I2,' ERR=',E10.2,' EPS=',E10.2,      890
     *' KJ=',I2)                                                        900
      CALL IWIN(24,AJ,WORK)                                             910
```

```
  29  CONTINUE                                                          920
       AXX=AXX+T(NJ+1)                                                  930
      XA=XB                                                             940
      YA=YB                                                             950
      IL=IL+1                                                           960
      IF(IL.LE.NX)GOTO 18                                               970
  50  CONTINUE                                                          980
      ANINT=AXX                                                         990
      RETURN                                                           1000
      END                                                              1010
```

```
      FUNCTION WINK(XL,SG,KJ,ICOS,AZ,AM)                                10
C                                                                        20
C  FUNCTION MODIFIED BY BROEDERS, INR  JUNE,1975                         30
C                                                                        40
      DIMENSION XL(1),SG(1)                                              50
      DATA ICOMA/20/                                                     60
      COMMON M(4),NOUT                                                   70
      IF(KJ.NE.0)GOTO 1                                                  80
C     WINK=0.5*(1.+AZ*AM)                                                90
      WINK=     (1.+AZ*AM)                                              100
      GOTO 10                                                           110
    1 CONTINUE                                                          120
      IF(AM.LT.XL(1).OR.AM.GT.XL(ICOS))GOTO 2                           130
      IF(ICOS.GT.ICOMA)GOTO 3                                           140
      CALL IPOL(ICOS,XL,SG,AM,WINK,XL(ICOS+1))                          150
      GOTO 10                                                           160
    3 CONTINUE                                                          170
      DO 4 II=2,ICOS                                                    180
      I=II                                                              190
      IF(AM.LE.XL(I))GOTO 5                                             200
    4 CONTINUE                                                          210
    5 WINK=FIPOL(XL(I-1),AM,XL(I),SG(I-1),SG(I))                        220
      GOTO 10                                                           230
    2 CONTINUE                                                          240
      WRITE(NOUT,100)AM,XL(1),XL(ICOS)                                  250
   10 RETURN                                                            260
  100 FORMAT(' ***WARNING 9.1 , THE ANGLE',1PE14.6,'  IS NOT IN THE RANG 270
     *E',E14.6,' ,',E14.6,' .')                                         280
      END                                                               290
```

```
      SUBROUTINE HIDR(BU,BL,K,A,*)                                       10
      REAL*8 A,X1,X2,B1,B2                                               20
      B1=BU                                                              30
      B2=BL                                                              40
      X2=DSQRT(0.5*(1.0+B1))                                             50
      X1=DSQRT(0.5*(1.0+B2))                                             60
      GOTO (1,2,3,4,5,6),K                                               70
    1 A=X2**2-X1**2                                                      80
      RETURN 1                                                           90
    2 A=2.0/3.0*(X2**3-X1**3)                                           100
      RETURN 1                                                          110
    3 A=3.0/4.0*(X2**4-X1**4)-0.5*(X2**2-X1**2)                         120
      RETURN 1                                                          130
    4 A=0.5*(X2**5-X2**3-X1**5+X1**3)                                   140
      RETURN 1                                                          150
    5 A=0.125*(35.0/6.0*(X2**6-X1**6)-7.5*(X2**4-X1**4)+1.5*(X2**2-     160
     1X1**2))                                                           170
      RETURN 1                                                          180
    6 A=0.125*(9*(X2**7-X1**7)-14*(X2**5-X1**5)+5.*(X2**3-X1**3))       190
      RETURN 1                                                          200
      END                                                               210
```

```
      FUNCTION AKOR(B14,BL4,K,AM4)                                       10
      IMPLICIT REAL*8 (A-H,O-Z)                                          20
      REAL*4 B14,BL4,AM4,AKOR                                            30
      Q0(X)=0.75*X*X                                                     40
      Q1(X)=0.5*(X**3)                                                   50
      Q2(X)=3./16.*X*X*(3*X*X-2)                                         60
      Q3(X)=0.75*(X**3)*(X*X-1)                                          70
      Q4(X)=1./32.*((X*X-1.)*(35.*X*X-10)-1)*X*X                         80
      Q5(X)=3./16.*(X**3)*(X*X-1.)*(9*X*X-5)                             90
      B1=DBLE(B14)                                                      100
      BL=DBLE(BL4)                                                      110
      AM=DBLE(AM4)                                                      120
      GAM=1./AM                                                         130
      IF(GAM.LT.0.99)GOTO 7                                             140
      A1=DSQRT((B1+1.)/2)                                               150
      A2=DSQRT((BL+1.)/2.)                                              160
      GOTO 8                                                            170
    7 CONTINUE                                                          180
      A1=ANG(B1,GAM)                                                    190
      A2=ANG(BL,GAM)                                                    200
    8 CONTINUE                                                          210
      GOTO(1,2,3,4,5,6),K                                               220
    1 AKOR8=Q0(A1)-Q0(A2)                                               230
      GOTO 90                                                           240
    2 AKOR8=Q1(A1)-Q1(A2)                                               250
      GOTO 90                                                           260
    3 AKOR8=Q2(A1)-Q2(A2)                                               270
      GOTO 90                                                           280
    4 AKOR8=Q3(A1)-Q3(A2)                                               290
      GOTO 90                                                           300
    5 AKOR8=Q4(A1)-Q4(A2)                                               310
      GOTO 90                                                           320
    6 AKOR8=Q5(A1)-Q5(A2)                                               330
   90 AKOR=SNGL(AKOR8)                                                  340
      RETURN                                                            350
      END                                                               360
```

```
      SUBROUTINE EGRENZ(E,ABN,IK,IV,WORK)                                10
      RETURN                                                             20
      END                                                                30
C     BERECHNUNG DES QUERSCHNITTS IN DER THERMISCHEN GRUPPE              10
C                                                                        20
      SUBROUTINE THERM (NE,NTY,TYP)                                      30
      REAL*8 MAT,TYP(NTY),FEST(5),A,B,C,D,P,F,G,H,Z,X,O,Q,U,SGNCO,PRSGI  40
     1,R                                                                 50
      INTEGER*2 IHC(2),IMP(2)                                            60
      DIMENSION N(4),E(2),S(2)                                           70
      COMMON MAT,ISTRUK,ISPA,NOUT,LIZ,NAAF,NEND,KL                       80
      EQUIVALENCE(IHC(1),HM)                                             90
      DATA IMP/'PU','U '/                                               100
      WRITE (NOUT ,9000)                                                110
 9000 FORMAT(1HO/1HO/' PROGRAMM KENNZIFFER 10')                         120
      WRITE (NOUT ,9001)                                                130
 9001 FORMAT(' PROGRAMM ZUR BERECHNUNG DER THERMISCHEN QUERSCHNITTE'/)   140
      N(1)=3                                                            150
      CALL DOPW (8HBEST    ,FEST(2))                                    160
      CALL DOPW (8HTHERM   ,A)                                          170
      CALL DOPW (8HSGF     ,B)                                          180
      CALL DOPW (8HSGA     ,C)                                          190
      CALL DOPW (8HSGC     ,D)                                          200
      CALL DOPW (8HALPHA   ,P)                                          210
      CALL DOPW (8HETA     ,F)                                          220
      CALL DOPW (8HNUE     ,G)                                          230
      CALL DOPW (8HSGG     ,H)                                          240
      CALL DOPW (8HMUEL    ,Z)                                          250
      CALL DOPW (8HSGN     ,X)                                          260
      CALL DOPW (8HSGI     ,O)                                          270
      CALL DOPW (8HSG2N    ,Q)                                          280
      CALL DOPW (8HSGT     ,U)                                          290
      CALL DOPW (8HCHI     ,R)                                          300
      CALL DOPW (8HSGNCO   ,SGNCO)                                      310
      CALL DOPW (8HPROBSGI ,PRSGI)                                      320
      HM=MAT                                                            330
      IAR=0                                                             340
      ISGT=0                                                            350
      IE=0                                                              360
      SC=0.                                                             370
      LL=0                                                              380
      IF(IHC(1).EQ.IMP(1))  GO TO 802                                   390
      IF(IHC(1).NE.IMP(2))  GO TO 822                                   400
  802 LAR=1                                                             410
      DO 803 JJ=1,NTY                                                   420
      IF(TYP(JJ).EQ.C)  GO TO 805                                       430
      IF(TYP(JJ).NE.B)  GO TO 803                                       440
  805 LL=LL+1                                                           450
      IF(LL-2)803,801,803                                               460
  803 CONTINUE                                                          470
      IF(LL-2)807,801,807                                               480
  807 WRITE(NOUT,808) MAT                                               490
  808 FORMAT(1HO/' ***WARNING 10. 1 : THE GROUP CROSS SECTION SGC CAN NO 500
     1T BE CALCULATED FOR ',A9/' BECAUSE THE REACTION TYPES SGF AND SGA  510
     2ARE NOT SPECIFIED IN THE INPUT')                                  520
      GO TO 801                                                         530
  822 LAR=0                                                             540
      DO 821 JJ=1,NTY                                                   550
      IF(TYP  (JJ).EQ.C)  GO TO 801                                     560
  821 CONTINUE                                                          570
      GO TO 807                                                         580
  801 I=0                                                               590
      WRITE (LIZ)I,A                                                    600
      FEST(1)=MAT                                                       610
      IC=0                                                              620
      DO 26 I=1,NTY                                                     630
      IF(TYP(I).EQ.U)  GO TO 27                                         640
   26 CONTINUE                                                          650
      GO TO 22                                                          660
   27 LL=0                                                              670
      SGT=0.                                                            680
      IC=1                                                              690
      DO 20 I=1,NTY                                                     700
      IF(TYP(I).EQ.X)  GO TO 21                                         710
      IF(TYP(I).EQ.C)  GO TO 21                                         720
      IF(TYP(I).EQ.O)  GO TO 21                                         730
      IF(TYP(I).NE.C)  GO TO 20                                         740
   21 LL=LL+1                                                           750
      IF(LL-4)20,22,22                                                  760
   20 CONTINUE                                                          770
      IF(LL-4)23,22,22                                                  780
   23 WRITE(NOUT,25) MAT                                                790
   25 FORMAT(1HO/' ***WARNING 10. 5 : THE GROUP CROSS SECTION SGT CAN NO 800
     1T BE CALCULATED FOR ',A9/' BECAUSE THE REACTION TYPES SGN, SGA, SG 810
     2I AND SG2N ARE NOT SPECIFIED IN THE INPUT')                       820
   22 DO 1 I=1,NTY                                                      830
      IF(TYP(I).EQ.U)  GO TO 1                                          840
      KSIK=0                                                            850
      IF(TYP(I).NE.P.AND.TYP(I).NE.F)  GO TO 871                        860
      IF(LAR.EQ.0)  GO TO 875                                           870
      KSIK=1                                                            880
      FEST(3)=H                                                         890
      GO TO 872                                                         900
  875 WRITE(NOUT,876) MAT,TYP(I)                                        910
  876 FORMAT(1HO/' ***WARNING 10. 2 : THE GROUP CROSS SECTION FOR ',2A8, 920
     1' CAN NOT BE CALCULATED BECAUSE THE VALUE OF SGF IS ZERO')        930
      GO TO 1                                                           940
  874 KSIK=2                                                            950
      FEST(3)=B                                                         960
      GO TO 872                                                         970
  879 KSIK=3                                                            980
      FEST(3)=G                                                         990
      GO TO 872                                                        1000
  871 FEST(3)=TYP(I)                                                   1010
  872 CALL NOFLOC (J,N,FEST,K,K)                                       1020
      IF(J)2,2,3                                                       1030
```

```
  2 WRITE (NOUT,4) TYP(I),MAT                                                    1040
  4 FORMAT(1HO/' ***WARNING 10. 3 : THE CROSS SECTION TYPE ',A9,' IS N 1050
   1OT AVAILABLE IN THE KEDAK LIBRARY FOR MATERIAL ',A9)                         1060
    T=0.                                                                        1070
    GO TO 890                                                                   1080
  3 E(1)=FEST(4)                                                                1090
    S(1)=FEST(5)                                                                1100
    IF(E(1)-0.0253)24,5,6                                                       1110
  6 WRITE (NOUT,7) TYP(I),MAT                                                   1120
  7 FORMAT(1HO/' ***WARNING 10. 4 : IN THE KEDAK LIBRARY IS NO ENERGY  1130
   1POINT LESS THAN OR EQUAL TO 0.0253'/' AVAILABLE FOR THE CROSS SECT 1140
   2ION TYPE ',A9,' FOR MATERIAL ',A9)                                          1150
    GO TO 1                                                                     1160
 24 CALL NDFNXT(J,N,FEST,K,K)                                                   1170
    IF(J)2,2,8                                                                  1180
  8 E(2)=FEST(4)                                                                1190
    S(2)=FEST(5)                                                                1200
    IF(E(2)-0.0253) 3,10,11                                                     1210
 10 E(1)=E(2)                                                                   1220
    S(1)=S(2)                                                                   1230
  5 IF(TYP(I).EQ.G.OR.TYP(I).EQ.Z.OR.TYP(I).EQ.X)  GO TO 30                     1240
    T=S(1)*0.8862269                                                            1250
    GO TO 9                                                                     1260
 30 T=S(1)                                                                      1270
    GO TO 9                                                                     1280
 11 SE=S(1)+(0.0253-E(1))*((S(2)-S(1))/(E(2)-E(1)))                             1290
    IF(TYP(I).EQ.G.OR.TYP(I).EQ.Z.OR.TYP(I).EQ.X)  GO TO 31                     1300
    T=SE*0.8862269                                                              1310
    GO TO 9                                                                     1320
 31 T=SE                                                                        1330
  9 IF(KSIK.EQ.3)  GO TO 881                                                    1340
    IF(KSIK.EQ.2)  GO TO 877                                                    1350
    IF(KSIK.EQ.0)  GO TO 890                                                    1360
    TT=T                                                                        1370
    GO TO 874                                                                   1380
877 IF(T.EQ.0)  GO TO 875                                                       1390
    TT=TT/T                                                                     1400
    IF(TYP(I).EQ.F)  GO TO 879                                                  1410
    T=TT                                                                        1420
    GO TO 890                                                                   1430
881 T=T/(1.+TT)                                                                 1440
890 WRITE (NOUT,12) MAT,TYP(I),NE                                               1450
 12 FORMAT(1H /1H ,A9,A9,I10)                                                   1460
    WRITE (NOUT,13) T                                                           1470
 13 FORMAT(E16.8)                                                               1480
    K=5                                                                         1490
    WRITE(LIZ) K,MAT,TYP(I),NE                                                  1500
    K=1                                                                         1510
    WRITE(LIZ) K,T                                                              1520
    IF(TYP(I ).EQ.C)  GO TO 810                                                 1530
    IF(TYP(I ).EQ.B)  GO TO 812                                                 1540
    IF(IC.EQ.0) GO TO 1                                                         1550
    IF(TYP(I).EQ.X)  GO TO 28                                                   1560
    IF(TYP(I).EQ.O)  GO TO 28                                                   1570
    IF(TYP(I).EQ.Q)  GO TO 28                                                   1580
    GO TO 1                                                                     1590
810 SC=SC+T                                                                     1600
    IE=1                                                                        1610
    IF(INR.EQ.1)  GO TO 818                                                     1620
    INR=1                                                                       1630
    IF(IC.EQ.1)  GO TO 28                                                       1640
    GO TO 1                                                                     1650
812 SC=SC-T                                                                     1660
    IF(INR.EQ.1)  GO TO 818                                                     1670
    INR=1                                                                       1680
    GO TO 1                                                                     1690
 28 SGT=SGT+T                                                                   1700
    IE=0                                                                        1710
    ISGT=ISGT+1                                                                 1720
    IF(ISGT.LT.4)  GO TO 1                                                      1730
    WRITE(NOUT,12) MAT,U,NE                                                     1740
    WRITE(NOUT,13) SGT                                                          1750
    K=5                                                                         1760
    WRITE(LIZ) K,MAT,U,NE                                                       1770
    K=1                                                                         1780
    WRITE(LIZ) K,SGT                                                            1790
    GO TO 1                                                                     1800
818 WRITE(NOUT,12) MAT,D,NE                                                     1810
    WRITE(NOUT,13) SC                                                           1820
    K=5                                                                         1830
    WRITE(LIZ)K,MAT,D,NE                                                        1840
    K=1                                                                         1850
    WRITE(LIZ) K,SC                                                             1860
    IF(IC.EQ.1.AND.IE.EQ.1)  GO TO 28                                           1870
  1 CONTINUE                                                                    1880
    SNCO=1.                                                                     1890
    PSGI=1.                                                                     1900
    SG=0.                                                                       1910
    CHI=0.                                                                      1920
    WRITE(NOUT,12) MAT,SGNCO,NE                                                 1930
    WRITE(NOUT,13) SNCO                                                         1940
    K=5                                                                         1950
    WRITE(LIZ) K,MAT,SGNCO,NE                                                   1960
    K=1                                                                         1970
    WRITE(LIZ)K,SNCO                                                            1980
    WRITE(NOUT,12) MAT,PRSGI,NE                                                 1990
    WRITE(NOUT,13) PSGI                                                         2000
    K=5                                                                         2010
    WRITE(LIZ) K,MAT,PRSGI,NE                                                   2020
    K=1                                                                         2030
    WRITE(LIZ) K,PSGI                                                           2040
    FEST(3)=B                                                                   2050
    CALL NDFLOC (J,N,FEST,K,K)                                                  2060
    IF(J) 900,900,901                                                           2070
901 WRITE (NOUT,12) MAT,R,NE                                                    2080
    WRITE (NOUT,13) CHI                                                         2090
    K=5                                                                         2100
    WRITE (LIZ) K,MAT,R,NE                                                      2110
    K=1                                                                         2120
    WRITE (LIZ) K,CHI                                                           2130
900 KL=KL+1                                                                     2140
    RETURN                                                                      2150
    END                                                                         2160
```