KERNFORSCHUNGSZENTRUM

KARLSRUHE

Juni 1973 KFK 1784

Institut für Neutronenphysik und Reaktortechnik
Projekt Schneller Brüter

MIGRØS - 2: A Program Written in FORTRAN for the Calculation of Microscopic Group Constants from Nuclear Data

Compiled by
H. Huschke, B. Krieg

GESELLSCHAFT
FÜR
KERNFORSCHUNG M.B.H.

KARLSRUHE

GESELLSCHAFT FÜR KERNFORSCHUNG M. B. H.
KARLSRUHE

Kernforschungszentrum Karlsruhe

KFK 1784

Institut für Neutronenphysik und Reaktortechnik
Projekt Schneller Brüter

MIGRØS - 2 : A Program Written in FORTRAN for the Calculation of Microscopic Group Constants from Nuclear Data

Compiled by

H. Huschke and B. Krieg

with contributions from

H. Huschke, B. Krieg, B. Schatz, I. Siep, P. Vertes, H. Wiese

Gesellschaft für Kernforschung m.b.H., Karlsruhe

Abstract

MIGRØS-2 allows the production of microscopic group constants of the ABN - type. The Karlsruhe nuclear data file KEDAK is used as the nuclear data basis. All group constants necessary for diffusion-, consistent P1 -, and S_n-calculations, taking the anisotropy into account up to P_5 , can be calculated.
A description of the code and the underlying theory is given. An input and an output description, a sample problem and the program lists are provided.

Zusammenfassung:

MIGRØS-2 erlaubt die Bereitstellung von mikroskopischen Gruppenkonstanten vom ABN-Typ. Als Datenbasis wird die Karlsruher Kerndatenbibliothek KEDAK benutzt. Es können alle Gruppenkonstanten berechnet werden, die für Diffusions-, konsistente P_1- und anisotrope S_n-Rechnungen benötigt werden.
Der Code und die zugrundeliegende Theorie werden beschrieben.
Es werden ein Eingabe - und Ausgabebeschreibung, ein Rechenbeispiel und die Programmlisten bereitgestellt.

Table of Contents:

INTRODUCTION

The code MIGROS-2 has been established to produce microscopic group constants for arbitrary isotopes. MIGROS-2 allows the production of group cross section sets of the ABN-type [1]. The Karlsruhe nuclear data file KEDAK [2] is used as the nuclear data basis. The code has been further developed from the code MIGROS [3], which has been used so far for the production of the Karlsruhe 26-group cross section sets. The microscopic group constants, which are calculated by MIGROS-2, can be used for the production of macroscopic group cross sections for diffusion, consistent P_1- and for S_n- calculations, taking the anisotropy into account up to P_5. They are :

- average group cross sections for infinite dilution (without resonance self shielding) for all types of neutron reactions, from energy dependent cross sections tabulated point by point;
- energy resonance self shielding factors and average group cross sections for infinite dilution for capture, fission, elastic scattering and total neutron reaction from resolved resonance parameters, from statistical resonance parameters and from energy dependent cross sections, tabulated point by point, in the resonance region;
- matrices of the elastic scattering up to the P_5-approximation from angular distributions;
- matrices of the zero'th moment of inelastic scattering from inelastic exitation cross sections or by an evaporation model;
- 1/v-average group values;
- fission spectra;
- cross sections for the thermal energy region (one energy group).

The code MIGROS-2 has a modular structure, which 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. The output of the results is given in two forms; on paper and on an external unit.
The input of MIGROS-2 is very versatile. If the user does not use the standard

input, he has to prove whether or not the input is physically meaningful and the methods in the used modules are adequate. In the following a short description of the task of MIGROS-2 is given.

The calculation of average group cross sections from pointwise data on KEDAK.

Group averages for all types of cross sections that are available on KEDAK are calculated. A trapezoidal rule for the integration is used. As integration points the energy points on KEDAK are used. Besides the average group cross-sections group values for the average cosine of the elastic scattering, for the number of secondaries per fission, for α and η are calculated.

The calculation of energy resonance self shielding factors and average group cross sections from resolved resonance parameters and from statistical parameters.

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.
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.

The calculation of energy resonance self shielding factors from pointwise data.

The same types of self shielding factors that are calculated from resonance parameters can also be calculated from pointwise data by a tropezoidal rule. They can only be calculated for the temperature for which the cross sections are tabulated.

The calculation of the zero'th and higher moments of the elastic scattering transfer elements.

There exist two approaches. In the first one average transfer elements from one group into another or into the same group are calculated. The average over the outscattering group may be weighted.
In the second approach, the outscattering group is subdivided into several intervals. To describe the transfer from one group to another, for each outscattering group the average values over the intervals are calculated. In both cases an integration is done over the in-scattering groups.
Both approaches expect tabulated angular distributions. The angles must be the same for all energies, at which the distributions are tabulated.
The two approaches use different interpolation and quadrature procedures. In the first one the angular distributions are transformed from the centre of mass system to the laboratory system. The interpolations in the energy and in the angle are done by polinomials of the order four. The integration over the in-scattering group is performed as integration over the corresponding angle interval in the laboratory system by a Simpson rule, the integration over the outscattering group is performed by a trapezoidal rule.
In the second approach the interpolation for the angle in the centre of mass system is done by a linear interpolation, the interpolation in energy is performed logarithmic. The integration over the in-scattering groups is transformed to an integration over the corresponding angle intervals in the centre of mass system. Both integration, over the angle intervals and over the outscattering groups is done by a Romberg procedure.

The calculation of the inelastic scattering matrix.

For the calculation of the inelastic scattering matrix in the range of discrete levels excitation cross sections are used. The total inelastic scattering cross section and the excitation cross sections are interpolated linearly. All energy integrations are done by a trapezoidal rule.
At higher energies the Weißkopf evaporation model is used.

The calculation of the fission spectra.

Fission spectra are calculated by a Watt-formula. The fragment kinetic energy per nucleon and the Watt fragment nuclear "temperature" are used.

Thermal cross sections.

One thermal group with a Maxwellian spectrum is assumed.

References

/1/ L.P. Abagjan, N.V. Bazazjanc, I.I. Bondarenko, M.N. Nikolaev
Gruppenkonstanten schneller und intermediärer Neutronen für die Berechnung von Kernreaktoren.
KFK-tr-144

/2/ B. Hinkelmann, B. Krieg, I. Langner, J.J. Schmidt, D. Woll
Status of the Karlsruhe evaluated nuclear data file KEDAK at June 1970.
KFK 1340

/3/ H. Huschke et.al.
Gruppenkonstanten für dampf- und natriumgekühlte schnelle Reaktoren in einer 26-Gruppendarstellung.

1. The organization of MIGRØS-2

1.1 The logical structure of MIGRØS-2

The code MIGRØS-2 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. Also in these the group constants are output on paper and on an external storage unit. The available computational modules are given in table I.

The 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 the 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 FORTRAN-IV, except for the routine DATAMAIN, which is written in 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.

MIGROS-2 is organized in an overlay structure, given in table II.

1.2 The control module

The control module has three tasks:

- to read all input information exept 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 DATAMAIN und MAIN a central data array is provided, whose length can be defined by the user in the IBM/OS control language (see chapter 2).

In the subroutine INPUT, all input information exept 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 the control is actually transferred to the module. All information of the central data array is transferred by parameter lists in the entry sub-routines of the computational modules. A description is given in table III.

Also there is an unlabeled CØMMØN-array, described in table IV.

1.3 The organization of the central data array XL

The ASSEMBLER-routine DATAMAIN provides a central array named XL for the subroutine MAIN. The length of XL is defined by the user in the PARM.G-parameter of the EXEC-card in the IBM/OS control language. 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 that necessary for the variable dimensioning of the input arrays in the XL-array is retained, e.g., the number of group boundaries, the number of points of the weighting function, the number of computational modules that shall be used etc. The input unit is "backspaced" to the beginning and 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 every call of a computational module the length of the non-permanent section of the XL-array is checked to determine, if it is long enough for the working arrays of the module. The length of these working arrays are dependent 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 the 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 the working array is so large that the XL-array is not long enough the computational module in question is passed 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 the case, that there are specified no weighting functions for the group cross sections and matrices by input, the following two functions are used:

```
FUNCTIØN PHI(E)
PHI = 1./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.

```
FUNCTIØN PHI1 (L,E)
PHI1 = 1./E ** L
RETURN
END
```

E is the energy in [eV]
L = l + 1, l = Legendre moment.

This weighting function is used for the first and higher Legendre moments in the module 6 (not in module 9).

Table I

number of the module	described in	content	names of the subroutines and functions	entry subroutine
1	chapter 4	energy resonance self shielding factors from resolved Breit-Wigner resonance parameters	DOPW, EXPPX, FGEM, NDF, PHI, PSIXI, STOSS, WIRQ, WIRQU	FGEM
2	chapter 5	energy resonance self shielding factors from statistical Breit-Wigner parameters	DELTA, DMIT, DØPW, EPSI, EZZ, FSTAT, GAFM, GAMG, GAMN, NDF, PHASE, PHI, PØL, QUER, SIGC, SUCH, TAB	FSTAT
3	chapter 9	energy resonance self shielding factors from neutron cross sections given point by point in energy	DØPW, FSTRUK, NDF, PHI	FSTRUK
4	chapter 3	average group cross sections, for infinite dilution (without resonance self shielding from point by point data in the energy and average group values $\bar{\mu}$, η, α, ν	DØPW, NDF, PHI, SUND	SUND

number of the module	described in	content	names of the subroutines and functions	entry subroutine
5	chapter 6	zero'th moment of the inelastic scattering from discrete levels and from an evaporation model	AKED, DNFAK, DØUB, EXD, NDF PHI, SCAT, TRA, XKØN	SCAT
6	chapter 7	zero'th and higher moments of the elastic scattering from angular distributions	ADD, FLUMMI, GRUPIN, G, IN, FØRM, IPØLA, IPØLIN, LECAL, LEGANS, LEGINT, LEGIST, LEGPØL, LØØKO, LØØK1, LØØK2, LØØK3, MAKRØ, MIXSGT, MUKØN, NDF, PHI, PHIL, PRINT, PUNK, PUSUM, SPRAL, SUM, TRAFØ, TRAPEZ	FLUMMI
7	chapter 12	fission spectra	DØPW, NDF, SPALT	SPALT
8	chapter 11	1/V-average group values	DØPW, EDV, PHI	EDV
9	chapter 8	zero'th and higher moments of elastic scattering for the "REMO"-correction	AKØR, AMESH, ANINT, BCM, EGRENZ, FXINT, HIDR, ICSØP, INTEN, ISØFAL, IWIN, IWØ KEDDAT, LMI, MASSIN, NDF, NØRM, PHI, PTL, REMØ, REMP SEARCH, SINT, SMØRN, SUCHM, WAHRS, WINK, ZWIN	REMØ

number of the module	described in	content	names of the subroutines and functions	entry subroutine
1o	chapter 1o	group cross sections in the thermal group	DØPW, NDF, THERM	THERM
control module	chapter 2		DATAMAIN, DØPW, EING, FREEFØ, FSTAE, INPUT, MAIN, NDF	

Table II The overlay structure of MIGRØS-2

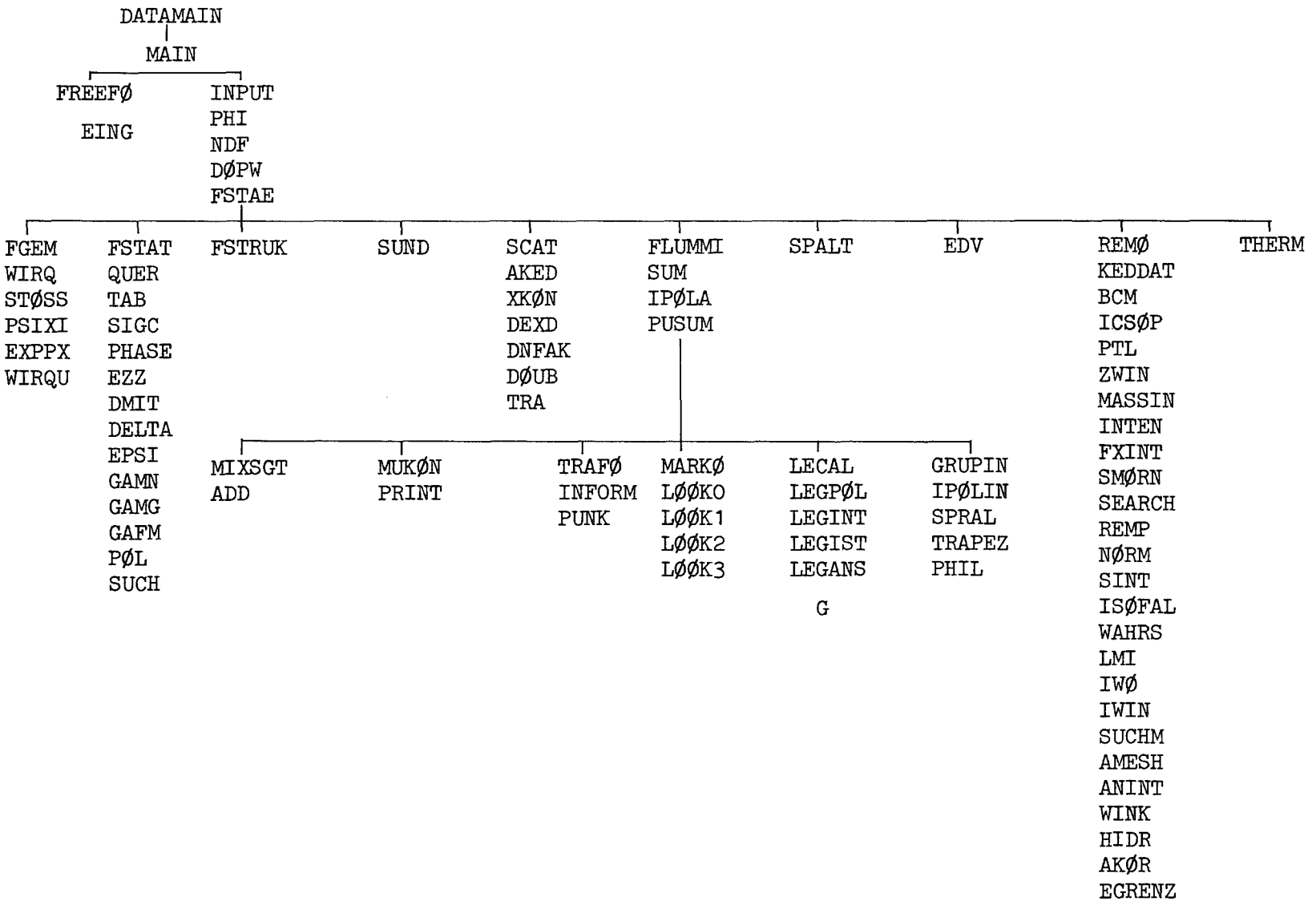


Table III

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	15
NMAT	Real 8	NAME(I), I=1, NMAT	25
NMAT	Real 4	TZ(I), I=1, NMAT	25
NE	Real 4	ENG(I), I=1, NE	5
NFE	Real 4	EF(I), I=1, NFE	7
NFE x NSPEC	Real 4	(F(I,J), I=1, NFE), J=1, NSPEC	7
3 x NA	Integer 4	(NR(I,J),I=1,3)J=1, NA	9
NT	Real 4	TEMP(I), I=1, NT	11
MI+1	Real 4	SIGO(I),I=1, MI	13
NA	Integer 4	NGRE(K), K=1, NCALL	9, 34, 33
NA x NE	Integer 4	(NI (K,I),I=1, NGRE) K=1, NCALL	9, 5, 34, 33
NA x NE	Integer 4	(N2)K,I), I=1, NGRE K=1, NCALL	9, 5, 34, 33
NA x NE	Integer 4	(NFG(K,I=1, NGRE) K=1, NCALL	9, 5, 34, 33
NA x NE	Integer 4	(NFI(K,I), I=1, NGRE K=1, NCALL	9, 5, 34, 33
2 x NE	Integer 4	this subarray is defined, but information is actually only stored if module 9 is called	5

Table III, cont.

b) The non-permanent section

Besides the permanent section a non-permanent section is defined, when a computational module is actually 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 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.

b1) Module 1

length of the subarray	type	content of the subarray	see card n of the input description
MI x 7	Real 4	SUM, auxiliary array	13
NE x 3	Real 4	SUØ, " "	5
max (3oo,r)	Real 4	ER, " "	
max (3oo,r)	Integer 4	L, " "	
max (3oo,r)	Real 4	GJ, " "	
max (3oo,r)	Real 4	GAT, " "	
max (3oo,r)	Real 4	GAN, " "	
max (3oo,r)	Real 4	GAG, " "	
max (3oo,r)	Real 4	GAF, " "	
5 x max (4oo,i)	Real 4	STE, " "	

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.

b2) Module 2

length of the subarray	type	content of the subarray	see card n of the input description
3 x 5 x MI	Real 4	SE auxiliary array	13
3 x 5 x MI	Real 4	SM " "	13
5 x MI	Real 4	XEUGZ " "	13

b3) Module 3

length of the subarray	type	content of the subarray	see card n of the input description
NE x 4	Real 4	XINTE, auxiliary array	5
MI x NE x 5	Real 4	ZA, " "	13, 5
MI x NE x 4	Real 4	XN, " "	13, 5
MI x NE x 6	Real 4	SE, " "	13, 5
NE	Real 4	XII, " "	5
MI x NE	Real 4	ZB, " "	13, 5
NE	Real 4	XI, " "	5
max (1500,i)	Real 4	EMU, " "	-
max (1500,i)	Real 4	XMU, " "	-
3 x max (1500,j)	Real 4	SN, " "	-
3 x max (1500,j)	Real 4	EN, " "	-

i = number of $\bar{\mu}_e$-values on the KEDAK library for the isotope and energy range in question.

j = maximum number of σ_a-, σ_e-, or σ_f-values on the KEDAK library for an isotope and energy range in question.

b4) Module 4

length of the subarray	type	content of the subarray	see card n of the input description
NE	Real 4	SGC, auxiliary array	5
NE	Real 4	DUE, " "	5
NE	Real 4	XINTE, " "	5
NE	Real 4	ZINT, " "	5
NE	Real 4	XNEN, " "	5
NE	Real 4	STREU, " "	5
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 on the KEDAK library.

b5) Module 5

length of the subarray	type	content of the subarray	see card n of the input description
NE	Real 8	WAHR, auxiliary array	5
NE	Real 8	PRØB, " "	5
NE	Real 8	VW, " "	5
NE	Real 8	QUER, " "	5
NE + 1	Real 8	E, " "	5
max (700,i)	Real 8	ET, " "	-
max (25,j)	Real 8	AE, " "	-
NE	Real 4	SU, " "	5
NE	Real 4	QUØT, " "	5
NE	Integer 4	LBA, " "	5
NE	Real 4	WEIN, " "	5
NE + 1	Real 4	AG, " "	5

length of the subarray	type	content of the subarray	see card n of the input description
max (7oo,i)	Real 4	SGIT, auxiliary array	-
max (25,j)	Integer 4	KMAX, " "	-
max (4oo,j,k)	Real 4	SGIP, " "	-
max (4oo,i)	Real 4	WERT, " "	-

i = number of σ_{in}-values for one isotope on the KEDAK-library.

j = number of exitation levels for one isotope on the KEDAK-library.

k = number of exitation cross sections for one isotope on KEDAK-library.

b6) Module 6

length of the subarray	type	content of the subarray	see card n of the input description
max (i,4oo)	Real 4	A, auxiliary array	-
max (i,4oo)	Real 4	B, " "	-
max (i,4oo)	Real 4	EA, " "	-
max (i,4oo)	Real 4	EB, " "	-
max (i,4oo)	Real 4	E, " "	-
max (j,1ooo)	Real 4	EN, " "	-
max (j,1ooo)	Real 4	SGN, " "	-
max (j,1ooo)	Real 4	ECØ, " "	-
max (j,1ooo)	Real 4	SCØ, " "	-
max (j,1ooo)	Real 4	V, " "	-
max (j,1ooo)	Real 4	W, " "	-
max (j,1ooo)	Real 4	F, " "	-
k	Real 4	AR, " "	-
k	Real 4	FU, " "	-
NE + 1	Real 4	ABN, " "	5

length of the subarray	type	content of the subarray	see card n of the input description
NE + 1	Integer 4	INT, auxiliary array	5
NE + 1	Real 4	GR, " "	5
NE + 1	Real 4	FEKØE, " "	5
NE	Real 4	R, " "	5
NE	Real 4	RSP, " "	5
k x i	Real 4	SGNC, " "	-
l x i	Real 4	FEKØ, " "	-
6 x l x NE	Real 4	ELSIG, " "	5
2 x NE	Real 4	ELTØT, " "	5
max (m,3ooo)	Real 4	ET, " "	-
max (m,3ooo)	Real 4	ST, " "	-

i = 3oo + maximum number of energy points for the reactor type SGNC on the KEDAK-library for four neighbouring energy groups.

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

k = number of angle-mesh-points for the reaction type SGNC on KEDAK.

l = maximum nuber of elements of the elastic scattering matrix for one outscattering group.

m = maximum number of energy points for the reaction type SGT on KEDAK in four neighbouring groups for a mixture of isotopes.

b7) Module 7

length of the subarray	type	content of the subarray	see card n of the input description
NE	Real 4	X, auxiliary array	5

b8) Module 8

length of the subarray	type	content of the subarray	see card n of the input description
NE	Real 4	E, auxiliary array	5
NE	Real 4	V, " "	5
NE	Real 4	Y, " "	5
max (NFE, 1o x NE)	Real 4	ES, " "	5
max (NFE, 1o x NE)	Real 4	F, " "	5

b9) Module 9

length of the subarray	type	content of the subarray	see card n of the input description
XL-array minus the permanent section	Real 4	WØRK, auxiliary array	-

b1o) Module 1o

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

Table IV Structure of the unlabled CØMMØN-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	3
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	9
1	Integer 4	J, at the end of each module J must be enlarged by one	9

References

/1/ J.J. Schmidt
Neutron Cross Sections for Fast Reactor Materials
KFK 12o, 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 134o, EANDC(E), 136 "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

2. Input and output of MIGRØS-2

2.1 Description of the input

In the following input description the expression "card" is used for the information that is read by one READ-statement. The input is unformatted. The following rules must be observed: The information of one "card" may actually be punched on several cards. Column one of the first physical card must not be blank, for the following physical cards belonging to the same READ-statement it must be blank. The information of two words must be separated by at least one blank. Alphanumeric information may consist of eight symbols or less. It is represented in the form 'TEXT bbbb'. The blanks and apostrophes are obligatory. For alphanumeric information consisting of five or less symbols the following representation is also allowed: αTEXTα. In this case no blanks are necessary. They are only necessary, if several words are linked: αTEX1α αTEX2α or linked αTEX1bTEX2bα.

2.1.1 Input description

Card 1

MAT		name of the material in the KEDAK-nomenclature /1/
ISTRUK	= o:	light or medium weight material, no temperature dependent resonance cross-sections
	= 1:	heavy isotopes, temperature dependent resonance cross sections

Card 2

αBLØCα	1	constant

Card 3

ISPA	= o:	non-fissile isotope
	= 1:	fissile isotope

Comment: If card 2 and card 3 are not defined, it is assumed that the isotope is fissile, if the last figure of the material name is odd.

Card 4

αBLØCα	2	constant

Card 5

NE	number of group boundaries
(ENG(I), I=1, NE)	group boundaries in (eV) ENG(I) < ENG(I + 1)

Comment: There is no limitation for the number of groups.
If "card 4" and "card 5" are not defined, as standard input the group boundaries of the 26-group ABN-set /2/ are used.
o.215, o.465, 1.o, 2.15, 4.65, 1o.o, 21.5, 46.5, 1oo, 215, 465, 1ooo, $2.15.1o^3$, $4.65.1o^3$, $1o^4$, $2.15.1o^4$, $4.65.1o^4$, $1o^5$, $2.1o^5$, $8.1o^5$, $1.4.1o^6$, $2.5.1o^6$, $4.o.1o^6$, $6.5.1o^6$, $1o^7$.

Only the group boundaries of the non-thermal groups must be specified.

Card 6

αBLØCα	3	constant

Card 7

NSPEC	number of weighting functions
NFE	number of energy points
(EF(I), I = 1, NFE)	energy points for the macroscopic weighting functions in (eV) ordered with increasing energy
((F(I,J), I = 1, NFE), J = 1, NSPEC)	Corresponding values of the macroscopic weighting functions
Comment:	The weighting functions need not be normalized. The macroscopic weighting function represents the resonance free part of the weighting, normally a collision density $\Sigma(E)$. $\phi(E)$ is expected (Σ = total cross section, $\phi(E)$ = neutron flux density) The weighting functions (F(1,J), I = 2, NSPEC) are only used in the module 6.
	The number of weighting functions should be the same as the number of moments of the elastic scattering matrix. If only one weighting function is given, it will be used for all moments of the elastic scattering matrix.
	The number of energy points is arbitrary. The weighting function

must cover the whole energy range, in which weighted group constants shall be calculated.

If card 6 and card 7 are not provided, the following standard is used:

F(I,1) is given by the FUNCTIØN PHI (E) and (F(I,L), L=2, NLE + 1) by FUNCTIØN PHI1 (L,E) (NLE is defined in card 23).

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

```
FUNCTIØN PHI1 (L,E)
PHI1 = 1./E x x L)
RETURN
END
```

E: energy
See also card 27

Card 8

αBLØCα	4	constant

Card 9

NA	number of calls of any computational modules
((NR(I,J), I=1,3), J=1,NA)	NR(1,J) identification number of the module to be called (see table I. in chapter 1)

NR(2,J) number of the first energy group,

NR(3,J) number of the last energy group, for which the module NR(1,J) is called.

Comment: The numbers of the energy groups are fixed by the chosen group boundaries in card 4 and card 5. the groups are numerated from 1 to NE-1, starting with the group of the highest energy.

NR(2,J), NR(3,J) must be ordered with increasing energy, e.g. NR(2,J) $\geq$ NR(3,J). The module NR(1,J) is executed for all groups from NR(2,J) to NR(3,J). A module can be specified several times. There is no limitation for NA. In the case of scattering matrices, NR(2,I) and NR(3,J) are the outscattering groups. The transfer elements for all inscattering groups belonging to an outscattering group are calculated.

In the case when one of the modules 1 or 2 for the calculation of selfshielding factors is called, the following two cards are necessary:

Card 1o

αBLØCα	5	constant

Card 11

NT	number of temperatures
(TEMP(I), I=1, NT)	temperatures in ^{o}K
Comment:	If card 1o and card 11 are not specified, the following standards are used:
	$3oo^{o}K$, $9oo^{o}K$, $21oo^{o}K$ for heavy isotopes (ISTRUK = 1)
	$o^{o}K$ for light and medium weight isotopes, (ISTRUK = o).
	There is no limitations for the number of temperatures.

For the case when one of the modules 1, 2 or 3 for the calculation of self shielding factors is called, the following two cards are necessary:

Card 12

αBLØCα	6 constant

Card 13

MI	number of background cross sections σ_o
(SIGO(I), I=1, MI)	background cross sections σ_o in (barn)
Comment:	If card 12 and card 13 are not specified, the following standards are used: MI = 7, σ_o = o, 1o, $1o^2$, $1o^3$, $1o^3$, $1o^4$, $1o^5$, $1o^6$ barns
	There is no limitation for the number of σ_o-values.

If module 4 or module 10 is called, the following two cards must be specified:

Card 14

αBLØCα	7	constant

Card 15

NTYP	number of cross section types
(ITYP(I), I=1, NTYP)	names of the cross section types.
Comment:	The number of cross section types is not limited. All cross sections types available on the Karlsruhe nuclear data file KEDAK /1/ can be computed. For the names the KEDAK-nomenclautre must be used. If card 14 and card 15 are not specified, the following standards are used: MUEL, NUE, SGA, SGF, SGI, SGN, SG2N. In the case that SGA and SGF are computed, always SGC ≡ SGA - SGF is computed too. SGC can also be specified as cross section type in the input, although it is no KEDAK-type.

If module 1 is called, the following four cards are necessary:

Card 16

αBLØCα	8	constant

Card 17

NRES		number of resonances
Comment:		For the calculation of the cross sections at the energy E contribution from NRES resonances above E and NRES resonances below E are taken into account. If card 16 and 17 are not specified, a standard, NRES = 1o, is used.

Card 18

αBLØCα	9	constant

Card 19

ERRØR		allowed integration error
Comment:		ERRØR corresponds to ε in chapter 4, formulas (4.18), 4.19). If card 18 and card 19 is not specified, a standard, ERRØR = o.o5, is used.

If the module 5 is called, the following two cards are necessary:

Card 2o

αBLØCα	1o	constant

Card 21

XNUE		parameter for the Weisskopf evaporation model
Comment:		XNUE corresponds to the parameter ν in chapter 6. If card 2o and card 21 are not specified the standard XNUE = o.16 is used.

If the module 6 is called, the following eight cards are necessary:

Card 22

αBLØCα	11	constant

Card 23

ISEL	parameter, which defines the averaging procedure for the transferelements. ISEL = 2: The transferelements are the group averaged transfer cross sections normalized to the group averaged total elastic cross section. ISEL = 1: The transferelements are the group averaged, to the total elastic cross sections normalized elastic transfer cross sections.
NLA	lowest Legendre moment
NLE	highest Legendre moment
Comment:	NLA ist always set to zero by the program. NLE must be smaller or equal to five. If NLE < 1, NLE is set to one by the program. If card 22 and card 23 are not specified, the following standards are used:

ISEL = 2 for ISTRUK = o
ISEL = 1 for ISTRUK = 1
NLA = o
NLE = 5

Card 24

αBLØCα	12	constant

Card 25

NMAT	number of materials in a composition
(NAME(I), TZ(I), I=1, NMAT)	
NAME:	names of the materials
TZ:	atomic densities x $1o^{-24}$
Comment:	card 24 and card 25 are only necessary if the fine structure of the weighting function for a defined composition is to be taken into account (see chapter 7)

Card 26

αBLØCα	13	constant

Card 27

MAZ(1)	= o:	all Legendre moments are weighted with the macroscopic weighting function of the zero'th moment (see weighting function in card 7, F(I,1)).
	= 1:	each Legendre moment is weighted with it's own macroscopic weighting function (see card 7, F(I,J)).
MAZ(2)	= o:	all Legendre moments are weighted with the microscopic weighting function of the zero'th moment ∿ 1/Σ(E), Σ(E)!

macroscopic total neutron cross section for a composition.

= 1: the microscopic weighting function for the l^{-th} Legendre moment is $\sim \{ 1/\Sigma \}^{l+1}$

Comment: If card 26 and card 27 are not specified, the following standards are used:
MAZ(1) = o, MAZ(2) = o

Card 28

αBLØCα 14 constant

Card 29

NS maximum number of groups in one "macro" group.

NK number of basic energypoints used in that energy range in a group, for which scattering into neighbouring groups is possible.

NR Number of basic energy points used in that energy range in a group, for which no out-scattering into neighbouring groups is possible.

Comment: If card 28 and card 29 are not specified, the following standards are used:
NS = 4, NK = 7o, NR = 16

If module 9 is called, the following five cards are necessary:

Card 3o

αBLØCα	15	constant

Card 31

ERR	allowed integration error.
NJM	$2^{NJM} + 1$ is the number angles for the integration.
NUJM	$2^{NUJM} + 1$ is the maximum number of energy points for the integration.
Comment:	If card 3o and card 31 are not specified, the following standards are used: ERR = o,o5 NJM = 6 NUJM= 1o ERR, NJM, NUJM correspond to ε, NJM, NUJM in appendix IV

Card 32

αBLØCα	16	constant

Card 33

ISELR	= 1:	The transferelements from subintervals of the out-scattering group into other groups are interval averaged transfer cross sections, normalized to the interval averaged total elastic cross section.

ISELR	= o:	The transfer cross sections are first normalized to the total elastic cross sections. The average of the outscattering interval is performed afterwards.
NLRA		lowest Legendre moment
NLRE		highest Legendre moment
NCALL	= o:	The way of subdiving the groups, given by card 5, shall be the same for all groups. It is assumed, that the groups are subdivided into 14 fine groups and the fine groups are subdivided into five intervals. The subdivision is always performed equidistant in lethargy. The result of this procedure are 7o intervals per group.
NCALL > o	:	If the intervals shall be constructed in a different way as for NCALL = o, NCALL is the number of calls of module 9. This number must be the same as specified in card 9.

If NCALL > o, the next card must be specified NCALL-times.

Card 34

NGRE	number of subdividing procedures in one call of module 9.

(N1(I),N2(I),NFG(I),NFI(I),I=1,NGRE)

N1(I)	number of the first energy group subdivided by the I-th procedure
N2(I)	number of the last energy group subdivided by the I-th procedure
NFG(I)	number of fine groups per group in the I-th procedure
NFI(I)	number of intervals per fine group in the I-th procedure.
Comment:	If card 32 and card 33 are not specified, the following standards are used: ISELR = 1 for ISTRUK = o ISELR = o for ISTRUK = 1 NLRA = o NLRE = 5 NCALL = o NFG = 14 NFI = 5 In this case, card 34 must be omitted. In the case that card 32, card 33 and card 34 are specified, ist must be noted, that N1(I) $\geq$ N2(I) and N1(I) > N1(I+1), N2(I) > N2(I+1). (See also comment to card 9).

Card 35

αENDEα	17	constant
Comment:		This is the last card of the input for one material. It must not be omitted.

The cards 1 to 35 must be repeated for each material. The last card of the input must be

αENDEα	18	constant

2.1.2 Description of the necessary external units and memory capacity

MIGRØS-2 needs the following external units:

unit number

8	for the input with FREEFØ.
1	Karlsruhe nuclear data library KEDAK.
3	unit for the unformatted output of the results.
1o	is only necessary in the module 6 as working unit.

The necessary memory capacity must be specified by the user by the PARM.G-parameter in the EXEC-card of the IBM-job control language. The length of the PARM.G-array depends on the input information. The memory capacity, necessary for the single modules, is given in the following:
(The symbols of the input description are used).

Control module

$$2 \times NTYP + 3 \times NMAT + NFE \times (NSPEC + 1) + NT + MI + 1 + 3 \times NE + 4 \times NA \times (1 + NE)$$

words. In the case, that one of these values are not specified by the input, the standard must be used: NTYP = 6, NFE = 1, NSPEC = 1, NT = 3, MI = 7, NMAT = 1.
The memory demand of that called computational module with the largest memory demand must be added to the memory demand of the control module.

Number of the module	Memory demand of the module
1	7 x MI + 3 x NE + 7 x max (3oo, number of resonances on KEDAK) + 5 x max (4oo, maximum number of energy points, necessary for the integration over one energy group)-words. Comment: The number of integration points can not be estimated at the beginning of a calculation. If the assumed 4oo words are not sufficient, the dimension of the corresponding array is enlarged automatically by the control module, provided that the PARM.G-array is large enough. If the PARM.G-array is not large enough, the module is passed. In thise case it is recommended to duplicate the number of words for the integration array in the PARM.G-array.
2	35 x MI - words
3	6 x NE + 16 x MI x NE + 2 x max (15oo, number of MUEL-values on KEDAK in the wanted energy range) + 6 x max (15oo, number of SGA-values, number of SGN-values, number of SGF-values in KEDAK in the wanted energy range)-words.

4 6 x NE + 2 x max (1500, number of SGN-values, number of SGF-values on KEDAK in the wanted energy range)-words

5 12 x NE + 3 x (NE + 1) + 3 x max (700, number of SGI-values on KEDAK above the threshold for inelastic scattering) + 3 x max (25, number of inelastic exitation levels) + max (25 x 400, number of inelastic exitation levels times the number of the energy points for the exitation cross section belonging to the first level) + max (400, number of SGI-values above the threshold for inelastic scattering)-words.

6 5 x max (400, ISM) + 7 x max (1000, ISD) + 4 x (NE + 1) + 4 x NE + max (400 x 21, ISM x ICØS) + max (400 x 2, ISM x NECU) + 6 x max (2, NECU) x NE + 2 x ICØS + 2 x max (4000, NTT)-words

ISM: 300 + maximum number of energy points for the SGNC on KEDAK within four neighbouring energy groups.

ISD: ISM + maximum number of SGN- or MUEL-values on KEDAK within one energy group.

ICØS: number of angle points for the SGNC on KEDAK.

NECU: maximum energy loss by elastic scattering measured in energy groups (= 2 for scattering into the neighbouring group).

NTT: number of SGT-values for a given composition in four neighbouring energy groups.

7 NE-words

8 3 x NE + 2 x max (1o x NE, NFE)-words

9 39 + NM1 x IMAX + (3 + NUJM) + ICØS x (2 + NIV) + NIV + IMAX + 2 x NJM + 3 x NDAT + NE + NFIN x IZV + BUF - words.

NM1: NLRE +1

NFIN: number of energy points in one energy group

NDAT: maximum number of SGT- or SGN-values on KEDAK in one energy group.

NIV: number of energy points for the SGNC on KEDAK

BUF: max (NDAT, 2 + IMAX x NFIN)

IZV: max (4, IMAX x NM1)

IMAX: maximum energy loss by elastic scattering measured in energy groups (identical with NECU in module 6).

ICØS: identical to module 6

1o -

The REGIØN-parameter on the JOB-card is given by the length of the PARM.G-array in K-bytes + 17o K-bytes for the MIGRØS-programs and the buffer.

2.2 Description of the output

2.2.1 Printed output

Each computational module has an output of the results on paper. In table V an explanation of the symbols is given.

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.

2.2.3 Output of error messages

In table VII a list of error messages and warnings is given. In this list only those messages are given which are not self explaining.

Table V

Module 1

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

Temperatures are given in ^{o}K, the group boundaries in eV, cross sections in barns.

Module 2

Symbol	content		defined by formula	required KEDAK-types
SIGMA G	average group cross sections for infinite dilution	radiative capture	(5.37)	
SIGMA N		elastic scattering	(5.38)	
SIGMA F		fission	(5.37)	
SIGMAN1	identical with SIGMA N		-	ISØT1
SIGMAT1	SIGMA G + SIGMA N + SIGMA F		-	ISØT2
SIGMA o	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		
Temperatures are given in ^{o}K, group boundaries in eV, cross sections in barns				

Module 3

Symbol	content		defined by formula	required KEDAK-types
SIGMA A	average group cross sections for infinite dilution,	absorption	(9.1o)	SGA
SIGMA C		capture		
SIGMA N		elastic scattering		SGN
SIGMA F		fission		SGF
SIGMA No1		$\sigma_e \cdot \bar{\mu}_e$	(9.11)	
SIGMA N1	identical to SIGMA No1		-	SGT
SIGMA T1	SIGMA C + SIGMA N + SIGMA F		-	MUEL
FA	flux weighted resonance self shielding factors,	absorption	(9.1)	
FC		capture		
FN		elastic scattering		
FF		fission		
FNo1	flux weighted resonance self shielding factor for	$\sigma_e \cdot \bar{\mu}_e$	(9.3)	
FN1	current weighted resonance self shielding factor for $\sigma_e \cdot \bar{\mu}_e$		(9.8)	
FT1	current weighted total resonance self shielding factor		(9.5)	
SIGO	background cross section σ_o			

Group boundaries are given in eV, cross sections in barns

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 HbbbbbØ1 is calculated, also a type STR is calculated, which corresponds to formula (3.6).

Module 5

Symbol	content	defined by formula	underlying KEDAK-type
PRØBSGI	inelastic scattering probabilities, in the discrete region	(6.6), (6.7)	SGI, ISØT2
	inelastic scattering probabilities, in the continuous range	(6.15)	SGI,SGIZ,ISOT2
In the first column the numbers of the outscattering groups are printed. The numbers above the values of PRØBSGI are the inscattering groups.			

Module 6

Symbol	content	defined by formula	underlying KEDAK-type
SGNC0	zero'th moment of elastic scattering matrix, normalized to the total elastic cross section		SGN,
SGNC1	1^{st} moment		SGNC,
SGNC2	2^{nd} moment		MUEL,
SGNC3	3^{th} moment		SGT
SGNC4	4^{th} moment		
SGNC5	5^{th} moment		

Module 7

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

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.			

Module 1o

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 (1o.1) to (1o.5).

Table VI (The symbols of table V are used)

Module 1

1. record: o , 'MIGR----'
2. record: n , material name, temperature in [°K], number of the energy group, lower group boundary in [eV], upper group boundary in [eV]
3. record: n , SIGMA G, SIGMA N, SIGMA F, SIGMA N1, SIGMAT1
4. 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 4-bytes words in the record. The material names are 8-bytes alphanumerical words. All other words are R x 4. The 8-bytes alphanumeric words are counted as two words in n. These conventions are the same for all ohter modules. Exceptions are mentioned. "-" in the label names must be interpreted as blank.

Module 2

1. record: o , 'FSTAT---'
2. record: n , material name, temperature in [°K], number of the energy group, lower group boundary in [eV], upper group boundary in [eV].
3. record: n , SIGMA G, SIGMA N, SIGMA F, SIGMAN1, SIGMAT1
4. record: n , SIGMA 0, FG, FN, FF, FN1, FT1

. .

. for all SIGMA 0-values

Module 3

1. record: o , 'FSTRK---'
2. record: n , material name, number of the energy group, lower group boundary in [eV], upper group boundary in [eV]
3. record: n , SIGMA A, SIGMA N, SIGMA NO1, SIGMA N1, SIGMA T1
   for non heavy isotopes (ISTRUK = o)
   n , SIGMA C, SIGMA N, SIGMA F, SIGMA NO1, SIGMA N1, SIGMA T1
   for heavy isotopes (ISTRUK = 1)
4. record: n , SIGO, FA, FN, FNO1, FN1, FT1
   . for non heavy isotopes (ISTRUK = o)
   . n , SIGO, FC, FN, FF, FNo1, FN1, FT1
   . for heavy isotopes (ISTRUK = 1)
   repeated for all SIGO-values

Module 4

1. record: o , 'SGKE----'
2. record: n , highest energy group (lowest number), lowest energy group
3. record: n , material name, name of reaction type (8-byte, alphanumeric)
4. record: n , group constant of the type defined by the 3^{rd} word in the $3.^{rd}$ record, for all energy groups, specified by the 2^{nd} 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.

Module 5

1. record: o , 'SMTØT---'
2. record: n , material name, total number of outscattering groups
3. record: n , number of the outscattering group, elements of
. the matrix PRØBSGI in the sense that the first
. element describes scattering within the group,
. then scattering into the neighbouring group etc.

repeated for all outscattering groups.

Module 6

1. record: o , 'FLUM----'
2. record: n , material name, number of outscattering groups, number of Legendre moments.
3. record: n , number of the outscattering groups, group averaged total elastic cross section, group averaged cosine for elastic scattering.

repeated for all outscattering groups.

4. 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.

Module 7

1. record: o , 'SPALT---'
2. record: n , material name, energy of the fission inducing neutron in [eV], number of the lowest energy group, number of the highest energy group.
3. record: n , CHI for all groups specified in the 2nd record, arranged with increasing energy.

Module 8

1. record: o , 'S1/V----'
2. 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

1. record: o , 'REMØ----'
2. record: n , material name, total number of outscattering groups, total number of Legendre moments.
3. 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.
4. 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.

Module 1o

1. record: o , 'THERM---'
2. record: n , material name, name of the reaction type, number of the thermal group.
3. record: n , value of the group constant specified in the 2nd record

Table VII Error messages and warnings

*** 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 chapter 5, formula (5.24).

*** 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. In this cases, the self shielding factors are not calculated and negative figures are printed. See chapter 5, and Appendix III, formula (25).

*** WARNING 2.06

Comment: The reason for this warning might be the same as in *** 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/ B. Krieg
Handling and Service Program for the Karlsruhe Nuclear Data File KEDAK.
Part I: Managment and Retrieval Programs
KFK 1725, 1972

/2/ L.P. Abayjan, N.O. Bazazjanc, I.I. Bondarenko, M.N. Nikolaev
Gruppenkonstanten schneller und intermediärer Neutronen für die Berechnung von Kernreaktoren
KFK-tr-144

3. The calculation of average group cross sections from tabulated neutron cross sections. Module 4.

3.1 The average group cross sections are defined by

$$ {}^{k}\tilde{\sigma}_{x,g} = \frac{\int_{(g)} {}^{k}\sigma_{x}(E)\,\phi(E)\,dE}{\int_{(g)} \phi(E)\,dE} \qquad (3.1) $$

k = isotope

x = neutron reaction (n,x)

g = energy group

$\phi(E)$ is the neutron flux density. In the resonance region, normaly 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

$$ {}^{k}\bar{\mu}_{e,g} = \frac{\int_{(g)} {}^{k}\bar{\mu}_{e}(E)\,{}^{k}\sigma_{e}(E)\,\phi(E)\,dE}{\int_{(g)} {}^{k}\sigma_{e}(E)\,\phi(E)\,dE} \qquad (3.2) $$

- the average number of secondaries per fission

$$ {}^{k}\nu_{g} = \frac{\int_{(g)} {}^{k}\nu(E)\,{}^{k}\sigma_{f}(E)\,\phi(E)\,dE}{\int_{(g)} {}^{k}\sigma_{f}(E)\,\phi(E)\,dE} \qquad (3.3) $$

f = fission

- the average α-value

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

γ = radiative capture

- the average η-value

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

For which type of neutron reaction an average cross-section shall be calculated can be choosen by input. There must be information available on KEDAK-library.

Besides that, the following group average

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

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

3.2 The integration in the averages (3.1) to (3.4) are done by a trapezoidal rule. As integration points the energy points at which the nuclear data on the KEDAK-library are tabulated and the group boundaries are used. The values of the cross sections at the boundaries are calculated by linear interpolation or extrapolation from the tables on KEDAK. The weighting function is either interpolated linearly from tables or is given by a function.

3.3 The following subroutines is 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 : one-dimensional field containing the energy group boundaries in [eV].

NFE : number of points of the neutron flux density.
= o, if the function PHI(E) is used.

REFE : one-dimensional field containing the energy points of the neutron flux density in [eV].

EFE : one-dimensional field containing the neutron flux density.

ITYP : number of cross section types.

ITNAM : one-dimensional field containing the names of these reaction types for which the average group cross sections shall be calculated.

LDIM : dimension of the following fields SE and FSE which is max (1500, number of σ_e(E)-values on KEDAK, number of σ_f(E)-values on KEDAK in all regarded energy groups).

The following parameters are work fields used by the subroutine SUND :

SGC, DUE, XINTE, ZINT, SNEN, STREU	one-dimensional fields of the length MM
SE, FSE	one-dimensional fields of the length LDIM .

The following parameter is calculated in the subroutine

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

: n , number, by which LDIM should be increased.

4. The calculation of 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

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

k = isotope

x = neutron reaction (n,x)

g = energy group

T = temperature in ^{o}K

σ_o = background cross section in barns

where

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

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.

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 (4.3), (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 capture and fission ,

---

* (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 = capture, fission, where

$${}_r\sigma_{ox} = 4\pi \lambda^2(E_r)\, g \cdot \frac{\Gamma_n(E_r)\,\Gamma_x(E_r)}{\Gamma^2(E_r)} \cdot \left(\frac{E}{E_r}\right)^{l-1/2} \qquad (4.9)$$

$${}_r\sigma_{oc} = 4\pi \lambda^2(E_r) \cdot g \cdot \frac{\Gamma_n(E_r)}{\Gamma(E_r)} \cdot \left(\frac{E}{E_r}\right)^{l-1/2} \qquad (4.10)$$

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

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

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

$\Delta = \frac{4kTE_r}{A}$ = Doppler width

Γ = total width

$g = \frac{2I+1}{2(2i+1)}$, I = total spin, i = spin of the nucleus

$\delta_l = \frac{R'}{\lambda\!\!\!^{-}} - \text{arctg}\ \frac{R'}{\lambda\!\!\!^{-}} \cdot l$ for l = o,1

R' = effective radius of the nucleus

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

Γ_n = neutron width

Γ_x = fission or capture width

σ_p = potential cross section

For T → 0, that means Θ → ∞, and

$$\Psi(\theta\to\infty,\ x)=\frac{1}{1+x^2} \qquad (4.14)$$

$$\chi(\theta \to \infty, x) = \frac{x}{1+x^2} \tag{4.15}$$

For resonances at negative resonance energies the formulas (4.9) and (4.1o) are modified to

$$_r\sigma_{ox} = 4\pi\lambda_o^2 \cdot g \cdot \frac{\Gamma_n(E_r)\,\Gamma_x(E_r)}{\Gamma^2(E_r)} \cdot E^{l-1/2} \tag{4.16}$$

$$_r\sigma_{oc} = 4\pi\lambda_o^2 \cdot g \cdot \frac{\Gamma_n(E_r)}{\Gamma(E_r)} \cdot E^{l-1/2} \tag{4.17}$$

where $\lambda_o = \lambda\!\!\!^{-}\ (1\ \mathrm{eV})$.

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. A trapezoidal rule is used. To keep the number of integration points as small as possible, which is necessary, because the calculation of the function values is very time consuming, the integration points are not taken equidistant. 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: $X^o = (X_1^o, X_2^o, \ldots X_n^o) = (E_{g+1}, E_{r,i}\ (i=1, n-2), E_g)$

$Y^o = (Y_1^o, Y_2^o, \ldots Y_n^o)$

E_{g+1} lower group limit

E_g upper group limit

$E_{r,i}$ resonance energy of the i-th resonance in energy group g.

Second step: $X^1 = (X_1^o, \frac{X_1^o+X_2^o}{2}, X_2^o, \ldots X_n^o) = (X_1^1, X_2^1, \ldots X_{n+1}^1)$

$Y^1 = (Y_1^1, \ldots Y_{n+1}^1)$

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

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

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

The condition

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

where ε is a given error limit, must be satisfied.

If condition (4.18) is not fulfilled, the second step is repeated until condition (4.18) is fulfilled, let's say, after repeating the second step (l-1) times.

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

$$Y^1 = (Y_1^1, \ldots Y_{n+1}^1)$$

Third step: $a = \frac{1}{2}(X_3^1 - X_2^1) \cdot (Y_2^1 + Y_3^1)$

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

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

The condition

$$\frac{b-a}{a} < \varepsilon \qquad \text{must be satisfied .} \qquad (4.19)$$

If the condition is fulfilled, the integral over the interval $\left[X_1^1, X_3^1\right]$ is given as

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

and the algorithm is repeated in the interval $\left[X_3^1, X_{n+1}^1\right]$ starting with the integration points

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

If condition (4.19) is not fulfilled, the integral in the interval $\left[X_1^1, X_2^1\right]$ is calculated as

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

and the algorithm is repeated in the interval $\left[X_2^1, X_{n+1}^1\right]$ starting with the integration points

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

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 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)

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).

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 ^{o}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 resonance of one isotope.

GAN(IRE) : one-dimensional field containing the neutron half widths for all resonance 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 ^{o}K.

A : atomic weight.

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

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

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 : 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)

References

/1/ H. Späth, INR-Arbeitsbericht, private Communication.

/2/ C. Chiarella, A. Reichel
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.

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

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

${}^{k}\sigma_{x,g}$ = microscopic effective group cross section

k = isotope

x = neutron reaction (n,x)

g = energy group

T = temperatur in ^{o}K

σ_o = background cross section in barns.

The following approximation is used:

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

with

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

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

ΔE_j = energy interval around E_j

$\sigma_{x,g}(E_j)$ = is the effective cross section in the energy interval ΔE_j around E_j 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 choosen 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 capture and fission, and

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

${}^s\sigma_{r,g}(E_j)$ is the total resonance cross section, (c = 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 :

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

where

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

$\sigma_{o,max}$ 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 :

$$ {}_1\sigma_{x,g} = \frac{\sum_j {}_1\phi_j \cdot {}_1\sigma_{x,g}(E_j) \cdot \Delta E_j}{\sum_j {}_1\phi_j \cdot \Delta E_j} \qquad (5.1o) $$

${}_1\phi_j$ is a slowly varying, resonance free current density, normaly approximated by a collision density.

For (5.1o) the same approximation for averaging as for (5.4) is used.

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

$$ {}_1\sigma_{e,g}(E) = \sum_s \left\{ {}^s_1\sigma_{r,g}(E_j) - {}^s_1\sigma_{c,g}(E_j) - {}^s_1\sigma_{f,g}(E_j) + \sigma_p \right\} \qquad (5.11) $$

$$ {}_1\sigma_{t,g}(E) = \sum_s {}^s_1\sigma_{r,g} + \sigma_p \qquad (5.12) $$

The effective resonance cross section at the energy E_j and the series s is calculated by a modified theory*, first developed by R. Froelich /1/, /2/.

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

for fission and capture

* see appendix I

and

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

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 = temperatur

$\delta_l = \frac{R}{\lambda\!\!\!^{-}} - \operatorname{arctg}\frac{R}{\lambda\!\!\!^{-}} \cdot l \quad$ for $l = o,1$

R = effective radius of the nucleus

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

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

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

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.

$\langle {}^{s}\tilde{\sigma}_x \rangle$ — average cross section of the neutron reaction (n,x) for the series s

$\langle {}^{s}\tilde{\sigma}_r \rangle$ — average resonance cross section of the series s.

$$\langle \tilde{\sigma}_t \rangle = \sigma_o + \sigma_p + \sum_s \langle {}^{s}\tilde{\sigma}_r \rangle \quad , \qquad (5.19)$$

with

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

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

$$ {}^s\sigma_{p,eff} = \langle \sigma_t \rangle - \langle {}^s\sigma_r \rangle \tag{5.21} $$

$$ {}^s\beta = \frac{\langle \sigma_t \rangle}{{}^s\sigma_{oc}} \tag{5.22} $$

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

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

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.

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

with $\nu = 10$.

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

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

$\overline{{}^{os}D}$ 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 $\overline{{}^s\Gamma_x\cdot({}^s\beta,\,{}^s\theta)}$ are normaly 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.

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

ν degree of freedom

G here is the Γ-function

---

* see appendix II

In the case, where

$$\frac{\overline{{}^{s}D}}{\sqrt{2\pi}\cdot\Delta}\cdot\frac{\langle{}^{s}\tilde{\sigma}_{r}\rangle}{{}^{s}\tilde{\sigma}_{p,eff}}\cdot{}^{s}E_{r}<0.1 \tag{5.28}$$

the following approximations are used:

$$\overline{{}^{s}\Gamma\cdot J({}^{s}\beta,{}^{s}\theta)}\simeq\frac{\overline{{}^{s}D}\cdot\langle{}^{s}\tilde{\sigma}_{r}\rangle}{{}^{s}\tilde{\sigma}_{p,eff}}\left[1-\frac{\overline{{}^{s}D}}{\sqrt{2\pi}\Delta}\cdot\frac{\langle{}^{s}\tilde{\sigma}_{r}\rangle}{{}^{s}\tilde{\sigma}_{p,eff}}\cdot{}^{s}E_{r}\right] \tag{5.29}$$

$$\overline{{}^{s}\Gamma_{x}\cdot J({}^{s}\beta,{}^{s}\theta)}\simeq\frac{\overline{{}^{s}D}\cdot\langle{}^{s}\tilde{\sigma}_{x}\rangle\cos2\delta_{l}}{{}^{s}\tilde{\sigma}_{p,eff}}\left[1-\frac{\overline{{}^{s}D}}{\sqrt{2\pi}\Delta}\cdot\frac{\langle{}^{s}\tilde{\sigma}_{r}\rangle}{{}^{s}\tilde{\sigma}_{p,eff}}\cdot{}^{s}E_{x}\right] \tag{5.30}$$

for x = capture, fission.

The ${}^{s}E_{r}$, ${}^{s}E_{x}$ are defined as

$${}^{s}E_{r}=\frac{\overline{\{{}^{s}\Gamma_{n}\}^{2}}}{\{\overline{{}^{s}\Gamma_{n}}\}^{2}}=1+\frac{2}{\nu_{n}} \tag{5.31}$$

ν_n degree of freedom of the χ^2-distribution for the neutron half width.

$$ {}^{s}E_{\chi} = \frac{\overline{\left[\frac{\{{}^{s}\Gamma_n\}^2 \cdot {}^{s}\Gamma_{\chi}}{{}^{s}\Gamma}\right]}}{{}^{s}\Gamma_n \overline{\left[\frac{{}^{s}\Gamma_n \cdot {}^{s}\Gamma_{\chi}}{{}^{s}\Gamma}\right]}} \qquad (5.32) $$

The ${}^{s}E_{x}$ are calculated by numerical integration, with the χ^2-distributions defined in (5.21).

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

$$ \langle {}^{s}\tilde{\sigma}_{\chi} \rangle = \frac{2\pi^2}{{}^{s}D} \cdot \lambda^2 \cdot g \cdot \overline{{}^{s}\Gamma_n} \cdot {}^{s}S_{\chi} \qquad (5.33) $$

with

$$ {}^{s}S_{\chi} = \frac{\overline{\left[\frac{{}^{s}\Gamma_n \cdot {}^{s}\Gamma_{\chi}}{{}^{s}\Gamma}\right]}}{\overline{{}^{s}\Gamma_n}} \qquad (5.34) $$

and

$$ \langle {}^{s}\tilde{\sigma}_{r} \rangle = \frac{2\pi^2}{{}^{s}D} \cdot \lambda^2 \cdot g \cdot \overline{{}^{s}\Gamma_n} \cdot \cos 2\delta_l \qquad (5.35) $$

The ${}^{s}S_{x}$ are calculated by numerical integration with the χ^2-distributions defined in (5.21)

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

$$\overline{{}^{s}\Gamma_n} = \overline{{}^{os}\Gamma_n} \cdot \sqrt{E} \cdot \frac{R^2 + (1+l)\lambda^2}{R^2 + \lambda^2} \qquad (5.36)$$

for $l = o,1$.

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

$$\tilde{\sigma}^{\infty}_{x,g} = \frac{\sum_j \phi_j \left\{ \sum_s \langle {}^{s}\tilde{\sigma}_x \rangle \right\}}{\sum_j \phi_j} \qquad (5.37)$$

for capture and fission,

$$\tilde{\sigma}^{\infty}_{e,g} = \frac{\sum_j \phi_j \left\{ \sum_s \left(\langle {}^{s}\tilde{\sigma}_r \rangle - \langle {}^{s}\tilde{\sigma}_c \rangle - \langle {}^{s}\tilde{\sigma}_f \rangle \right) + \tilde{\sigma}_p \right\}}{\sum_j \phi_j} \qquad (5.38)$$

for elastic scattering, where ϕ_j is the weighting function 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:

$$\overline{f(\Gamma)} = \int_0^\infty f(\Gamma)\, F(\Gamma)\, d\Gamma \tag{5.39}$$

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

$$\int_{\Gamma_i}^{\Gamma_{i+1}} F(\Gamma)\, d\Gamma = \frac{1}{n} \qquad \text{for all intervals } i=1,n \tag{5.40}$$

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

$$\overline{\Gamma}_i = \frac{\int_{\Gamma_i}^{\Gamma_{i+1}} \Gamma\, F(\Gamma)\, d\Gamma}{\int_{\Gamma_i}^{\Gamma_{i+1}} F(\Gamma)\, d\Gamma} = n \cdot \int_{\Gamma_i}^{\Gamma_{i+1}} \Gamma\, F(\Gamma)\, d\Gamma \tag{5.41}$$

For χ^2-distributions for several degrees of freedom

$$\chi_i = \frac{\overline{\Gamma}_i}{\overline{\Gamma}} \quad ; \quad i = 1, n \tag{5.42}$$

are tabulated.

$$\overline{\Gamma} \equiv \int_0^\infty \Gamma \cdot F(\Gamma)\, d\Gamma \tag{5.43}$$

The integral (5.39) then is approximated by

$$\overline{f(\Gamma)} = \sum_{i=1}^{n} f(\overline{\Gamma}\cdot\chi_i) \cdot \int_{\Gamma_i}^{\Gamma_{i+1}} F(\Gamma)\, d\Gamma = \frac{1}{n} \sum_{i=1}^{n} f(\overline{\Gamma}\cdot\chi_i) \tag{5.44}$$

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 (5.41) 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

$$\overline{f(\Gamma_1,\Gamma_2)} = \int_0^\infty d\Gamma_1 \int_0^\infty d\Gamma_2\, f(\Gamma_1,\Gamma_2)\cdot F_1(\Gamma_1)\cdot F_2(\Gamma_2) \tag{5.45}$$

are approximated by

$$\overline{f(\Gamma_1,\Gamma_2)} = \frac{1}{n_1\cdot n_2} \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} f(\overline{\Gamma_1}\cdot\chi_{1,i}\,,\,\overline{\Gamma_2}\cdot\chi_{2,j}) \tag{5.46}$$

with

$$\chi_{1,i} = \frac{\overline{\Gamma_{1,i}}}{\overline{\Gamma_1}} \quad , \quad \chi_{2,j} = \frac{\overline{\Gamma_{2,j}}}{\overline{\Gamma_2}} \quad . \tag{5.47}$$

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: 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)

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), (5.11) 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 = radius of the nucleus.

CHI(25,4) : 2-dimensional field, containing the χ_i as defined in equation (5.42) for second 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(1oo) : 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 100.

GFA(1o, 1oo) : 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.

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 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 cross sections in [barn],
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).

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 (5.32) and (5.34), 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 (5.42) 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 = radius of the nucleus.

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

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

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

EY(1oo) : 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 100.

GF(1o, 1oo) : 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), for capture.

EZC : defined by equation (5.31).

EZF : defined by equation (5.32), for fission.

DRSG : defined by equation (5.34), for capture.

DRFS : defined by equation (5.34), 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, 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 (5.36).

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 = 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 [barn], λ 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(1oo)	: one-dimensional field, containing the energies, at which the average fission widths are tabulated [eV].
GF(1o, 1oo)	: 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 [^{o}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/^{o}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 [^{o}K],
NS	: number of resonance series.
DEL	: $\frac{4k}{A} \cdot 1o^6$; k = Boltzmann constant in [eV/^{o}K], A = mass number.

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

In this function cos $2\delta_l$ is calculated, where $\delta_l = R/\lambda\!\!\!^{-} - \text{arctg}\,\frac{R}{\lambda\!\!\!^{-}} \cdot l$. 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 : $\Lambda_o^2 = E \cdot \lambda^2$ [eV·barn].

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

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

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

E : energy in [eV].

NS : number of resonance series.

XA : $\Lambda_o^2 = E \cdot \lambda^2$ [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 $\overline{\Gamma}_n^o \cdot 1o^3$ for all resonance series, $\overline{\Gamma}_n^o$ 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.

References

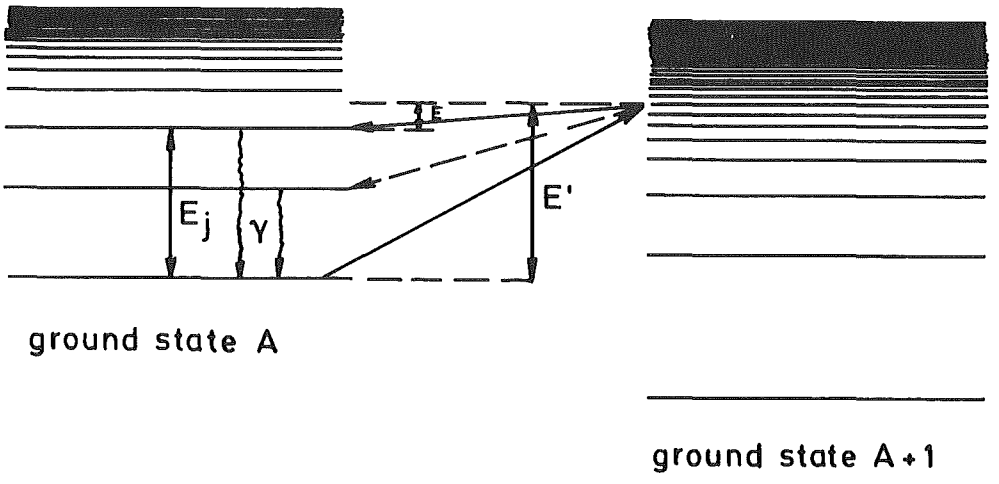
/1/ R. Froelich
Theorie der Dopplerkoeffizienten schneller Reaktoren unter Berücksichtigung der gegenseitigen Abschirmung der Resonanzen.
KFK 367 (1965)

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

6. The calculation of the matrices of the average zeroth moments of inelastic scattering. Module 5.

6.1 Description of the inelastic scattering process

Capture of a neutron with incident energy E' by a nucleus of atomic mass A leads to the formation of a compound nucleus A + 1 with excitation energy $AE = E_B + E'$ where E_B is the binding energy of the neutron in the compound nucleus. The compound nucleus decays then by emission of a neutron to an excited level of the residual nucleus, and the transition to the ground state occurs by γ-emission.



The excitation levels of the residual nucleus are either discrete ones or are belonging to the so-called continuum. The levels in the continuum cannot be resolved experimentally and concerning their position one can make statements only from statistical theory. In the discrete region the energies of the excitation levels are well-known from experiment.

The general expression for the probability of inelastic scattering out of any energy group g to any group h for an isotope k is given by Yiftah, Okrent, Moldauer /3/ in the following form:

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

Here is E' the incident neutron energy and E the energy of the scattered neutron. $\phi(E')$ represents the energy dependent neutron flux. P (E' → E) indicates the transition probability of the inelastically scattered neutrons. For its determination one has to distinguish between the range of resolved excitation levels of the residual nucleus and the so-called continuum range in which the levels of the residual nucleus are undistinguishable.

6.1.1 Energy groups with discrete excitation levels for inelastic scattering

For given incident neutron energies E' in group g and outgoing neutron energies E in group h inelastic scattering can occur only to those excitation levels for which $E = E' - E_j$ where E_j is the energy of the jth level.
The transition probability therefore is a δ-function which has the value one, if the above condition is fulfilled and zero, if not. Thus we have

$$ {}^{k}\sigma_i(E')\,P(E'\to E) = \sum_{j=1}^{N} {}^{E_j}\sigma_i(E')\,P_j(E'\to E) $$

$$ = \sum_{j=1}^{N} {}^{E_j}\sigma_i(E')\,\delta(E'-E-E_j) \qquad (6.2) $$

where N is the number of excitation levels of the isotope considered,

P_j the probability of the transition to the jth level of the residual nucleus and σ_i^{Ej} the inelastic excitation cross section of the jth level. With this special form of the transition - probability the double integration in equation (6.1) can be reduced to a single one over the energy group h to which the scattering occurs.

$$ {}^k\sigma^{\infty}_{i,g\to h} = \frac{\sum_j \int_{(h)} dE\, {}^k\sigma_i^{E_j}(E+E_j)\,\varphi(E+E_j)}{\int_{(g)} \varphi(E')\,dE'} \qquad (6.3) $$

With the transformation $E + E_j \to E'$ it follows:

$$ {}^k\sigma^{\infty}_{i,g\to h} = \frac{\sum_j \int_{E_{h+1}+E_j}^{E_h+E_j} dE'\, {}^k\sigma_i^{E_j}(E')\,\varphi(E')\,\chi(E_{g+1} \le E' \le E_g)}{\int_{E_{g+1}}^{E_g} \varphi(E')\,dE'} \qquad (6.4) $$

By the distribution function χ it was taken into account that the incident neutron energy E' should be contained in a 26-group g. On the other hand it must be of course

$$E_{h+1} + E_j \le E' \le E_h + E_j$$

because of the integration over this range. The integration therefore has to be extended only over the interval $[E_u, E_o]$ with the following definition

$$E_u = \begin{cases} E_{g+1}, & \text{if } E_{h+1} + E_j < E_{g+1} \\ E_{h+1} + E_j, & \text{if } E_{h+1} + E_j \geq E_{g+1} \end{cases}$$

$$E_o = \begin{cases} E_g, & \text{if } E_h + E_j > E_g \\ E_h + E_j, & \text{if } E_h + E_j \leq E_g \end{cases} \qquad (6.5)$$

Instead of the neutron flux the collision density $F(E') = \Sigma_t(E')\,\phi(E')$ was taken as weighting spectrum since outside the resonance region $\Sigma_t(E')$ can be considered as constant and then $F(E') \sim \phi(E')$ (see also /5/). The formula (6.4) then becomes the form:

$$k\sigma^{\infty}_{i,g\to h} = \frac{\sum_j \int_{E_{h+1}+E_j}^{E_h+E_j} dE'\, {}^k\sigma_i^{E_j}(E')\, F(E')\, \chi(E_{g+1} \leq E' \leq E_g)}{\int_{E_{g+1}}^{E_g} F(E')\, dE'} \qquad (6.6)$$

The matrix elements $\sigma_{i,g\to h}$ are normalized in the computer program SCAT (described under section 6.2.1) to the total inelastic scattering cross section value over group g

i.e.

$$k\sigma^{\infty}_{i,g} = \frac{\int_{(g)} \sigma_i(E')\, F(E')\, dE'}{\int_{(g)} F(E')\, dE'} \qquad (6.7)$$

The total inelastic scattering cross sections and the inelastic excitation cross sections are taken from the Karlsruhe Neutron Nuclear Data File KEDAK /6/.

6.1.2 Energy groups with unresolved excitation levels for inelastic scattering

If the incident neutron energy is high enough, to excite energy levels in the "continuum region" of the residual nucleus A, the level densities are calculated using the formula of Weisskopf.

Let U be the excitation energy of the nucleus of mass A and C and ν free parameters, then according to Weisskopf the level density $\omega(U)$ is

$$w(U) = C \exp(2\sqrt{\nu A U}) \tag{6.8}$$

The probability of inelastic scattering of a neutron from incident energy E' to final energy E is given by the statistical model as

$$P_i(E' \rightarrow E) = NE \exp(-E/\Theta(E')) \tag{6.9}$$

where N is a normalization constant and Θ is the "nuclear temperature", which is related to the level density of the nucleus by

$$\frac{1}{\Theta(E')} = \frac{d}{dU} \ln w(U) \Big|_{U=E'} \tag{6.10}$$

For our special formula (6.8) this results in

$$\Theta(E') = \sqrt{\frac{E'}{\nu A}} \quad [\text{MeV}] \quad \begin{cases} E' \text{ in MeV} \\ \nu \text{ in MeV}^{-1} \end{cases} \tag{6.11}$$

The free parameter ν is an input quantity for the program. Szwarcbaum et al. /2/ recommend $\nu = 0.16\ \text{MeV}^{-1}$ for all nuclei, whereas in the YOM-cross-section-set /3/ $\nu = 0.0961\ \text{MeV}^{-1}$ had been used. The figure 1 shows the influence of the parameter ν on the spectrum of the inelastically scattered neutrons. As an example the inelastic scattering of neutrons with an incident energy $E' = 8.5$ MeV on U 238 was taken, using $\nu = 0.16$, $\nu = 0.0961$ and $\nu = 0.06$. Figure 2 shows the spectra for neutrons inelastically scattered by U 238 using $\nu = 0.16$ and for $E' = 10.5$ MeV, $E' = 8.5$ MeV and $E' = 6.5$ MeV. With (6.8) and (6.11) inserted into (6.1) the cross section for inelastic scattering of a neutron on material k from group g to group h is given by

$$\begin{aligned} {}^{k}\sigma_{i,g\to h}^{\infty} &= \frac{\int_{(g)} dE'\, {}^{k}\sigma_i(E')\, F(E')\, N\, \Theta(E')^2 \exp\left(-\frac{E_{h+1}}{\Theta(E')}\right)\left(\frac{E_{h+1}}{\Theta(E')}+1\right)}{\int_{(g)} F(E')\, dE'} \\ &= \frac{\int_{(g)} dE'\, {}^{k}\sigma_i(E')\, F(E')\, N\, \Theta(E')^2 \exp\left(-\frac{E_{h}}{\Theta(E')}\right)\left(\frac{E_{h}}{\Theta(E')}+1\right)}{\int_{(g)} F(E')\, dE'} \end{aligned} \tag{6.12}$$

In (6.12) the integration over the final energy group, which can be done analytically, has already been carried out.

The integration over E' can be carried out numerically only. As the original program was written for the IBM 7074 computer and we had only a limited region of computer storage for the inelastic scattering routine, the following approximation, the same as in /2/ and /3/ was used. For the nuclear temperature $\Theta(E')$ the value averaged by $F(E')$ over the energy-group g is taken. With this the integration over E' in (6.12) can be carried out easily with the result

$$
\begin{aligned}
{}^{k}\sigma^{\infty}_{i,g\to h} = {}^{k}\sigma^{\infty}_{i,g} \cdot N \Bigg[& \Theta_g^2 \exp\left(-\frac{E_{h+1}}{\Theta_g}\right)\left(\frac{E_{h+1}}{\Theta_g}+1\right) \\
& - \Theta_g^2 \exp\left(-\frac{E_h}{\Theta_g}\right)\left(\frac{E_h}{\Theta_g}+1\right)\Bigg] \qquad (6.13) \\
= {}^{k}\sigma^{\infty}_{i,g} \; {}^{k}\tilde{P}_{i,g\to h} \cdot N &
\end{aligned}
$$

the normalization constant N is obtained by the relation.

$$
\sum_{h\geq g} {}^{k}\sigma^{\infty}_{i,g\to h} = {}^{k}\sigma^{\infty}_{i,g} \quad \text{, that means} \qquad (6.14)
$$

$$
N = \frac{1}{\sum\limits_{h\geq g} {}^{k}\tilde{P}_{i,g\to h}}
$$

so that finally the probability for inelastic scattering of a neutron by material k from group g to group h is

$$ {}^{k}P_{i,g\to h} = \frac{{}^{k}\tilde{P}_{i,g\to h}}{\sum\limits_{h\geq g} {}^{k}\tilde{P}_{i,g\to h}} \qquad (6.15) $$

Different from Szwarcbaum et al. /2/ and from the ABN-set /4/ we calculate the transition probabilities ${}^{k}P_{i,g\to h}$ for all groups h, which can be reached from group g until down to thermal energies. For groups of small energy however, the quantities E_{h+1}/Θ_g and E_h/Θ_g are very small compared to one (Θ_g is around o.5 MeV for U 238 and neutron incident energy E' = 8.5 MeV). When calculating the expression (6.13) on the computer two almost equal quantities have to be substracted, which results in numerical inaccuracies. As a consequence i.e. the values of ${}^{k}P_{i,g\to h}$ were not monotonically descending for h $\geq$ 2o in the energy-structure of the 26-group-ABN-set /4/ and sometimes even became negative. As a direct double precision calculation on the IBM 36o/65 did not completely eliminate the inaccuracies, we programmed a double precision function, that calculates

$$ \sum_{n=1}^{\infty} \frac{x^n}{n!} = \exp(x) - 1 = \tilde{F}(x) $$

By use of this function and **using** the following abbreviations

$$ x_h = \frac{E_h}{\Theta_g} \qquad x_{h+1} = \frac{E_{h+1}}{\Theta_g} \qquad \Delta x_h = x_h - x_{h+1} $$

the expression, which has to be calculated to obtain ${}^{k}P_{i,g\to h}$ (6.13) is

$$ \Theta_g^2 \exp(-x_{h+1}) \left[-\Delta x_h - \tilde{F}(-\Delta x_h) - x_{h+1}\tilde{F}(-\Delta x_h) - \Delta x_h \tilde{F}(-\Delta x_h) \right] \qquad (6.16) $$

With this numerical procedure values for ${}^{k}P_{i,g\to h}$ are calculated, that are monotonically descending for $h \geq 2o$.

6.1.3 Energy groups, where the excitation levels of the residual nucleus are partly resolved and partly unresolved.

For nearly all materials the last neutron incident energy, which can be treated with the discrete level method, lies within a 26 group, so that two different methods for calculation of the $P_{i,g\to h}$ have to be used in the same group. The results for the lower and upper part of the group are linked together as follows. Let ΔE_g^d be the energy range of group g, where the discrete level method is used, and ΔE_g^c the energy range, where the statistical model is used. Then for group g the transition probability for inelastic scattering is calculated according to the formula

$$ {}^{k}P^{(d+c)}_{i,g\to h} = d_g\,{}^{k}P^{d}_{i,g\to h} + c_g\,{}^{k}P^{c}_{i,g\to h} \qquad (6.17) $$

In (6.17) $d_g\,{}^{k}P^{d}_{i,g\to h}$ is the transition probability to group h of neutrons, whose incident energies lie in the range of resolved excitation levels of the residual nucleus within group g, that means

$$ d_g\,{}^{k}P^{d}_{i,g\to h} = \frac{\int_{\Delta E_g^d} dE' \int_{(h)} dE\; {}^{k}\sigma_i(E'\to E)\,F(E')}{\int_{(g)} dE'\; {}^{k}\sigma_i(E')\,F(E')} $$

and correspondingly (6.18)

$$ c_g\,{}^{k}P^{c}_{i,g\to h} = \frac{\int_{\Delta E_g^c} dE' \int_{(h)} dE\; {}^{k}\sigma_i(E'\to E)\,F(E')}{\int_{(g)} dE'\; {}^{k}\sigma_i(E')\,F(E')} $$

In the program ${}^{k}P^{d}_{i,g\to h}$ and ${}^{k}P^{c}_{i,g\to h}$ are both normalized in the following manner

$$\sum_{h\geq g} {}^{k}P^{d}_{i,g\to h} = 1 \quad \text{and} \quad \sum_{h\geq g} {}^{k}P^{c}_{i,g\to h} = 1 \tag{6.19}$$

so that

$$d_g = \frac{\int dE' \, {}^{k}\sigma_i(E') F(E')}{\Delta E^{d}_{g}} \Big/ \int_{(g)} dE' \, {}^{k}\sigma_i(E') F(E'), \qquad c_g = \frac{\int dE' \, {}^{k}\sigma_i(E') F(E')}{\Delta E^{c}_{g}} \Big/ \int_{(g)} dE' \, {}^{k}\sigma_i(E') F(E') \tag{6.2o}$$

A special subroutine for the calculation of (n, 2n) transition probabilities is being developped. So far the inelastic scattering transition probabilities are used for (n, 2n) reactions too.

6.2 Description of the computer program

The computer program for the calculation of the inelastic scattering matrices called SCAT is a subroutine of the managing program. It consists of the following subprograms:

A K E D, T R A, X K O N

Furthermore it uses the computer programs for retrieval of KEDAK-data NDFOPN, NDFLOC, NDFNXT. The function of the above computer-programs is outlined below.

6.2.1 S C A T

SCAT (NX, EG, XNUE, NFE, EF, FI, NE 27, WAHR, PROB, VW, QUER, E, NET, ET, NAE, AE, SU, QUOT, LBA, WEIN, AG, NETP, SGIT, NAEP, KMAX, ISG, ISGP, SGIP, IWE, IWP, WERT).

The parameters which have to be defined before calling SCAT are:

NX	:	number of energy group boundaries
NE 27	:	NX + 1
EG(NX)	:	energy group boundaries in eV
NFE	:	= o in the case the weighting spectrum is given by a function
		= constant equal to the number of points at which the weighting spectrum is given in this case
EF(NFE)	:	energy points of the weighting spectrum
FI(NFE)	:	values of the weighting spectrum
NET	:	dimension corresponding to the number of points of the inelastic scattering cross section on KEDAK for energies up to E (NAB + 1)
NAE	:	dimension corresponding to the number of inelastic excitation levels
ISG	:	dimension corresponding to the maximum of the number of KEDAK energy points for the different inelastic excitation levels
IWE	:	dimension corresponding to the number of KEDAK energy points in the "discrete" region (up to E (NAB + 1)

Only working fields are the following quantities:

NETP, NAEP, ISGP, IWP, SGIT (NET), LBA(NX), VW(NX), QUER(NX), PROB(NX), AG(NX), E(NX) and a group of parameters delivered by the subroutine AKED:

ET(NET), SGIP (NAE, ISG), JMAT, KMAX (NAE), AE (NAE), SU (NX), QUOT (NX), WERT (IWE)

Quantities calculated in SCAT are

WAHR(NX) = WEIN(NX) : normalized probabilities for inelastic scattering out of an energy group g into a group h.

The functions of the program SCAT are:

Calculation of the scattering matrices and organisation of the output for one material. This is done by the following successive steps:

1. Determination of the integration limits E_u, E_o for a given j, g, h.
2. linear interpolation of ${}^k\sigma_i^{E_j}(E')$ and F(E') at E_u, E_o
3. calculation of the integral over E_u, E_o by trapezoidal rule
4. return to 1. and next j by keeping the g and h; summation over all j excitation levels for a given g, h, and division by $\int_{(g)} F(E')\,dE'$ (calculated in AKED)
5. return to 1. and next h by keeping g; calculation of $\sum_{h=1}^{g} {}^k\sigma_{ig\to h}^{\infty}$ and normalization of the probabilities

$$ {}^kP_{i,g\to h} = \frac{{}^k\sigma_{i,g\to h}^{\infty}}{\sum_{h=1}^{g} {}^k\sigma_{i,g\to h}^{\infty}} $$

6. return to 1. and next g and so on until g becomes the energy group, where the excitation levels are partly resolved and partly unresolved. Then instead of 6. the subroutine XKON is called and 5. is calculated only for the part of group g in which the excitation levels are resolved (see section 6.1.3).

6.2.2 AKED

The subroutine AKED is called in SCAT with the following arguments AKED (E, ET, SGIP, JMAT, KMAX, LMAX, SU, QUOT, WERT, AE, EMAX, EMIN, IA, NAB, NFE, EF, FI, NE, NX, NET, NETF, NETP, SGIT, NAE, NAEF, NAEP, ISG, ISGF, ISGP, IWE, IWF, IWP).

Parameters which have to be defined before calling AKED are:

NX	:	number of boundaries of the energy groups not necessarily including the thermal energy group
NE	:	number of energy group boundaries including the thermal energy group
	=	NX + 1 in the case the energy groups defined externally do not contain a thermal energy group (o.oo1 eV - o.o25 eV); NX in the case they do contain the thermal energy group
E(NE)	:	energy group boundaries
NFE	:	= o in the case the weighting spectrum is given by a function
	=	constant equal to the number of points at which the weighting spectrum is given in this case
EF(NFE)	:	energy points of the weighting spectrum
FI(NFE)	:	values of the weighting spectrum
NET	:	dimension corresponding to the number of points of the inelastic scattering cross section on KEDAK for energies up to E (NAB + 1)
NAE	:	dimension corresponding to the number of inelastic excitation levels
ISG	:	dimension corresponding to the maximum of the number of KEDAK energy points for the different inelastic excitation levels
IWE	:	dimension corresponding to the number of KEDAK energy points in the "discrete" region (up to E (NAB + 1))

working fields in AKED are the following:

SGIT (NET), FELD (6), KFEL (6), NFEL (6), NEFT, NETP, NAEF, NAEP, ISGF, ISGP, IWP, IWF.

Parameters which are determined in AKED and are transferred to SCAT are:

ET(NET) : KEDAK energies

SGIP(NAE,ISG) : two dimensional field filled by the inelastic excitation cross sections for a level NAE

JMAT : number of inelastic excitation levels for the material considered

KMAX(NAE) : number of energy points for the inelastic excitation cross sections of the different levels.

SU(NX) : one dimensional field giving the integral of the collision density $\int_{(g)} F(E)\,dE$ about a particular energy group g

QUOT(NX) : one dimensional field giving the value of the integral $\dfrac{\int_{(g)} {}^{k}\sigma_i(E')F(E')dE'}{SU}$

WERT(IWE) : one dimensional field giving the value of the weighting function at the KEDAK energies

AE(NAE) : one dimensional field indicating the energies of the excitation levels

EMAX : upper energy limit of the "discrete" region

EMIN = ET(1) : last KEDAK energy at which ${}^{k}\sigma_i$ is still equal to zero

IA : number of the energy group in which EMIN is lying, i.e. lowest energy group out of which inelastic scattering is possible

NAB : number of the energy group in which EMAX is lying, i.e. where the excitation levels are to be considered to be partly resolved and partly unresolved.

AKED has the following functions:

1. reading of $\sigma_i(E')$ and the corresponding energy values E'
   reading of $\sigma_i^{E_j}(E')$ and the corresponding energy values E' above the treshold of the (n, n') process

2. linear interpolation of F(E') at the KEDAK energy points

3. linear interpolation of F(E') (by calling TRA) and $\sigma_i(E')$ at the energy boundaries of a given group structure

4. Integration of $\int_{(g)} F(E')\,dE'$ and $\int_{(g)} F(E')\,\sigma_i(E')\,dE'$ by using the trapezoidal rule

5. calculation of $\int_{(g)} F(E')\,\sigma_i(E')\,dE' / \int_{(g)} F(E')\,dE'$ and return to 3, and next g until the last g is reached i.e. the energy group NAB where the excitation levels are partly resolved and partly unresolved.

6.2.3 TRA

This subroutine has the following arguments:

TRA (EFI, FIS, NFE, EF, FI). The parameters which have to be defined before the subroutine call are:

NFE : = o in the case the weighting spectrum is given by a function
= constant equal to the number of points at which the weighting spectrum is given in this case.

EF(NFE) : energy points of the weighting spectrum

FI(NFE) : values of the weighting spectrum

The two other parameters are determined in TRA.

EFI : energy at which the weighting function is calculated

FIS : value of the weighting function at EFI.

The weighting spectrum is either given by a function (NFE = o) and is then available over CALL FUNCTION PHI(E) or is given pointwise.

6.2.4 The subroutine XKON

XKON (NZG, NUGR, DI, EMAX, W, A, NE, ENG, NF, E, F, XNUE, NX)

Arguments submitted by the calling program:

NZG : group number of that energy group, in which inelastic scattering occurs partially on unresolved excitation levels of the residual nucleus

NUGR : number of energy group g, from which the neutron starts before the process of inelastic scattering.

DI : normalization factor, that corresponds to c_g^k in formula (6.19).
DI is different from o. only for NUGR = NZG.

EMAX : highest energy of incident neutron, for which inelastic scattering occurs on resolved levels of the residual nucleus.

A : mass number of the residual nucleus.

ENG(NE) : one dimensional array, which contains the limits of the energy groups. (NE - 1) = number energy groups.

NF : If NF is equal to 1, the weighting function for the averaging of the nuclear temperature is submitted by a function subprogram. Otherwise NF means the number of energy points, E(NF), at which the value of the weighting function, F(NF), is submitted by input.

E(NF), F(NF) : energies and corresponding values of the weighting function, submitted by input. If NF is equal to 1, E and F are not used by XKON.

NX : dimension of the vector field for the transition probabilities for inelastic scattering.

quantities, calculated by XKON

W(NX) : double precision vector field, which by XKON is filled with Pi, g→h (see formula (6.15)) for a

group g corresponding to NUGR and all down-scattering groups h with equal or lower energy than g.

For

the numerical methods, using the function EXD(X) are applied as described above. The function EXD(X) called in XKON performs a double precision calculation of $\sum_{n=1}^{\infty} \frac{X^n}{n!} = \exp(X) - 1$. The function DNFAK(N) called in EXD(X) supplies the double precision values of N!

6.2.5 Output for one material

The program SCAT has an output on tape in the framework of the MIGROS - output and an output on listing. The output on listing has the following form:

1. line: SUBROUTINE SCAT

2. line:

2 Materialname Number of energy groups out of which inelastic scattering occurs

3. and eventually further lines

The scattering probabilities P_i, g→h in the form:

g	g + 1	g + 2	g + 3	.....
Pi, g→h	Pi, g→h + 1	Pi, g→h + 2	Pi, g→h + 3	

References

/1/ J.M. Blatt, V.F. Weisskopf, "Theoretical Nuclear Physics", J.Wiley & Sons, 1952, chapter VIII

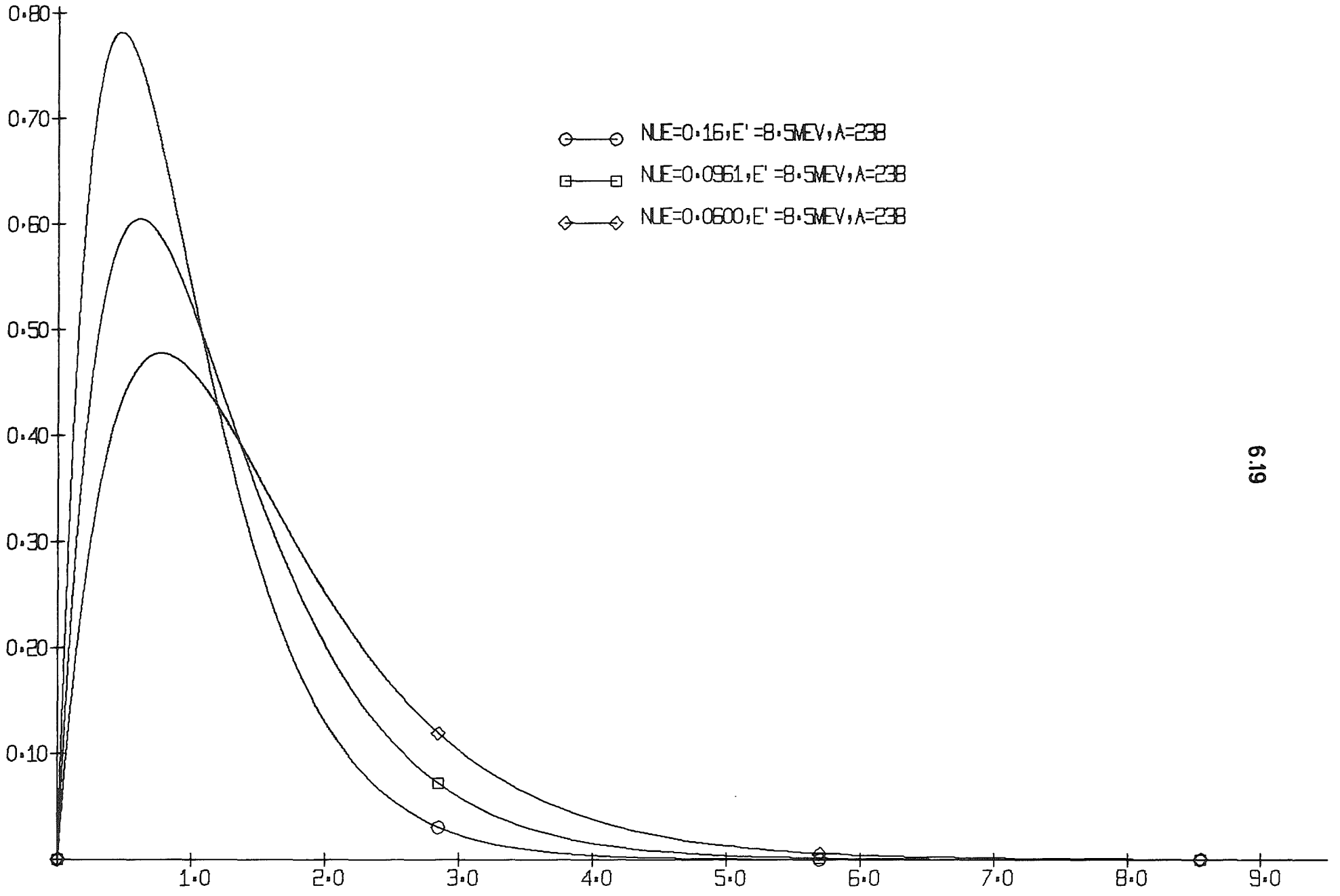
/2/ G. Szwarcbaum, M. Sieger, S. Yiftah, "Inelastic scattering of high-energy neutrons in fast reactors", Proc. of the 3. International Conference on the Peaceful Uses of Atomic Energy, Genf 1964, Volume 6, page 189

/3/ S. Yiftah, D. Okrent, P.A. Moldauer, "Fast Reactor Cross Sections", Pergamon Press, 1960

/4/ L.P. Abagjan, N.O. Bazazjanc, I.I. Bondarenko, M.N. Nikolaev, "Gruppenkonstanten schneller und intermediärer Neutronen für die Berechnung von Kernreaktoren", KFK-tr-144

/5/ H. Huschke, KFK 770 (1968)

/6/ I. Langner, J.J. Schmidt, D. Woll, KFK 750 (1968)



FIG·00001 P IN(E'→E)=N*E*EXP(-E/THETA)

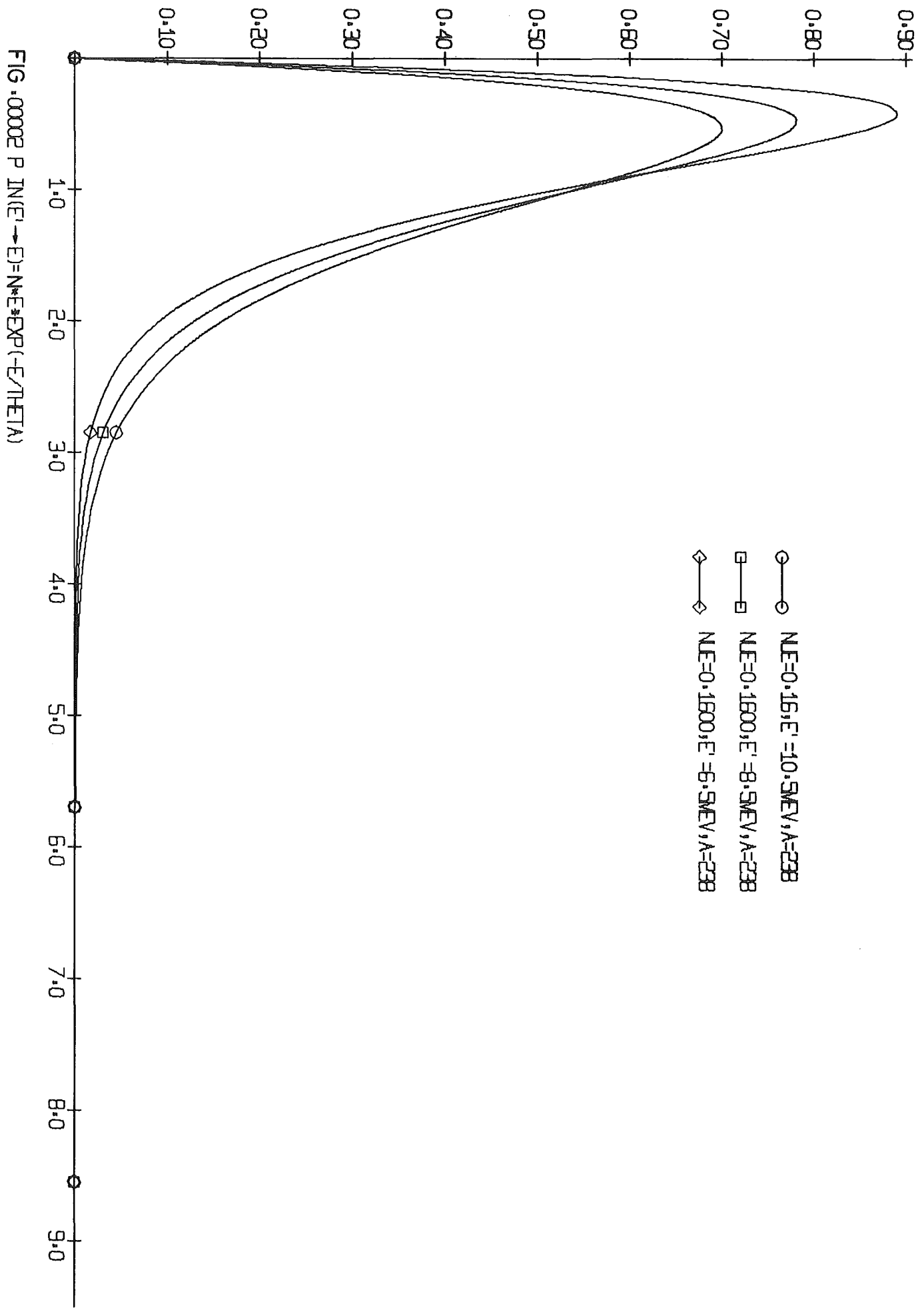


FIG .00002 P IN(E'→E)=N*E*EXP(-E/THETA)

7. Microscopic Multigroup Scattering Matrices for Elastic Neutron Scattering in a P_l-Approximation, $l \leq 5$ *. Module 6.

7.1 Definition of the quantities calculated in this module

Given 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 neutron,

$\bar{\mu}_o$ = scattering cosine in the c.m.-system, (KEDAK type SGNC),

$\bar{\mu}(E)$ = mean scattering cosine for elastic neutron scattering at energy E in the laboratory system (KEDAK type MUEL),

$\sigma_t(E)$ = total microscopic neutron reaction cross section at energy E (KEDAK type SGT),

and given a prescription for the approximation of the weighting functions $\Psi_l(E)$, $l = o, 1, .., 5$, this module calculates as final results three sets of quantities: the elastic cross section in the g-th group

$-\int_g$ means $\int_{Eg}^{Eg-1}$ with the group boundaries $E_1 > E_2 > .. > E_G$ -

$$\sigma^g = \int_g dE\, \sigma(E)\, \Phi_o(E) \Big/ \int_g dE\, \Phi_o(E) \,, \quad g = 1, 2, 3, \ldots, G \qquad (7.1)$$

---

* A detailed report (ref.1) of the code FLUMMI which is an extended version of this MIGRØS 2 module will be published as a KFK-report (in German). Further references will be found there.

the normalized matrixelements for scattering from group h into group g

$$s_\ell^{h\to g} = \frac{1}{\sigma^h}\int_h dE\,\sigma(E)\,w_\ell(E\to g)\,\Phi_\ell(E)\Big/\int_h dE\,\Phi_\ell(E) \qquad (7.2)$$

$$\ell = 0,1,2,3,4,5, \quad g,h = 1,2,\ldots,G, \quad g \geq h$$

and the mean scattering cosine in the g-th group

$$\bar{\mu}^g = \sum_{h\geq g} s_1^{g\to h}, \qquad g = 1,2,3,\ldots,G \qquad (7.3)$$

In (7.2) the quantity $w_1(E\to g)$ is defined as

$$w_\ell(E\to g) = \int_g dE'\,w_\ell(E,E'), \qquad (7.4)$$

where

$$w_\ell(E,E') = \begin{cases} \frac{d}{dE'}\int_{-1}^{\mu_o(E,E')} d\mu_o\, 2\pi\, w(E,\mu_o)\,P_\ell(\mu_o) & \text{if } E'\leq E\leq E'/\alpha \\ 0 & \text{otherwise} \end{cases} \qquad (7.5)$$

Here $\mu_o(E,E')$ is the scattering cosine for scattering from energy E to energy E' in the laboratory system:

$$\mu_o(E,E') = \frac{A+1}{2}\sqrt{\frac{E'}{E}} - \frac{A-1}{2}\sqrt{\frac{E}{E'}} \quad , \tag{7.6}$$

A = atomic weight of the scattering nucleus in neutron mass units, $P_l(\mu_o)$ is the l-th Legendre polynomial, $\alpha = \left(\frac{A-1}{A+1}\right)^2$

Further $w(E,\mu_o)$ is the angular distribution for elastic neutron scattering in the laboratory system, related to $\bar{w}(E,\bar{\mu}_o)$ through

$$w(E,\mu_o) = \bar{w}\left(E,\bar{\mu}_o(\mu_o)\right)\frac{d\bar{\mu}_o(\mu_o)}{d\mu_o} \quad , \tag{7.7}$$

where

$$\bar{\mu}_o(\mu_o) = \frac{1}{A}\left(\mu_o^2 - 1 + \mu_o\sqrt{\mu_o^2 - 1 + A^2}\right)$$

and therefore

$$\frac{d\bar{\mu}_o(\mu_o)}{d\mu_o} = \frac{1}{A}\,\frac{\left(\mu_o + \sqrt{\mu_o^2 - 1 + A^2}\right)^2}{\sqrt{\mu_o^2 - 1 + A^2}}$$

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 c.m.-system we have

$$W_l(E,E') = \begin{cases} \dfrac{d}{dE'}\,\dfrac{1}{2A}\displaystyle\int_{-1}^{\mu_o(E,E')} d\mu_o\,\frac{\left(\mu_o + \sqrt{\mu_o^2 - 1 + A^2}\right)^2}{\sqrt{\mu_o^2 - 1 + A^2}}\,P_l(\mu_o) & \text{if } E' \leq E \leq E'/\alpha \\ 0 & \text{otherwise} \end{cases}$$

hence

$$w_\ell(E \to g) = \frac{1}{2A} \int_{\hat{\mu}_0(E,E_g)}^{\hat{\mu}_0(E,E_{g-1})} d\mu_0 \, \frac{\left(\mu_0 + \sqrt{\mu_0^2 - 1 + A^2}\right)^2}{\sqrt{\mu_0^2 - 1 + A^2}} \, P_\ell(\mu_0) \qquad (7.8)$$

where

$$\hat{\mu}_0(E,E_g) = \begin{cases} -1 & \text{if } E \gg E_g/\alpha \text{ and } E_g > \hat{E} \\ +1 & \text{if } E \lesssim E_g \text{ and } E_g > \hat{E} \\ \mu_0(E,E_g) & \text{if } E_g < E < E_g/\alpha \text{ and } E_g > \hat{E} \\ -1 & \text{if } E_g = \hat{E} \end{cases} \qquad (7.9)$$

Here $\hat{E}$ is the lower limit of the considered energy region (In LECAL $\hat{E}$ = ABN (IM + 1)). With (7.4) scattering to energies below $\hat{E}$ is avoided, in particular: there is not scattering out of the lowest group.

In the case of anisotropy in the c.m.-system we have

$$w_\ell(E \to g) = 2\pi \int_{\hat{\mu}_0(E,E_g)}^{\hat{\mu}_0(E,E_{g-1})} d\mu_0 \, w(E,\mu_0) \, P_\ell(\mu_0) \qquad (7.10)$$

7.2 Integration, energy- and cosine-mesh, interpolation, and weighting

The multigroup constants to be determined according to (7.1) and (7.2) are integrals over weighting functions and cross sections given at discrete energies with a varying density of these energy points. In the energy integrals we have as weighting functions the Legendre moments $\Phi_l(E)$ of the angle- and energy-dependent flux density $\Psi(E,\mu)$, approximated by the product of a slowly varying macro-spectrum and a possibly rapidly varying micro-spectrum. In angular integrations the Legendre polynomials $P_l(\mu)$ appear as weighting functions.

The numerical technique applied for integration is a follows:

- integrals are approximated by finite sums;
  angular integration is performed with Simpson's rule since the cosine mesh can easily be spaced uniformly;
- energy integration is performed with the trapezoidal rule because of the varying density of the discrete cross section energies and the need for a fine mesh in the outgroup scattering region (defined below);
- the number of discrete points is chosen so that the program calculates cases which can be treated analytically with a maximum absolute error of $4 \cdot 10^{-4}$ in the normalized scattering matrix elements.

Interpolation of the SGN, MUEL, and SGT is linear; energy and angle interpolation of the SGNC is performed using polynomials of degree four.

The angular integrals are those in equ. (7.8) and (7.10). Since the Legendre polynomial $P_l(\mu_o)$ has l zeros in $[-1, +1]$, the integrals change sign , and there is partial cancellation.

The effect of cancellation increases with l, but this can be overcome by a cosine mesh with a number of meshpoints increasing with l.

For the computation of the integral in (7.1o) - unisotropy in the c.m.-system - the following table gives the number NST(L) of the cosine meshpoints in $[-1, +1]$ for the L-th moment:

L	o	1	2	3	4	5
NST(L)	81	81	161	161	321	321

The integration according to (7.1o) is performed by LEGANS. The integral in (7.8) is analytically given and does not depend on energy. The integrals

$$B_\ell(\omega) = \frac{1}{2} \int_{-1}^{\omega} d\mu_o \frac{d\bar{\mu}_o}{d\mu_o} P_\ell(\mu_o) \qquad (7.11)$$

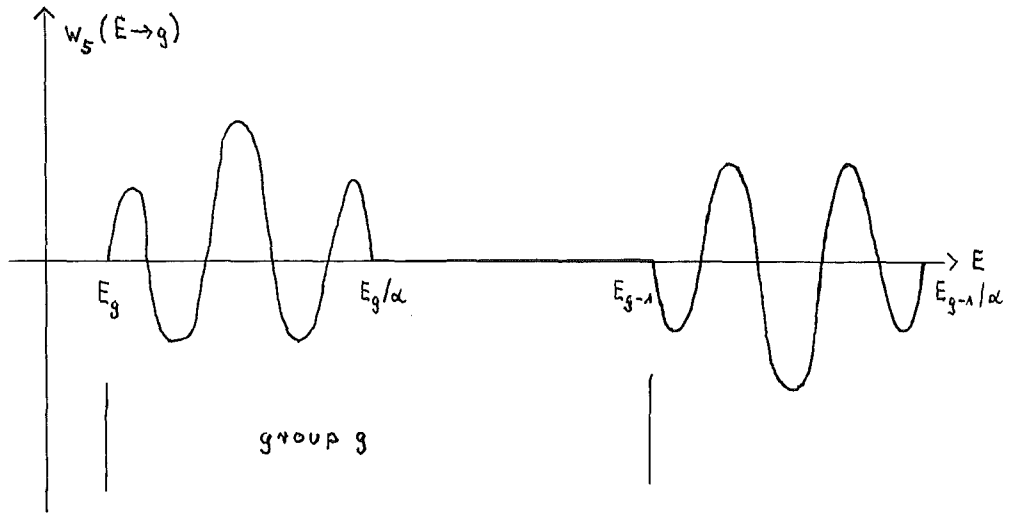
with $\bar{\mu}_o(\mu_o)$ according to (7.7) need be calculated only once for all groups in the region of isotropic scattering in the c.m.-system. So we can afford to determine $B_1(\omega)$ at NST(5) = 321 ω-points in $[-1, +1]$. The integration is done analytically, using different forms and approximations of the above integral for A = 1, $1 < A \leq 3o$, A > 9o, A = atomic weight of the scattering nucleus (see ref. 1).

The calculation of the $w_1(E \to g)$ according to (7.8) is performed by LEGIST, by interpolating in the table of the $B_1(w)$ determined by LEGINT.

The energy integral that requires the finest energy mesh is

$$\int_h dE\, \sigma(E)\, w_\ell(E \to g)\, \Phi_\ell(E) \qquad (7.12)$$

The $w_l(E \to g)$ are of a form qualitatively shown in the following figure for l = 5:



The intervall $[\, E_g,\ E_g/\alpha \,]$ from which scattering to energies $E < E_g$ is possible is called outgroup scattering region; if $E_g/\alpha < E_{g-1}$, the intervall $[\, E_g/\alpha,\ E_{g-1} \,]$, from which scattering occurs only to energies $E \geq E_g$, is called **ingroup scattering** region.

In the outgroup scattering region, $w_l(E \to g)$ may change its sign several times. To describe this behavior properly we need a sufficiently fine energy mesh (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 $\ln \frac{E_{g-1}}{E_g} = \Delta u_g \lesssim 0.7$

NK = number of discrete energies in the outgroup scattering region, uniformly spaced in lethargy
= 70,

NR = number of discrete energies in the ingroup scattering region, uniformly spaced in lethargy
= 16

is an appropriate choice; other values can be specified by input.

NR should be large enough to quarantee a sufficiently accurate pointwise representation of the makro-weighting spectrum if there are only a few discrete SGN-energies.
The whole group is an outgroup scattering region if $E_g/\alpha \geq E_{g-1}$; in this case NK discrete energies are assigned to the group.
These NK + NR discrete energies per group are called basic points; they are determined in PUNK. Together with the discrete SGNC-energies found on KEDAK they form the coarse mesh corresponding to which the $w_l(E \to g)$ are calculated in LECAL.

In GRUPIN the coarse mesh and the discrete SGN-energies are joined by means of PUSUM to form the fine mesh. Linear interpolation of the $w_l(E \to g)$ and the $\sigma(E)$ to the discrete energy points of the fine mesh yields a pointwise representation of the $\sigma_l(E \to g) = \sigma(E) \cdot w_l(E \to g)$ which contains on one hand the information available from KEDAK (without smoothing by interpolation), and on the other hand the oszillatory behavior of the $\sigma_l(E \to g)$ in the outgroup scattering region.

The weighting function $\Phi_l(E)$ is approximated by the product of a macro- and a micro-spectrum. In the following table the twelve possible forms of approximation of $\Phi_l(E)$ are listed.

Macro-spectrum	Micro-spectrum	MAZ(1)	MAZ(2)	NSPEC
$1/E$	1	o	o	o
$1/E$	$1/\Sigma_t(E)$	o	o	o
$1/E$	$1/(\Sigma_t(E))^{l+1}$	o	1	o
$1/E^{l+1}$	1	1	o	o
$1/E^{l+1}$	$1/\Sigma_t(E)$	1	o	o
$1/E^{l+1}$	$1/(\Sigma_t(E))^{l+1}$	1	1	o
$F_o(E)$	1	o	o	1
$F_o(E)$	$1/\Sigma_t(E)$	o	o	1
$F_o(E)$	$1/(\Sigma_t(E))^{l+1}$	o	1	1
$F_l(E)$	1	1	o	l+1
$F_l(E)$	$1/\Sigma_t(E)$	1	o	l+1
$F_l(E)$	$1/(\Sigma_t(E))^{l+1}$	1	1	l+1

MAZ(1), MAZ(2) and NSPEC are input parameters controlling the weighting of the higher moments. The fine-structure mixture from which Σ_t is determined, and macro-pointspectra are input quantities.

Now the integral (7.12) is determined in the following way:
Let $E_1 < E_2 < \ldots < E_{IKK}$ be the discrete energies of the fine mesh in group h, where E_1, E_{IKK} are the lower and upper boundary of group h. We put

$$f(E) = \sigma(E) \cdot w_\ell(E \to g) \cdot m(E)$$

- m(E) denotes the macro-spectrum; then (7.12) reads

$$\int_h dE\, f(E) \cdot g(E)$$

where g(E) denotes the micro-spectrum. After determination of $m(E_i)$, i = 1,2,...,IKK, by interpolation or with FUNCTIØN PHI or FUNCTIØN PHIL, we have

$$\int_h dE\, f(E)\, g(E) = \sum_{i=1}^{IKK-1} \int_{E_i}^{E_{i+1}} dE\, f(E)\, g(E)$$

$$\approx \sum_{i=1}^{IKK-1} \overline{f}_i \cdot \Delta_i^g E \qquad (7.13)$$

where $\overline{f_i} = 0.5\,(F(E_i) + f(E_{i+1}))$ and $\Delta_i^g E = \int_{E_i}^{E_{i+1}} dE\, g(E)$. The $\Delta_i^g E$ are called weighted intervall lengths (see GRUPIN, SPRAL, TRAPEZ). If fine-structure weighting is not taken into account, $\Delta_i^g E$ reduces to $\Delta E = E_{i+1} - E_i$ and (7.13) is the usual trapezoid sum. In the case of fine-structure weighting $\int dE\, g(E)$ is evaluated with the trapezoidal rule.

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 of degree 4
PUSUM	joining of point sets
MAKRØ	construction of a macro-group structure
MIXSGT, ADD	calculation of the total macroscopic cross section for fine-structure weighting
TRAFØ	transformation of angular distributions
INFØRM	printing of additional information: groups, macro-groups, distributions of SGNC and SGN, group lethargy widths, group integrals of the zeroth moment of the weighting spectrum, number of discrete SGN- and SGT-energies per macro-group, number of fine-mesh energy points per macro-group
PUNK	generation of a basic energy mesh
(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 $w_1(E \to g)$ according to (7.8) and (7.1o)
LEGPØL	calculation of pointwise Legendre polynomials
LEGINT	calculation of Legendre integrale 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 (7.1o)
GRUPIN	weighted energy integration according to (7.2)

IPØLIN	linear interpolation
SPRAL	presentation of the moment-dependent total weighting spectrum as described in chapter 7.2
PHI(FUNCTIØN)	PHI(E) = 1/E
PHIL(FUNCTIØN)	PHIL(L,E) = $1/E^L$
MUKØN	final determination of group constants according to (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. For a detailed description of the routines themselves see ref. 1.

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)

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(I), I=1, 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) $\begin{cases} > 1o^{-3} & : \text{NEGR} = \text{NE27}, \text{ABN(NEGR)}=1o^{-3} \\ = 1o^{-3} & : \text{NEGR} = \text{NX} \\ < 1o^{-3} & : \text{ERRØR 6.8} \end{cases}$

NGR = NEGR-1

Now we have for further use in this module

NGR = number of energy groups

NEGR = number of group boundaries

(ABN(I),I=1,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 = o always)

NLE = last Legendre moment to be calculated (input or standard)

NSPEK = macro-weighting spectrum control parameter (NSPEK = 1: spectrum from FUNCTIØN PHIL; we have KSPE = KSPEK = o in GRUPIN; NSPEK > 1: NSPEK = number of discrete energies of the macro-weighting spectrum; we have KSPE = 1 and KSPEK = NSPEK in GRUPIN)

LSPEK = number of values of the macro-weighting spectrum if NSPEK > 1, LSPEK = 1 otherwise

(ESP(I),I=1,NSPEK) = discrete energies of the macro-weighting spectrum if NSPEC > 1, no meaning otherwise (input)

(SPEK(I),I=1,LSPEK) = values of the macro-weighting spectrum (the first NSPEK values for the o. 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) = o) (input)

NTK = micro-weighting spectrum pointer (NTK = 1: the fine-structure mixture from which the micro-weighting spectrum is to be calculated is given in the arrays MAT and DAT; NTK = o: no fine-structure weighting)

KT = number of different nuclei in the fine-structure mixture (input)

(MAT(I),I=1,KT) = nuclei in KEDAK notation in the fine-structure mixture (input)

(DAT(I),I=1,KT) = densities in particles per ccm times $1o^{-24}$ of the nuclei in the fine-structure mixture (input)

NTTT = estimated number of discrete energies of the micro-spectrum

(MAZ(I),I=1,2) = control parameters concerning the weighting of the higher moments (input)

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 out-group 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(NX), SGNC(ICØS, ISM), FEKØ(ISM, NECU), ELSIG(6, NECU, NX), ELTØT(2, NX), ET(NTTT), ST(NTTT)

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(I),I=1,M) = summands

Results: $S = \sum_{I=1}^{M} A(I)$

SUBRØUTINE IPØLA (M, A, B, N, X, Y, T)

Purpose: Continuous and diffentiable interpolation with polynomials of degree four (for details see ref. 1)

Arguments: M = number of given points
(A(I),I=1,M) = given abszissae
(B(I),I=1,M) = given ordinates
N = number of the given new abszissae
(X(I),I=1,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(I),I=1,N) = new ordinates corresponding with the given new abszissae

SUBRØUTINE PUSUM (KA, A, KE, E, B)

Purpose: Joining of point sets

Arguments: KA = number of elements in the array A
(A(I),I=1,KA) = first point set (increasing)
KE = number of elements in the array E
(E(I),I=1,KE) = second point set (increasing)

Auxiliary array: B(KE)

Results: KE = number of different points in A and E
(E(I),I=1,KE) = different points in A and the given E (increasing)

SUBRØUTINE MAKRØ (ALFA, ISØ, IL, IM, NGR, ABN, ISD, ISM, ISDP, NS, NK, NECU, NUEB, V, W, LST, INTT, INT, NEGR, ISEL)

CØMMØN STØFF, ISTRUK, ISPA, NØUT

Purpose: A macro-group is defined as an energy region consisting of one group or several groups adjoining in pairs. 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
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 out-group scattering region per group

NGR = number of energy groups
NEGR = number of energy group boundaries
(ABN(I),I=1,NEGR) = energy group boundaries
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
STØFF = nucleus in KEDAK notation for which scattering matrices etc. shall be calculated
NØUT = printed-output unit
ISEL = pointer for additional output

Auxilary arrays: V(ISD), W(ISD), LST(2, NGR)

Results: INTT = number of macro-group boundaries
(INT(I),I=1,INTT) = macro-group boundaries given by group indices
ISDP = increment of ISD if ISD is found to be too small during execution
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)

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(I),I=1,KT) = nuclei in the mixture

(DAT(I),I=1,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 $\lceil$ EA, EE $\rfloor$.

NØUT = printed-output unit

Results:

NT = number of discrete energies of the mixture in the intervall $\lceil$ EA, EE $\rfloor$

(ET(I),I=1,NT) = discrete energies in $\lceil$ EA, EE $\rfloor$

(ST(I),I=1,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

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(I),I=1,NT) = hitherto determined discrete energies

(ST(I),I=1,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 polynomial 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(I),I=1,NT) = discrete energies up to E

(ST(I),I=1,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

$$P(E|ET,ST) = P(E|ET(1), ET(2),\ldots,ET(NT); ST(1), ST(2),\ldots,ST(NT))$$

$$= \begin{cases} 0 & \text{if } E < ET(1) \text{ or } E > ET(NT) \\ ST(J) & \text{if } E = ET(J) \\ ST(J-1) + \dfrac{ST(J) - ST(J-1)}{ET(J) - ET(J-1)} (E-ET(J-1)) & \\ & \text{if } ET(J-1) < E < ET(J) \end{cases}$$

provided ET(1) < ET(2) < ... < 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(I,J),I=1,IC),J=1,NE) = angular distributions in the c.m.-system
- (A(I),I=1,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(I),I=1,IC) = cosine meshpoints in the laboratory system
- ((S(I,J),I=1,IC),J=1,NE) = angular distributions in the laboratory system

SUBRØUTINE INFØRM (ALFA, NEGR, ABN, R, RSP, IL, IM, INTT, INT, NST, NSTIS, IR, ISTT, K, NTK, NTT, NØUT)

Purpose: Printing of additional information if ISEL < o

Arguments:
ALFA, NEGR, ABN, IL, IM, INTT, INT, NØUT see MAKRØ
(R(I),I=1,NEGR-1) = group lethargy widths
(RSP(I),I=1,NEGR-1) = group integrals over the total weighting spectrum of zeroth order
(NST(I),I=1,6), 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 ≠ o

SUBRØUTINE PUNK (NGR, NEGR, ABN, NA, NE, NEN, ALFA, NK, NR, ISM, ISMP, ISN, E)

Purpose: Generation of a basic energy mesh uniformly spaced in lethargy

Arguments:
NGR = number of energy groups
NEGR = number of energy group boundaries
(ABN(I),I=1,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 = $\left(\frac{A-1}{A+1}\right)^2$, A = atomic weight of the scattering nucleus in neutron mass units

NK = number of basic points in outgroup scattering region

NR = maximum number of basic points in ingroup scattering region

ISM = maximum number of basic points plus discrete SGNC-energies per macro-group

Results:

ISN = calculated number of basic points in the macro-group defined through NA, NE

(E(I),I=1,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 LØØK1 (ISD, K, E, SGN, EØ, EE, NT)

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(I),I=1,K) = discrete energies at which data a given
- (SGN(I),I=1,K) = data read from KEDAK (SGN, MUEL or SGT)

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(I),I=1,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 = 1 if ICØS is too small
= o otherwise
(AR(I),I=1,ICØS) = SGNC cosine meshpoints from KEDAK
((SGNC(I,J),I=1,ICØS),J=1,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 NDFNXT of the KEDAK routine NDF.

SUBRØUTINE LØØK3 (NE, EA, ISØ, NGR, ABN, ISM, ISMP, LST, NEGR, ISEL)

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(I),I=1,NE) = SGNC-energy mesh on KEDAK for the considered nucleus
(LST(I),I=1,NGR) where LST(I) = number of energies EA(N) with ABN(I+1)

$\leq$ EA(N) < ABN(I)

ISØ see 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 $w_1(E \to g)$ according to equations (7.8) and (7.1o)

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 = o otherwise)

(LEG(I),I=1,6) = sequence of calculated moments

NLE = upper Legendre index (input)

NANF, MEND = 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(I),I=1,NEGR) = energy group boundaries

ICØS = number of cosine meshpoints of the SGNC on KEDAK

(AR(I),I=1,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(I),I=1,ISN) = basic points plus discrete SGNC-energies in the macro-group to be calculated (coarse mesh)

((SGNC(I,J),I=1,ICØS),J=1,ISN) = angular distributions in the laboratory system

(NST(I),I=1,6) = 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 = o

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 = o: Legendre integrals are calculated,
ITA = 1: Legendre integrals have already been calculated)

NF = unit on which the $w_l(E \to g)$ 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: $w_l(E \to g)$ 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 = o (here: maximum length of A)

Results:
- (A(I),I=1,NST) = uniformly spaced cosine meshpoints
- (X(I),I=1,NST) = uniformly spaced cosine meshpoints
- (F(L,I),I=1,NST),L=1,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 = o, 1, 2, 3, 4, 5
- NAK = number of cosine meshpoints
- XMAT = atomic weight in neutron mass units

Results: (H(I),I=1,NAK) = uniformly spaced cosine mesh-points, H(1) = -1, H(NAK) = 1

D = spacing of the H(I)

(GRAL(L,I),L=1,6),I=1,NAK) where GRAL(L,I) $= 2 \cdot B_{L-1}(H(I))$

ITA = pointer (ITA = 1 after calculation)

Remarks: For A = 1, 1 < A ≤ 3o, A > 3o the above integral is treated numerically in different ways. For details see ref. 1.

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 mesh-points

(X(I),I=1,NST) = cosine mesh from LEGINT

D = spacing of the X(I)

((GRAL(L,I),L=1,6),I=1,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(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. (7.1o)-multiplication with 2π is performed in LECAL:

$$E(I) = \int_{GR(I+1)}^{GR(I)} d\mu_0 \, w(E,\mu_0) \, P_{L-1}(\mu_0)$$

Arguments:

L, NST, D, NEGR, IA, IB, GR see LEGIST

(X(I),I=1,NST) = cosine mesh from LEGPØL

(F(I),I=1,NST) = pointwise angular distribution corresponding with the X(I)

((PØL(L,I),L=1,6),I=1,NST) = Legendre polynomials pointwise from LEGPØL corresponding with the X(I)

Auxiliary arrays: PØLY(NST), A(NST)

Results: (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)

Purpose: Weighted energy integration according to (7.2)

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

NGR = number of energy groups

(EH(I),I=1,ISN) = basic points plus discrete SGNC-energies in the macro-group to be calculated

K = number of SGN

(H(I),I=1,K) = discrete SGN-energies

(F(I),I=1,K) = SGN corresponding with the H(I)

M = number of MUEL

(G(I),I=1,M) = discrete MUEL-energies

(EN(I),I=1,M) = MUEL corresponding with the G(I)

NTT = micro-weighting spectrum control parameter (NTT = 1: no micro-weighting; NTT > 1: micro-weighting with NTT = number of energy points of the micro-weighting spectrum)

(ET(I),ST(I),I=1,NTT) = micro-weighting spectrum if NTT > 1

(MAZ(I),I=1,2) = control parameters for the weighting of higher moments (input)

KSPE = pointer for macro-weighting (KSPE = o: weighting with FUNCTIØN PHI if MAZ(1) = o, with FUNCTIØN PHI and FUNCTIØN PHIL if MAZ(1) = 1; KSPE = 1: weighting with point-spectrum in ESP and SPEK according to MAZ(1)

KSPEK = number of discrete energies of the macro-weighting spectrum if KSPE = 1, = o otherwise

NSPEK = Max (1, KSPEK)

LSPEK = number of values of the macro-weighting spectrum if KSPE = 1 = 1 otherwise

(ESP(I),I=1,KSPEK) = macro-spectrum discrete energies if KSPE = 1; no meaning otherwise

(SPEK(I),I=1,LSPEK) = macro-spectrum values if KSPE = 1; no meaning otherwise

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-mesh consisting of the basic points (from PUNK), the discrete SGNC-energies, the discrete SGN- and MUEL-energies

(RSP(I),I=1,NGR) = energy group integrals of
the zeroth order weighting spectrum
(ELSIG(L,I,NN),NN=IL,IM),I=1,NUEB),L=1,NLE+1)
where with II = NN + I-1

$$ELSIG(L,I,NN) = \sigma_{L-1}^{NN \to II}$$

$$= \frac{\int_{NN} dE\, \sigma(E)\, w_{L-1}(E \to II)\, \Phi_{L-1}(E)}{\int_{NN} dE\, \Phi_{L-1}(E)}$$

SUBRØUTINE IPØLIN (M, A, B, N, X, Y, HR)

Purpose: Linear interpolation

Arguments:
M = number of given points
(A(I),B(I),I=1,M) = given points
N = number of given new abszissae
(X(I),I=1,N) = given new abszissae
where X(1) = A(1), X(N) = A(M)

Auxiliary array: HR(M)

Results: (Y(I),I=1,N) = new ordinates corresponding
with the X(I)

SUBRØUTINE TRAPEZ (M, E, F, G, W, H, L)

Purpose: Trapezoidal integration according to

$$W = \frac{1}{2} \sum_{I=2}^{M} (F(I)+F(I-1))\cdot E(I-1) \quad \text{if } L = o$$

$$W = \frac{1}{2} \sum_{I=2}^{M} (F(I)\cdot G(I)+F(I-1)\cdot G(I-1))\cdot E(I-1) \quad \text{if } L = 1$$

(see chapter 7.2)

Arguments: M = number of meshpoints
(E(I),I=1,M-1) = weighted intervall lengths
(F(I),I=1,M) = function to be integrated
(G(I),I=1,M) = weighting function
L = pointer for weighting (L = o: constant weighting function; L =1: weighting function not constant in G)

Auxiliary array: H(M)

Results: W(see above)

FUNCTIØN PHI(E) = 1/E
FUNCTIØN PHIL(L,E) = $1/E^L$

SUBRØUTINE MUKØN (ELSIG, ELTØT, NLE, NECU, NUEB, IL, IM, NGR)

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):

$$\sigma^{NN} = \sum_{II \geq NN} \sigma_o^{NN\to II},$$

$$S_L^{NN\to II} = \sigma_L^{NN\to II}/\sigma^{NN}, \quad L = o,1,\ldots,NLE,$$

$$\bar{\mu}^{NN} = \sum_{II \geq NN} S_1^{NN\to II}$$

Arguments: NLE = Legendre degree up to which scattering matrices are calculated
NUEB = scattering width
IL, IM = first and last calculated energy group
(((ELSIG(L,I,NN),NN=IL,IM),I=1,NUEB),L=1,NLE+1) where (see GRUPIN) ELSIG(L,I,NN) = $\sigma_{L-1}^{NN\to NN+I-1}$
NGR = number of energy groups (for dimensioning)
NECU = maximum scattering width (for dimensioning)

Results: (((ELSIG(L,I,NN),NN=IL,IM),I=1,NUEB),L=1,NLE+1)

where

ELSIG(L,I,NN) = $S_{L-1}^{NN\to NN+I-1}$ (see above)

((ELTØT(I,NN),NN=IL,IM),I=1,2) where

ELTØT(1,NN) = σ^{NN}

ELTØT(2,NN) = $\bar{\mu}^{NN}$ (see above)

Remark: Comparisons with cases which can be treated analytically (see ref. 1: FLUMMI tests) show 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.

SUBRØUTINE PRINT (ELSIG, ELTØT, NLA, NLE, NECU, NUEB, ISEL, NGR, KSPEK, MAZ, NTK, KIM)

CØMMØN STØFF, ISTRUK, ISPA, NØUT, KPR, NEND, NANF

Purpose: Printing and reserving of final results

Arguments:

ELSIG, ELTØT see MUKØN results

NLE, NECU, NUEB, NGR see MUKØN

NLA = first Legendre moment to be calculated (NLA = o 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

MAZ, NTK, KIM see FLUMMI

KSPEK corresponds to KSPE in GRUPIN

ISEL = pointer for additional output

NØUT = printed-output unit

KPR = unit on which all MIGRØS-results are stored

References

/1/ H.W.Wiese: FLUMMI - Ein FØRTRAN-IV-Programm zur Berechnung von Multigruppenkonstanten aus KEDAK-Daten für höhere Transportnäherungen der Neutronentransportgleichung
(to be published as a KFK-report (in German))

8. Calculation of the fine interval elastic scattering transfer matrices up to P_5 approximation and other quantities required for the REMO-correction. Module 9.

8.1 Basic formulae and notations

a) The fine interval system

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 lethargy. The fine interval width is denoted by ΔE_ℓ.

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 matrices are defined by

$$\langle {}^{\ell}P(E\to h) \rangle = \frac{\int_{\Delta E} dE\, \sigma_e(E)\, \pi_\ell(E\to h)\, F(E)}{\sum_h \int_{\Delta E} dE\, \sigma_e(E)\, \pi_o(E\to h)\, F(E)} \tag{8.3}$$

where

$$\pi_l(E \to h) = \frac{(A+1)^2}{4A} \cdot \frac{1}{E} \cdot \int_{\max(\alpha E,\, E_{h+1})}^{E_h} dE'\, \varphi(\mu_c)\, P_l(t) \qquad (8.4)$$

where $P_l(t)$ 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 labor system,

$$t = \frac{A+1}{2}\sqrt{\frac{E'}{E}} - \frac{A-1}{2}\sqrt{\frac{E}{E'}} .$$

$\varphi(\mu_c)$ = the angular distribution of the elastic scattering in the center of mass system. It should be normalized i.e.

$$\frac{1}{2}\int_{-1}^{+1} d\mu_c\, \varphi(\mu_c) = 1$$

($\varphi(\mu_c) \equiv 1$, for isotropic case)

It is practical to transform the integral (8.4) into

$$\pi_l(E \to h) = \frac{1}{2}\int_{\mu_{h+1}}^{\mu_h} d\mu_c\, \varphi(\mu_c)\, P_l(t(\mu_c)), \qquad (8.5)$$

where

$$t(\mu_c)=0.5\sqrt{1-(1-\mu_c)\frac{2A}{(A+1)^2}}\left\{A+1-\frac{A-1}{1-(1-\mu_c)\frac{2A}{(A+1)^2}}\right\} \quad (8.6)$$

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 unambigous 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 $1 \geq \mu > \mu_1$ 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 with the mesh points given by the nuclear data file KEDAK. At the end of the integration interval the cross-sections are interpolated.

For the integral (8.3) and (8.5) the Romberg integration method (see app.III) is used. The alternating sign of the Legendre poly-

nomial P_1 and the "ill-behaviour" of the $f(\mu_c)$ at some energy values require special consideration which are described in app. IV.

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-section 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 the inconsistency between the average cosine calculated from the angular distribution and the average cosine available on KEDAK.

There are two types of the above inconsistency:

a) The angular distribution of the scattered neutrons for the energy range in question are not given, but the retrieved average cosine $\overline{\mu_{ret}}$ is different from 2/3A. In this case a linear anisotropy is assumed i.e. the following center of mass angular distribution is used

$$f(\mu_c) = 1 + \left(\overline{\mu_{ret}} - \frac{2}{3A}\right) \cdot \frac{3}{1 - \frac{3}{5A^2}} \cdot \mu_c \qquad (8.7)$$

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.

$$W_s(\mu) = \sum_{l=0}^{\infty} \frac{2l+1}{2} \cdot b_{s,l} \cdot P_l(\mu), \quad b_{s,0} = 1, \; b_{s,1} = \bar{\mu}_{ang} \tag{8.8}$$

$\bar{\mu}_{ang}$ 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.

$$\overline{W_s}(\mu) = W_s(\mu) + \frac{3}{2}\left(\bar{\mu}_{ret} - \bar{\mu}_{ang}\right) P_1(\mu) \tag{8.8'}$$

and the correction to a transfer matrix element is

$$\Delta \pi_l(E \to h) = \frac{3}{2}\left(\bar{\mu}_{ret} - \bar{\mu}_{ang}\right) \int_{\mu_{h+1}}^{\mu_h} d\mu \, P_l(\mu) P_1(\mu) \tag{8.9}$$

where (μ_h, μ_{h+1}) is the angle interval in the labor atory system belonging to the scattering from E into the group H.

8.4 Strategy of the extrapolation

It is often the case that for a cross-section or angular distribution the energy interval given in the KEDAK file does not cover the energy range of the group system. In this case an extrapolation is necessary. As the difference between the last energy point and the end of the group energy range is generally not too large, additional energy point coinciding with the end of the group

is taken, with the cross-section value (or angular distribution) equal with the next one. (i.e. the extrapolation is horizontal)

8.5 The description of the program REMO and of the related subroutines

The subroutine REMO is called by the statement

```
CALL REMO (NG, ENG, NSP, F, E, ERR, NLA, NLE, NGRE, NFG, NFI, NJM, NUJM,
          ISEL, IWORK, WORK, L)
```

NG	The number of energy boundaries
ENG(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 formula to be obtained from (8.3), when $\sigma_s(E) = 1$, will be computed.
IWORK(I),WORK(I),I=1,L	Work-field
L	The length of the work-field.

In the subroutine system related to REMO the dynamical programming method is used, i.e. any dimensioned variable, the dimension of which depends on the task option is dimensioned with variable length. All of such variables are placed in the work field (WORK and IWORK) respectively) to be passed by the main control program. This field is generally transfered from one subroutine to the other and it contains a great deal of information to be passed. The first 34 words of WORK contain mainly the control information. (see Table VIII)

The function of the main subroutine REMO is the following:
To settle the control information contained in the Table VIII, and to determine the length of WORK.
To call the subroutine KEDLEC (see below) in order to retrieve the angular distributions in the energy region to be calculated.
REMO calls the subroutine

REMP (ENG, NFG, NFI, F, E, WORK, IWORK, IS) +

IS is the lowest energy group for which angular distributions are given.

The function of REMP: to organize the calculation by group.
It calls the following subroutines: KEDDAT, SINT, ISOFAL, ZWIN, NORM

The subroutine underlying the retrieval of KEDAK data has four entries.

α) KEDDAT (NAMIZ, NAMTYP, NW, NW1, FNW, NDAT, FA, FF, EP, EM, *, *, *)

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=L,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.

If the material and the type are not found then follow RETURN1 and RETURN2 respectively.

+ If the parameters of the subroutines are not described by the same symbols as in the program lists, symbols described before or in the input description are used.

b) DATNUM (NAMIZ, NAMTYP, NDAT, NW, EP, EM, *, *, *)

This entry is used when only NDAT is to be determined

c) 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 number of 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)

d) 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.

SUBROUTINE SINT (ENG(I), NFG(I), NFI(I), F, E, WORK, N, M)

SINT calculates the group averaged total and elastic scattering cross sections and average cosine in the group I.
M = IWORK(7)
For N = IWORK(5) SINT calculates $\langle\sigma_t\rangle$
For N = -IWORK(5) SINT calculates $\langle\sigma_s\rangle$ and $\langle\mu_s\rangle$
Called by REMP.

SUBROUTINE NORM (J2, J1, SGNC, WORK)

NORM normalizes the angular distribution from the J2-th up to the J1-th one.
Called by REMP.

SUBROUTINE ISOFAL (ENG(I), NFG(I), NFI(I), F, E, WORK)

ISOFAL divides the group I into fine intervals and organises the calculation of elastic transfer probabilities for the group I.
Called by REMP.

SUBROUTINE WAHRS (EP, EM, IMAX, WORK(N), ENG(I), NM1, NUJM, F, E, TE, WORK, PER)

N = IWORK (22)

NM1 = NLE+1

EP, EM are the higher and the lower boundary of the energy interval to be calculated [eV].

WAHRS divides the interval [EP, EM] further according to the principles given in 8.2.

Called by ISOFAL

SUBROUTINE LMI (EP, EM, E_1, E2, SG1, SG2, AMU1, AMU2, IMAX1, ENG(I), TE, NM1, NUJ, NUJM, F, E, WORK, PER (IMAX+2), IMAX,PL)

SG1, SG2, AMU1, AMU2, E1, E2 elastic scattering cross sections, retrieved average cosine and the related energy points [eV]

IMAX1 The maximum group change by a scattering in the interval [EP, EM]

Called by WAHRS.

FUNCTION ANINT (BU, BL, K, SG, XL, AZ, ICOS, WORK, T, NJM)

ANINT calculates the integral (8.5) and the correspondence of notations is the following

K = n

BU = μ_k

BL = μ_{k+1}

XL → μ_c

SG → $\int(\mu_c)$

ICOS number of mesh points

AZ = $(\overline{\mu}_{ret} - \frac{2}{3A})$

Called by NORM, LMI.

SUBROUTINE AMESH(BU, BL, Z, L2, NX, K)

AMESH prepares the division of angle interval [BU, BL] according to the roots of Legendre polynomial of order K.(see appendix IV)

Z L2,...Z NX-1 The roots of the K-th Legendre polynomials in the interval BU, BL

Called by ANINT.

SUBROUTINE HIDR (BU, BL, K, A, *)

In the case of hydrogen the integral (8.5) can analytically be calculated.
This is done by HIDR.
A = result of the calculation
Called by ANINT.

FUNCTION WINK (XL, SG, KJ, ICOS, AZ, XA)

WINK determines $\mathcal{G}'(\mu)\sigma_s$ by means of linear interpolation from the point-wise angular distribution /XA → μ/
Called by ANINT.

FUNCTION FXINT (EP, EM, SGN, ES, F, E, NSP, NDAT)

FXINT calculates the integral $\int_{EM}^{EP} dE\ \sigma(F)\ F(E)$ by means of trapezoidal rule.

SGN(I) cross-section
ES(I) energy mesh-points [eV]
Called by SINT.

FUNCTION BCM (EI, EO, WORK)

BCM gives the cosine of scattering angle in the center of mass system.
EI the energy of neutrons before scattering.
EO the energy of neutron after scattering.
Called by LMI.

FUNCTION ICSOP (E, ENG)

ICSOP gives the group number for energy E.
Called by REMO, LMI, FXINT, MASSIN.

FUNCTION (ANG, XA, A, XM)

ANG gives the cosine of scattering angle in labor system.
XA cosine of scattering angle in center of mass system.
A atomic mass.
XM= $(A+1)^2/2A$.
Called by ANINT.

FUNCTION PTL (N, X)

PTL gives the value $P_N(X)$
Called by ANINT.

SUBROUTINE ZWIN (K, EP, EM, ES, J2, J1)

ES(I),I=1,k energy mesh-points in [eV].
ZWIN gives the values J2, J1. These have the meaning: ES(J2),..
ES(J1) cover the energy interval EP, EM.
Called by REMP, LMI, FXINT, WAHRS.

SUBROUTINE MASSIN (WORK, ENG)

MASSIN calculates the mass dependent quantities and places them in the corresponding words of WORK /see Table 1./
Called by REMO.

SUBROUTINE INTEN (E, SG, SGNC, EA, ICOS)

INTEN interpolates the angular distribution in energy.
E is the energy for which the angular distribution is to be interpolated.
Called by LMI.

SUBROUTINE SMORN (PI, N, M1, IMAX, WORK)

SMORN normalizes the calculated elastic transfer matrixes in order to get the transfer probabilities (8.3.)
PI(NM1, IMAX) the elastic transfer matrix.
Called by ISOFAL.

SUBROUTINE SEARCH (NFG, NFI, WORK, IWORK, I)

SEARCH organizes the output of $\langle\sigma_t\rangle$, $\langle\sigma_s\rangle$, $\langle\mu_s\rangle$ for the group.
Called by REMO.

SUBROUTINE SUCHM (NFG, NFI, IWORK, WORK, MOM, I, ENG)

SUCHM organizes the output of $\langle\sigma\ (E_i \rightarrow h)\rangle$ for the group I.
Called by REMO

FUNCTION IWO (N, IWORK)

IWO gives the value IWORK(N).

SUBROUTINE IWIN (L, N, IWORK)

IWIN performs the statement IWORK(L) = N.
In the future program is intended to generalize to the inelastic case. The subroutines INRE, IMPE, EGRENZ serve for this purpose. For elastic scattering calculation these have no any influence.

SUBROUTINE AKOR (BU, BL, L, A)

It calculates the integral in (8.9) for average cosine correction. BU and BL are the c. of mass scattering angles corresponding to μ_2 and μ_1 respectively. L is the order of the moment, A is the mass of the scatterer.
Called by LMI.

Table VIII

Control information in the array WØRK

Word	Content	Comment
1	Adress of EA/1/	Energy mesh points for angular distribution
2	Adress of XL/1/	Angle mesh points
3	Adress of SGNC/1/	Angular distributions
4	I	The number of just calculated group
5	Adress of SGN/1/	Elastic scattering or total cross-section
6	Adress of AMU/1/	Retrieved average cosine
7	Adress of ES/1/	Energy mesh points for cross-sections
8	ISEL	
9	Adress of SG/1/	Work-field
1o	Adress of TE/1/	Work-field
11	Adress of PER/1/	Work-field
12	Adress of SP/1/	Field for the storage of results
13	Adress of BUF/1/	Buffer-field for output
14	NG	
15	NSP	
16	NLA	
17	NLE	
18	IMAX	Maximum group change+1
19	NJM	
2o	NUJM	
21	ICOS	Number of angle mesh points /now it is 21/
22	Address of the first free word of SP	
23	KJ	Control number of the anisotropy
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 integration procedure
28	A	
29	$((A+1)/(A-1))^2$	

Table VIII (cont.)

Word	Content	Comment
3o	$(A+1)^2/2A$	
31	$\log ((\frac{A+1}{A-1})^2)$	
32	Q = -o.1	
33	Address of T/1/	8-bytes work-field
34	Adrress of PL/1/	8-bytes work-field

9. The calculation of average group cross sections for infinite dilution and of energy resonance self shielding factors from energy point wise data in the resonance region. Module 3.

9.1 The flux weighted energy resonance self shielding factors are calculated for capture, fission, elastic scattering

$$ {}^{k}f_{x,g}(\sigma_o) = \frac{{}^{k}\tilde{\sigma}_{x,g}(\sigma_o)}{{}^{k}\tilde{\sigma}_{x,g}(\sigma_o \to \infty)} \qquad (9.1) $$

k = isotope
x = neutron reaction (n,x)
(n,e)= elastic scattering, (n,f)=fission,
(n,c)= total absorption - fission.
g = energy group
σ_o = back ground cross section in barns.

$$ {}^{k}\tilde{\sigma}_{x,g}(\sigma_o) = \frac{\left\langle \frac{{}^{k}\sigma_x(E)\cdot F(E)}{{}^{k}\sigma_t(E)+\sigma_o} \right\rangle}{\left\langle \frac{F(E)}{{}^{k}\sigma_t(E)+\sigma_o} \right\rangle}^{*} \qquad (9.2) $$

is the microscopic effective cross section.
F(E) collision density
$\sigma_t(E)$ is the microscopic total cross section.
Besides that, a flux weighted self shielding factor of the following type is calculated:

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

$$ {}_{1,0}f_{e,g}(\sigma_0) = \frac{\left\{ {}^{k}\sigma_e \cdot {}^{k}\bar{\mu}_e \right\}_g (\sigma_0)}{\left\{ {}^{k}\sigma_e \cdot {}^{k}\bar{\mu}_e \right\}_g (\sigma_0 \to \infty)} \tag{9.3} $$

with

$$ \left\{ {}^{k}\sigma_e \cdot {}^{k}\bar{\mu}_e \right\}_g (\sigma_0) = \frac{\left\langle \frac{{}^{k}\sigma_e(E) \cdot {}^{k}\bar{\mu}_e(E) \cdot F(E)}{{}^{k}\sigma_t(E) + \sigma_0} \right\rangle}{\left\langle \frac{F(E)}{{}^{k}\sigma_t(E) + \sigma_0} \right\rangle} \tag{9.4} $$

$\bar{\mu}_e(E)$ = average cosine for elastic scattering

The current weighted resonance self shielding factors are calculated for elastic scattering and for the total neutron cross section.

$$ {}^{k}_{1}f_{t,g}(\sigma_0) = \frac{{}^{k}_{1}\sigma_{t,g}(\sigma_0)}{{}^{k}_{1}\sigma_{t,g}(\sigma_0 \to \infty)} \tag{9.5} $$

$$ {}^{k}_{1}f_{e,g}(\sigma_0) = \frac{{}_{1}\left\{ {}^{k}\sigma_e \cdot {}^{k}\bar{\mu}_e \right\}_g (\sigma_0)}{{}_{1}\left\{ {}^{k}\sigma_e \cdot {}^{k}\bar{\mu}_e \right\}_g (\sigma_0 \to \infty)} \tag{9.6} $$

with

$$ {}^{k}_{1}\tilde{\sigma}_{t,g}(\sigma_o) = \frac{\left\langle \frac{{}^{k}\tilde{\sigma}_t(E)\cdot F(E)}{\{{}^{k}\tilde{\sigma}_t(E)+\sigma_o\}^2} \right\rangle}{\left\langle \frac{F(E)}{\{{}^{k}\tilde{\sigma}_t(E)+\sigma_o\}^2} \right\rangle} \qquad (9.7) $$

$$ \left\{ {}^{k}_{1}\tilde{\sigma}_e \cdot {}^{k}\bar{\mu}_e \right\}_g (\sigma_o) = \frac{\left\langle \frac{{}^{k}\tilde{\sigma}_e(E)\,{}^{k}\bar{\mu}_e(E)\,F(E)}{\{{}^{k}\tilde{\sigma}_t(E)+\sigma_o\}^2} \right\rangle}{\left\langle \frac{F(E)}{\{{}^{k}\tilde{\sigma}_t(E)+\sigma_o\}^2} \right\rangle} \quad , \qquad (9.8) $$

The average group cross sections for infinite dilution are defined:

$$ {}^{k}\tilde{\sigma}^{\infty}_{x,g} = \lim_{\sigma_o\to\infty} {}^{k}\tilde{\sigma}_{x,g}(\sigma_o) = \lim_{\sigma_o\to\infty} {}^{k}_{1}\tilde{\sigma}_{x,g}(\sigma_o) \qquad (9.9) $$

or

$$ {}^{k}\tilde{\sigma}^{\infty}_{x,g} = \frac{\langle {}^{k}\tilde{\sigma}_x(E)\cdot F(E)\rangle}{\langle F(E)\rangle} \qquad (9.10) $$

for capture, fission, elastic scattering and the total neutron reaction, and

$$\left\{ {}^{k}\tilde{\sigma}_e \, {}^{k}\bar{\mu}_e \right\}_g^{\infty} = \frac{\left\langle {}^{k}\tilde{\sigma}_e(E) \cdot {}^{k}\bar{\mu}_e(E) \cdot F(E) \right\rangle}{\left\langle F(E) \right\rangle} \qquad (9.11)$$

F(E) is a slowly varying weighting-function, normaly a collision density.

9.2 The microscopic cross sections are taken from energy point wise data on the KEDAK-library. The integrations are done by a trapezoidal rule. As integration points the energy points of the KEDAK-tables for $\sigma_t(E)$ and the group boundaries are used. In the averages (9.8) and (9.11) the energy points of the tables for $\sigma_e(E)$ and $\bar{\mu}_e(E)$ are used. If they are tabulated at different energies, they are linearly interpolated.
The weighting function is either interpolated from tables or calculated by a function.

9.3 The calculations are performed in the subroutine

FSTRUK (MI, SIGO, NE, ENG, NFE, REFE, EFE, XINTE, ZA, XN, SE, XII,
ZB, XI, MDIM, MDIMP, EMU, XMU, NER, NERP, SN, EN)

The following parameters must be defined:

MI	: number of σ_o-values.
SIGO	: one-dimensional field containing the σ_o-values [barn].
NE	: number of group boundaries.
ENG	: one-dimensional field containing the group boundaries [eV].
NFE	: number of energy points of the weighting spectrum.
REFE	: one-dimensional field containing the energy points of the weighting spectrum [eV].

EFE : one-dimensional field containing the weighting function at the energy points of field REFE.

MDIM : length of working fields, should be larger than the number of $\bar{\mu}_e$-values on KEDAK within one energy group.

NER : length of working fields, should be larger than the maximum number of values for σ_a, σ_e, σ_f on KEDAK within one energy group.

Working fields:

XINTE (NE,4), ZA (MI, NE, 5), XN (NI, NE, 4), SE (MI, NE, 6), XII (NE), ZB (MI, NE), XI (NE), EMU (MDIM), XMU (MDIM), SN (NER, 3), EN (NER, 3).

The following parameters are calculated in the subroutine:

MDIMP : o, if MDIM is large enough .
n, number, by which MDIM should be increased.

NERP : o, if NER is large enough .
n, number, by which NER should be increased.

1o. The calculation of group constants in the thermal group. Module 1o.

1o.1 There 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, and for the weighting function a Maxwell - distribution is assumed. So the thermal group cross sections are defined as

$$ {}^{k}\bar{\sigma}_{x,th} = \frac{\sqrt{\pi}}{2} \cdot {}^{k}\sigma_{x}\,(0{,}0253\ eV) \qquad (1o.1.) $$

k = isotope
x = neutron reaction (n,x) except (n,n) process
th = thermal

The thermal group cross sections are calculated by formula (1o.1.) for all types x of neutron reactions. Furthermore the following group constants are calculated :

- the average elastic scattering cross section

$$ {}^{k}\bar{\sigma}_{n,th} = {}^{k}\sigma_{n}\,(0{,}0253\ eV) \qquad (1o.2.) $$

- the average cosine of the elastic scattering

$$ {}^{k}\bar{\mu}_{e,th} = {}^{k}\mu_{e}\,(0{,}0253\ eV) \qquad (1o.3.) $$

- the average number of secondary neutrons per fission

$$ {}^{k}\bar{\nu}_{th} = {}^{k}\nu\,(0{,}0253\ eV) \qquad (1o.4.) $$

- the average α - value

$$ {}^{k}\bar{\alpha}_{th} = \frac{{}^{k}\sigma_{\gamma,th}}{{}^{k}\sigma_{f,th}} \qquad (1o.5.) $$

γ = radiative capture
f = fission

- the average η - value

$$\overline{{}^{k}\eta_{th}} = \frac{{}^{k}\nu_{th}}{1 + {}^{k}\alpha_{th}} \qquad (1o.6.)$$

1o.2. The following subroutine is necessary :

THERM (NE, NTY, TYP)

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.

11. The calculation of the average 1/v values. Module8 .

11.1 The average 1/v values are defined as

$$\left(\frac{1}{v}\right)_g = \frac{\int_{(g)} \frac{1}{v} \cdot F(E)\, dE}{\int_{(g)} F(E) dE} \qquad (11.1)$$

11.2 The numerical integration is performed by the following formula:

$$\left(\frac{1}{v}\right)_g = C \cdot \frac{\sum_{i=1}^{n} \left\{ \frac{F_i}{\sqrt{E_i}} + \frac{F_{i+1}}{\sqrt{E_{i+1}}} \right\} \cdot \left\{ E_{i+1} - E_i \right\}}{\sum_{i=1}^{n} \left\{ F_i + F_{i+1} \right\} \cdot \left\{ E_{i+1} - E_i \right\}} \qquad (11.2)$$

i : index for the integration points
E_i : energy in [eV]
F_i : weighting function
n : number of integration points in group g.
c : constant = $7{,}229286 \cdot 10^{-7}$

If the weighting function is given pointwise, as integration points the energy points of the weighting function are used. Therefore the user must take care of the number of energy points.
If the weighting function is given in an analytic form, ten integration points per groups, equidistant in energy, are used.

In the thermal group the 1/v value at o,o253 is taken.

11.3 The following subroutine is used:

EDV (MM,A, NEF, XS, G, E, V, Y, NES, ES, F)

The following parameters must be defined:

MM : number of group boundaries
A(MM) : group boundaries in [eV].
NEF : number of energy points of the weighting function.
XS(NEF): energy points of the weighting function in [eV]
G(NEF) : weighting function at the energy points XS (NEF)
NES : max (1o x number of groups boundaries, number of energy points of the weighting function)

E (MM), V(MM), Y(MM), ES(NES), F(NES)
one-dimensional working fields.

12. The calculation of the fission spectrum. Module 7.

12.1 For the calculation of fission spectra the Watt formula is used.

$$\chi(E) = \frac{\exp\left\{-\frac{E_f}{T}\right\}}{\sqrt{\pi \cdot E_f \cdot T}} \cdot \exp\left\{-\frac{E}{T}\right\} \cdot \sinh\left\{\frac{2}{T}\sqrt{E \cdot E_f}\right\} \qquad (12.1)$$

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

$$\chi_g = \frac{1}{2\sqrt{\pi}} \sqrt{\frac{T}{E_f}} \left\{ \exp(-x_{g+1}^2) - \exp(-x_g^2) - \exp(-y_{g+1}^2) + \exp(-y_g^2) \right\} - \frac{1}{2} \left\{ \operatorname{erf}(x_{g+1}) - \operatorname{erf}(x_g) + \operatorname{erf}(y_{g+1}) - \operatorname{erf}(y_g) \right\} \qquad (12.3)$$

$$x_g = \sqrt{\frac{E_g}{T}} - \sqrt{\frac{E_f}{T}} \; ; \quad x_{g+1} = \sqrt{\frac{E_{g+1}}{T}} - \sqrt{\frac{E_f}{T}}$$

$$y_g = \sqrt{\frac{E_g}{T}} + \sqrt{\frac{E_f}{T}} \; ; \quad y_{g+1} = \sqrt{\frac{E_{g+1}}{T}} + \sqrt{\frac{E_f}{T}}$$

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$

12.2 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[e V].

The following parameter is defined by the subroutine SPALT.

X(NE) one-dimensional field containing the fission spectrum.

Appendix I

A modified version of the formalism of Froelich /1/, /2/, for the calculation of energy resonance self shielding factors in the range of "statistical resonances".*

To take into account overlapping of resonances of the same series, Froelich makes the following assumption /2/, (formula 2.41a):

$$ {}^{s}\tilde{\sigma}_{p,eff} + {}^{s}_{r}\tilde{\sigma}_{oc} \cdot {}^{s}_{r}\psi \gg \sum_{r' \neq r} {}^{s}_{r'}\tilde{\sigma}_{oc} \cdot {}^{s}_{r'}\psi \qquad (1) $$

This condition is not fulfilled in the case of strong overlapping, if the resonances are higher than the background cross section ${}^{s}\sigma_{p.eff}$. Therefore a weaker condition will be used, namely

$$ {}^{s}\tilde{\sigma}_{p,eff} + \langle {}^{s}\tilde{\sigma}_{c} \rangle + {}^{s}_{r}\tilde{\sigma}_{oc} \cdot {}^{s}_{r}\psi \gg \left| \sum_{r' \neq r} {}^{s}_{r'}\tilde{\sigma}_{oc} \cdot {}^{s}_{r'}\psi - \langle {}^{s}\tilde{\sigma}_{c} \rangle \right| \qquad (2) $$

Expression 2.40 in /2/ can be modified to

$$ \sum_{r} \left\langle \frac{{}^{s}_{r}\tilde{\sigma}_{ox} \cdot {}^{s}_{r}\psi}{\left[{}^{s}\tilde{\sigma}_{p,eff} + {}^{s}\tilde{\sigma}_{c} + {}^{s}_{r}\tilde{\sigma}_{oc} \cdot {}^{s}_{r}\psi \right] \left[1 - \frac{\sum_{r' \neq r} {}^{s}_{r'}\tilde{\sigma}_{oc} \cdot {}^{s}_{r'}\psi - {}^{s}\tilde{\sigma}_{c}}{{}^{s}\tilde{\sigma}_{p,eff} + {}^{s}\tilde{\sigma}_{c} + {}^{s}_{r}\tilde{\sigma}_{oc} \cdot {}^{s}_{r}\psi} \right]} \right\rangle \qquad (3) $$

Using condition (2), expanding the second term of the denominator of (3) and neglecting quadratic terms in

$$ \sum_{r' \neq r} {}^{s}_{r'}\tilde{\sigma}_{oc} \cdot {}^{s}_{r'}\psi - \langle {}^{s}\tilde{\sigma}_{c} \rangle $$

, one gets

* in this appendix the same symbols as in /2/ are used.

the following expression:

$$\sum_r \frac{{}^s_r\tilde{\sigma}_{ox}}{{}^s_r\tilde{\sigma}_{oc}} \left\langle \frac{{}^s_r\psi}{\frac{\langle\tilde{\sigma}_t\rangle}{{}^s_r\tilde{\sigma}_{oc}} + {}^s_r\psi} \right\rangle + \langle {}^s\tilde{\sigma}_c \rangle \sum_r \frac{{}^s_r\tilde{\sigma}_{ox}}{\left\{{}^s_r\tilde{\sigma}_{oc}\right\}^2} \left\langle \frac{{}^s_r\psi}{\left\{\frac{{}^s\tilde{\sigma}_c}{{}^s_r\tilde{\sigma}_{oc}} + {}^s_r\psi\right\}^2} \right\rangle$$

$$- \sum_r \sum_{r' \neq r} \frac{{}^s_r\tilde{\sigma}_{ox} \cdot {}^s_{r'}\tilde{\sigma}_{oc}}{\left\{{}^s_r\tilde{\sigma}_{oc}\right\}^2} \left\langle \frac{{}^s_{r'}\psi \cdot {}^s_{r'}\psi}{\left\{\frac{\langle\tilde{\sigma}_t\rangle}{{}^s_r\tilde{\sigma}_{oc}} + {}^s_r\psi\right\}^2} \right\rangle \qquad (4)$$

with

$$\langle\tilde{\sigma}_t\rangle = \tilde{\sigma}_{p,eff} + \langle {}^s\tilde{\sigma}_c \rangle$$

The first and the third term of (4) are the same as in expression (2.42) in /2/, when ${}^s\sigma_{p.eff}$ is replaced by $\langle\sigma_t\rangle$.

To calculate the overlapping effect, the assumption is made:

$$\langle\sigma_t\rangle \gg {}^s_r\sigma_{oc} \cdot {}^s_r\psi \qquad (5)$$

This condition corresponds to the condition (2.50) and (2.51) in /2/.

With this condition, for the third term of (4) one gets the identically same result as for the second term of (2.42) in /2/.

$$\sum_r \sum_{r' \neq r} \frac{{}^s_r\tilde{\sigma}_{ox} \cdot {}^s_{r'}\tilde{\sigma}_{oc}}{\left\{{}^s_r\tilde{\sigma}_{oc}\right\}^2} \left\langle \frac{{}^s_r\psi \cdot {}^s_{r'}\psi}{\left\{\frac{\langle\tilde{\sigma}_t\rangle}{{}^s_r\tilde{\sigma}_{oc}} + {}^s_r\psi\right\}^2} \right\rangle \simeq \frac{{}^s\overline{D} \cdot \langle {}^s\tilde{\sigma}_x \rangle \cdot \langle {}^s\tilde{\sigma}_c \rangle}{\Delta\sqrt{2\pi}\,\langle\tilde{\sigma}_t\rangle^2} \cdot \varepsilon \qquad (6)$$

From condition (5), the following approximation for the denominator of the second term of (4) can be deduced:

$$\left\{\frac{\langle\tilde{\sigma}_t\rangle}{{}^s_r\tilde{\sigma}_{oc}} + {}^s_r\psi\right\}^2 \cong \frac{\langle\tilde{\sigma}_t\rangle}{\{{}^s_r\tilde{\sigma}_{oc}\}^2} \cdot \left\{\langle\tilde{\sigma}_t\rangle + {}^s_r\tilde{\sigma}_{oc} \cdot {}^s_r\psi\right\} \tag{7}$$

Then for the second term of (4) one gets

$$\frac{\langle{}^s\tilde{\sigma}_c\rangle}{\langle\tilde{\sigma}_t\rangle} \cdot \sum_r \frac{{}^s_r\tilde{\sigma}_{ox}}{{}^s_r\tilde{\sigma}_{oc}} \left\langle \frac{{}^s_r\psi}{\frac{\langle\tilde{\sigma}_t\rangle}{{}^s_r\tilde{\sigma}_{oc}} + {}^s_r\psi} \right\rangle \tag{8}$$

Now the first and the second term of (4) can be combined to

$$\left\{1 + \frac{\langle{}^s\tilde{\sigma}_c\rangle}{\langle\tilde{\sigma}_t\rangle}\right\} \sum_r \frac{{}^s_r\tilde{\sigma}_{ox}}{{}^s_r\tilde{\sigma}_{oc}} \left\langle \frac{{}^s_r\psi}{\frac{\langle\tilde{\sigma}_t\rangle}{{}^s_r\tilde{\sigma}_{oc}} + {}^s_r\psi} \right\rangle \tag{9}$$

and for this, one gets in the same manner as for the first term of (2.42) in /4/ the following expression.

$$\left\{1 + \frac{\langle{}^s\tilde{\sigma}_c\rangle}{\langle\tilde{\sigma}_t\rangle}\right\} \frac{\overline{{}^s\Gamma_x \cdot J({}^s\beta, {}^s\theta)}}{\overline{{}^sD} \cdot \cos 2\delta_l} \tag{10}$$

where now ${}^s\beta$ is given by

$${}^s\beta = \frac{\langle\tilde{\sigma}_t\rangle}{{}^s\tilde{\sigma}_{oc}} \tag{11}$$

So for the effective microscopic cross section one gets the modified result

$$ {}^s\sigma_{x,g}(E) = {}^s\sigma_{p,eff} \frac{\left[1+\frac{\langle {}^s\sigma_c\rangle}{\langle \sigma_t\rangle}\right]\overline{{}^s\Gamma_x \cdot J({}^s\beta, {}^s\theta)} - \overline{{}^sD}\cdot\langle {}^s\sigma_x\rangle\cdot\langle {}^s\sigma_c\rangle \cdot \varepsilon}{\overline{{}^sD}\cdot\cos 2\delta_l \qquad \Delta\sqrt{2\pi}\cdot\langle\sigma_t\rangle^2} \qquad (12) $$

$$ 1-\left[1+\frac{\langle {}^s\sigma_c\rangle}{\langle \sigma_t\rangle}\right]\frac{\overline{{}^s\Gamma\cdot J({}^s\beta, {}^s\theta)}}{\overline{{}^sD}} + \frac{\overline{{}^sD}\cdot\langle {}^s\sigma_c\rangle^2}{\Delta\sqrt{2\pi}\,\langle\sigma_t\rangle^2}\cdot\varepsilon $$

for capture and fission, and

$$ {}^s\sigma_{c,g}(E) = {}^s\sigma_{p,eff} \frac{\left[1+\frac{\langle {}^s\sigma_c\rangle}{\langle \sigma_t\rangle}\right]\frac{\overline{{}^s\Gamma\cdot J({}^s\beta, {}^s\theta)}}{\overline{{}^sD}} - \frac{\overline{{}^sD}\cdot\langle {}^s\sigma_c\rangle^2}{\Delta\cdot\sqrt{2\pi}\,\langle\sigma_t\rangle^2}\cdot\varepsilon}{1-\left[1+\frac{\langle {}^s\sigma_c\rangle}{\langle \sigma_t\rangle}\right]\frac{{}^s\Gamma\cdot J({}^s\beta, {}^s\theta)}{\overline{{}^sD}} + \frac{\overline{{}^sD}\cdot\langle {}^s\sigma_c\rangle^2}{\Delta\cdot\sqrt{2\pi}\cdot\langle\sigma_t\rangle^2}\cdot\varepsilon} \qquad (13) $$

for the total resonance cross section.

All symbols have the same meaning as in /2/, formula (2.68), except

$$ {}^s\beta = \frac{\langle\sigma_t\rangle}{{}^s\sigma_{oc}} \quad \text{instead of} \quad \frac{{}^s\sigma_{p,eff}}{{}^s\sigma_{oc}} . $$

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 770, p. 2-7, (1968)

Appendix II

An approximate calculation of current weighted resonance self shielding factors from statistical resonance parameters.

1. Introduction

For the calculation of resonance self shielding factors from statistical resonance parameters a formalism /3/, first developed by R. Froelich in his paper on Doppler theory /2/, was used in the first version of MIGROS, which did not allow the calculation of current weighted self shielding factors. An approximation is proposed, which allows to use the modified formalism for flux weighted self shielding factors of Froelich, given in Appendix I, also for current weighted self shielding factors.

The flux weighted f-factor for the neutrons reaction (n,x) in the energy group g for a resonance isotope may be written as

$$f_{x,g} = \frac{\sum_j \phi_j \cdot \sigma_{x,g}(E_j) \cdot \Delta E_j}{\sum_j \phi_j \cdot \sigma^{\infty}_{x,g}(E_j) \cdot \Delta E_j} \qquad (1)$$

The ΔE_j are energy intervals in the group g, ϕ_j is a weighting function, constant over ΔE_j.

$$\sigma_{x,g}(E) = \frac{\left\langle \frac{\sigma_x(E)}{\sigma_t(E)+\sigma_0} \right\rangle}{\left\langle \frac{1}{\sigma_t(E)+\sigma_0} \right\rangle} \qquad (2)$$

1)

is the effective cross section in the energy interval ΔE around E for the neutron reaction (n,x) for the resonance isotope.

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

$\tilde{\sigma}_x(E)$ microscopic cross section of the resonance isotope for the neutron reaction (n,x)

$\tilde{\sigma}_t(E)$ microscopic total cross section of the resonance isotope.

σ_o total back ground cross section per resonance atom.

$$\tilde{\sigma}^{\infty}_{x,g}(E) = \left\langle \tilde{\sigma}_x(E) \right\rangle \tag{3}$$

is the average cross section in ΔE around E. The relation

$$\tilde{\sigma}^{\infty}_{x,g}(E) = \lim_{\sigma_o \to \infty} \tilde{\sigma}_{x,g}(E) \tag{4}$$

means that for infinite dilution of the resonance isotope the effective cross section is the same as the average cross section. The interval ΔE is assumed to be so large that many resonances are in it. There is no problem in calculating the average cross section from statistical resonance parameters | 2 |, | 3 |, | 4 |. However, it is not so easy to calculate the effective cross section because of the overlapping of the resonances. The effective cross section is composed of the contributions of the single resonances series s

$$\begin{aligned} \tilde{\sigma}_{x,g}(E) &= \sum_s {}^s\tilde{\sigma}_{x,g}(E) && \text{for capture and fission} \\ \tilde{\sigma}_{t,g}(E) &= \sum_s {}^s\tilde{\sigma}_{c,g}(E) + \sigma_p && \text{for the total cross section} \end{aligned} \tag{5}$$

${}^s\tilde{\sigma}_{c,g}(E)$ is the total resonance cross section of series s (c = compound, not capture)

$$ {}^s\tilde{\sigma}_{x,g}(E) = \frac{\left\langle \dfrac{{}^s\tilde{\sigma}_x(E)}{{}^s\tilde{\sigma}_c(E) + \sum_{s' \neq s} {}^{s'}\tilde{\sigma}_c(E) + \sigma_p + \sigma_o} \right\rangle}{\left\langle \dfrac{1}{{}^s\tilde{\sigma}_c(E) + \sum_{s' \neq s} {}^{s'}\tilde{\sigma}_c(E) + \sigma_p + \sigma_o} \right\rangle} \tag{6}$$

${}^s\tilde{\sigma}_c(E)$ is the resonance part of the total cross section of series s.

$\tilde{\sigma}_p$ potential cross section

R. Froelich showed that under the assumption that

$$\frac{\sum_{s' \neq s} \left[{}^{s'}\tilde{\sigma}_c(E) - \langle {}^{s'}\tilde{\sigma}_c(E) \rangle \right]}{\tilde{\sigma}_p + \tilde{\sigma}_o + {}^s\tilde{\sigma}_c(E) + \sum_{s' \neq s}^{s'} \tilde{\sigma}_c(E)} \ll 1 \qquad (7)$$

at the resonances of series s, the effective cross section of series s can be approximated by

$${}^s\tilde{\sigma}_{x,g}(E) = \frac{\left\langle \frac{{}^s\tilde{\sigma}_x(E)}{{}^s\tilde{\sigma}_c(E) + \sum_{s' \neq s} \langle {}^{s'}\tilde{\sigma}_c(E) \rangle + \tilde{\sigma}_p + \tilde{\sigma}_o} \right\rangle}{\left\langle \frac{1}{{}^s\tilde{\sigma}_c(E) + \sum_{s' \neq s} \langle {}^{s'}\tilde{\sigma}_c(E) \rangle + \tilde{\sigma}_p + \tilde{\sigma}_o} \right\rangle} . \qquad (8)$$

This approximation is correct up to quadratic terms of expression (7).

Introducing

$${}^s\tilde{\sigma}_{p,\mathrm{eff}} = \tilde{\sigma}_o + \tilde{\sigma}_p + \sum_{s' \neq s} \langle {}^{s'}\tilde{\sigma}_c(E) \rangle \qquad (9)$$

one gets

$${}^s\tilde{\sigma}_{x,g}(E) = \frac{\left\langle \frac{{}^s\tilde{\sigma}_x(E)}{{}^s\tilde{\sigma}_c(E) + {}^s\tilde{\sigma}_{p,\mathrm{eff}}} \right\rangle}{\left\langle \frac{1}{{}^s\tilde{\sigma}_c(E) + {}^s\tilde{\sigma}_{p,\mathrm{eff}}} \right\rangle} . \qquad (10)$$

or in a slightly different form

$$ {}^s\tilde{\sigma}_{x,g}(E) = {}^s\tilde{\sigma}_{p,eff} \cdot \frac{\left\langle \dfrac{{}^s\tilde{\sigma}_x(E)}{{}^s\tilde{\sigma}_c(E) + {}^s\tilde{\sigma}_{p,eff}} \right\rangle}{1 - \left\langle \dfrac{{}^s\tilde{\sigma}_c(E)}{{}^s\tilde{\sigma}_c(E) + {}^s\tilde{\sigma}_{p,eff}} \right\rangle} \qquad (11) $$

This microscopic cross section of the series s is composed of the contributions of all resonances r of this series in the interval ΔE (if ΔE contains enough resonances, contributions from outside may be neglected).

$$ {}^s\tilde{\sigma}_{x,g}(E) = {}^s\tilde{\sigma}_{p,eff} \cdot \frac{\sum_r \left\langle \dfrac{{}^s\tilde{\sigma}_x^r(E)}{{}^s\tilde{\sigma}_c^r(E) + \sum_{r' \neq r} {}^s\tilde{\sigma}_c^{r'}(E) + {}^s\tilde{\sigma}_{p,eff}} \right\rangle}{1 - \sum_r \left\langle \dfrac{{}^s\tilde{\sigma}_c^r(E)}{{}^s\tilde{\sigma}_c^r(E) + \sum_{r' \neq r} {}^s\tilde{\sigma}_c^{r'}(E) + {}^s\tilde{\sigma}_{p,eff}} \right\rangle} \qquad (12) $$

Replacing the sum of all resonances by the statistical average times the average number of resonances in the interval ΔE, the modified formalism of Froelich, given in appendix I, approximates expression (11) by

$$ {}^s\tilde{\sigma}_{x,g}(E) = {}^s\tilde{\sigma}_{p,eff} \frac{\left[1 + \dfrac{\langle {}^s\tilde{\sigma}_c \rangle}{\langle \tilde{\sigma}_t \rangle}\right] \dfrac{\overline{{}^s\Gamma_x \cdot J({}^s\beta, {}^s\theta)}}{\overline{{}^sD \cdot \cos 2\delta_l}} - \dfrac{\overline{{}^sD} \cdot \langle {}^s\tilde{\sigma}_x \rangle \cdot \langle {}^s\tilde{\sigma}_c \rangle}{\Delta \sqrt{2\pi} \cdot \langle \tilde{\sigma}_t \rangle^2} \cdot \varepsilon}{1 - \left[1 + \dfrac{\langle {}^s\tilde{\sigma}_c \rangle}{\langle \tilde{\sigma}_t \rangle}\right] \dfrac{\overline{{}^s\Gamma \cdot J({}^s\beta, {}^s\theta)}}{\overline{{}^sD}} + \dfrac{\overline{{}^sD} \cdot \langle {}^s\tilde{\sigma}_c \rangle^2}{\Delta \sqrt{2\pi} \cdot \langle \tilde{\sigma}_t \rangle^2} \cdot \varepsilon} \qquad (13) $$

for x = fission, capture

$$ {}^{s}\tilde{\sigma}_{c,g}(E) = {}^{s}\tilde{\sigma}_{p,eff} \frac{\left[1+\frac{\langle {}^{s}\tilde{\sigma}_c\rangle}{\langle \tilde{\sigma}_t\rangle}\right]\frac{\overline{{}^{s}\Gamma\cdot J({}^{s}\beta,{}^{s}\theta)}}{\overline{{}^{s}D}} - \frac{{}^{s}D\cdot\langle {}^{s}\tilde{\sigma}_c\rangle^2}{\Delta\sqrt{2\pi}\,\langle \tilde{\sigma}_t\rangle^2}\cdot\varepsilon}{1-\left[1+\frac{\langle {}^{s}\tilde{\sigma}_c\rangle}{\langle \tilde{\sigma}_t\rangle}\right]\frac{\overline{{}^{s}\Gamma\cdot J({}^{s}\beta,{}^{s}\theta)}}{\overline{{}^{s}D}} + \frac{{}^{s}D\cdot\langle {}^{s}\tilde{\sigma}_c\rangle^2}{\Delta\sqrt{2\pi}\cdot\langle \tilde{\sigma}_t\rangle^2}\cdot\varepsilon} \qquad (14) $$

for the total resonance cross section.

Γ_x width for the neutron reaction (n,X)

Γ total width

$J(\beta,\theta)$ J-function |5|

$\theta = \frac{\Gamma}{\Delta}$

Δ Doppler width |5|

δ_l scattering phase shift

$\beta = \frac{\langle \tilde{\sigma}_t\rangle}{\tilde{\sigma}_{oc}}$

$\tilde{\sigma}_{oc}$ total resonance cross section in the peak of the resonance

$\overline{D}$ average level distance

$$ \overline{f(\Gamma_n,\Gamma_f)} \equiv \iint f(\Gamma_n,\Gamma_f)\cdot F_n(\Gamma_n)\cdot F_f(\Gamma_f)\,d\Gamma_n\,d\Gamma_f $$

$F_n(\Gamma_n)$ distribution of neutron width

$F_f(\Gamma_f)$ distribution of fission width

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

$\Omega(D)$ distribution for level distance.

$$\langle {}^s\sigma_x \rangle = \frac{2\pi}{{}^sD} \cdot \lambda^2 \cdot g \cdot \overline{\left[\frac{{}^s\Gamma_n \cdot {}^s\Gamma_x}{{}^s\Gamma}\right]}$$

$$\langle {}^s\sigma_c \rangle = \frac{2\pi}{{}^sD} \cdot \lambda^2 \cdot g \cdot \overline{{}^s\Gamma_n} \cdot \cos 2\delta_l$$

$$\langle \sigma_t \rangle = {}^s\sigma_{p,eff} + \langle {}^s\sigma_c \rangle$$

λ neutron wave length

g statistical parameter

The second term in the numerator and the third term in the denominator in (13), (14) are correction terms for overlapping of the resonances. They vanish for separated resonances.

The approximation of R. Froelich for the expression (12) is only valid, if the condition

$$ {}^s\sigma_{p,eff} + \langle {}^s\sigma_c \rangle + {}^s\sigma_c^r(E) \rangle \rangle \left| \sum_{r' \neq r} {}^s\sigma_c^{r'} - \langle {}^s\sigma_c \rangle \right| \qquad (15)$$

is fulfilled in the range of the resonance r.

2. The extension of the formalism of Froelich to current weighted resonance self shielding factors.

The current weighted total f-factor may be written as

$$ {}_1f_{t,g} = \frac{\sum_j \phi_j \cdot {}_1\tilde{\sigma}_{t,g}(E_j) \cdot \Delta E_j}{\sum_j \phi_j \cdot \tilde{\sigma}^{\infty}_{t,g}(E_j) \cdot \Delta E_j} \qquad (16) $$

$$ {}_1\tilde{\sigma}_{t,g}(E) = \frac{\left\langle \frac{\sigma_t(E)}{\{\sigma_t(E)+\sigma_o\}^2} \right\rangle}{\left\langle \frac{1}{\{\sigma_t(E)+\sigma_o\}^2} \right\rangle} \qquad (17) $$

is the effective current weighted cross section in the energy interval ΔE around E for the total neutron reaction of the resonance isotope.

The effective total cross section may be composed of several resonance series s

$$ {}_1\tilde{\sigma}_{t,g}(E) = \sum_s {}^s{}_1\tilde{\sigma}_{c,g}(E) + \sigma_p \qquad (18) $$

width

$$ {}^{s}_{1}\tilde{\sigma}_{c,g}(E) = \frac{\left\langle \dfrac{{}^{s}\tilde{\sigma}_c(E)}{\left\{ {}^{s}\tilde{\sigma}_c(E) + \sum_{s' \neq s} {}^{s'}\tilde{\sigma}_c(E) + \tilde{\sigma}_p + \tilde{\sigma}_o \right\}^2} \right\rangle}{\left\langle \dfrac{1}{\left\{ {}^{s}\tilde{\sigma}_c(E) + \sum_{s' \neq s} {}^{s'}\tilde{\sigma}_c(E) + \tilde{\sigma}_p + \tilde{\sigma}_o \right\}^2} \right\rangle} \qquad (19) $$

The numerator of (19) can also be written as

$$ \left\langle \frac{{}^{s}\tilde{\sigma}_c(E)}{\left\{ {}^{s}\tilde{\sigma}_c(E) + \sum_{s' \neq s} \left\langle {}^{s'}\tilde{\sigma}_c(E) \right\rangle + \tilde{\sigma}_p + \tilde{\sigma}_o \right\}^2 \cdot \left\{ 1 + \dfrac{\sum_{s' \neq s} \left[{}^{s'}\tilde{\sigma}_c(E) - \left\langle {}^{s'}\tilde{\sigma}_c(E) \right\rangle \right]}{\tilde{\sigma}_p + \tilde{\sigma}_o + {}^{s}\tilde{\sigma}_c(E) + \sum_{s' \neq s} \left\langle {}^{s'}\tilde{\sigma}_c(E) \right\rangle} \right\}^2} \right\rangle $$

Neglecting quadratic terms of

$$ \sum_{s' \neq s} \left\{ {}^{s'}\tilde{\sigma}_c(E) - \left\langle {}^{s'}\tilde{\sigma}_c(E) \right\rangle \right\} $$

in the second bracket, using condition (7) and expression (9), one gets

$$ \left\langle \frac{{}^{s}\tilde{\sigma}_c(E)}{\left\{ {}^{s}\tilde{\sigma}_c(E) + {}^{s}\tilde{\sigma}_{p,\,eff} \right\}^2} \right\rangle - 2 \cdot \left\langle \frac{{}^{s}\tilde{\sigma}_c(E) \cdot \sum_{s' \neq s} \left\{ {}^{s'}\tilde{\sigma}_c(E) - \left\langle {}^{s'}\tilde{\sigma}_c(E) \right\rangle \right\}}{\left\{ {}^{s}\tilde{\sigma}_c(E) + {}^{s}\tilde{\sigma}_{p,\,eff} \right\}^3} \right\rangle $$

Because the resonances, which belong to different series, are not correlated, the second term may be written as

$$ 2 \cdot \left\langle \frac{{}^{s}\tilde{\sigma}_c(E)}{\left\{ {}^{s}\tilde{\sigma}_c(E) + {}^{s}\tilde{\sigma}_{p,\,eff} \right\}^3} \right\rangle \cdot \left\langle \frac{\sum_{s' \neq s} \left\{ {}^{s'}\tilde{\sigma}_c(E) - \left\langle {}^{s'}\tilde{\sigma}_c(E) \right\rangle \right\}}{\left\{ {}^{s}\tilde{\sigma}_c(E) + {}^{s}\tilde{\sigma}_{p,\,eff} \right\}^3} \right\rangle $$

The second term is identically zero.

The same can be done for the denominator of (19), so that one gets

$$ {}^{s}_{1}\tilde{\sigma}_{c,g}(E) = \frac{\left\langle \dfrac{{}^{s}\tilde{\sigma}_{c}(E)}{\left\{ {}^{s}\tilde{\sigma}_{c}(E) + {}^{s}\tilde{\sigma}_{p,eff} \right\}^{2}} \right\rangle}{\left\langle \dfrac{1}{\left\{ {}^{s}\tilde{\sigma}_{c}(E) + {}^{s}\tilde{\sigma}_{p,eff} \right\}^{2}} \right\rangle} \qquad (20) $$

To calculate the current weighted effective cross section (20), one can use the formalism of Froelich described in chapter I, if the following condition is fulfilled:

$$ \left| {}^{s}\tilde{\sigma}_{c}(E) - \left\langle {}^{s}\tilde{\sigma}_{c}(E) \right\rangle \right| \ll \sum_{s'} \left\langle {}^{s'}\tilde{\sigma}_{c}(E) \right\rangle + \tilde{\sigma}_{p} + \tilde{\sigma}_{o} \qquad (21) $$

The numerator of (20) may be written as

$$ \left\langle \frac{{}^{s}\tilde{\sigma}_{c}(E)}{\left\{ \left[{}^{s}\tilde{\sigma}_{c}(E) - \left\langle {}^{s}\tilde{\sigma}_{c}(E) \right\rangle \right] + \left[{}^{s}\tilde{\sigma}_{p,eff} + \left\langle {}^{s}\tilde{\sigma}_{c}(E) \right\rangle \right] \right\}^{2}} \right\rangle $$

Using condition (21) and neglecting quadratic terms in

$$ \left| {}^{s}\tilde{\sigma}_{c}(E) - \left\langle {}^{s}\tilde{\sigma}_{c}(E) \right\rangle \right| $$

one gets

$$ \frac{1}{2 \cdot \left\{ {}^{s}\tilde{\sigma}_{p,eff} + \left\langle {}^{s}\tilde{\sigma}_{c}(E) \right\rangle \right\}} \cdot \left\langle \frac{{}^{s}\tilde{\sigma}_{c}(E)}{{}^{s}\tilde{\sigma}_{c}(E) + 0.5 \left\{ {}^{s}\tilde{\sigma}_{p,eff} - \left\langle {}^{s}\tilde{\sigma}_{c}(E) \right\rangle \right\}} \right\rangle $$

For the denominator of (20), one gets

$$\frac{1}{2\cdot\left\{{}^{s}\tilde{\sigma}_{p,eff}+\left\langle{}^{s}\tilde{\sigma}_{c}(E)\right\rangle\right\}}\left\langle\frac{1}{{}^{s}\tilde{\sigma}_{c}(E)+0.5\left\{{}^{s}\tilde{\sigma}_{p,eff}-\left\langle{}^{s}\tilde{\sigma}_{c}(E)\right\rangle\right\}}\right\rangle$$

Therefore, under condition (21) the current weighted effective cross section can be approximated by a flux weighted effective cross section of the form (11)

$${}^{s}_{1}\tilde{\sigma}_{c,g}(E)={}^{s}\tilde{\sigma}^{*}_{p,eff}\cdot\frac{\left\langle\frac{{}^{s}\tilde{\sigma}_{c}(E)}{{}^{s}\tilde{\sigma}_{c}(E)+{}^{s}\tilde{\sigma}^{*}_{p,eff}}\right\rangle}{1-\left\langle\frac{{}^{s}\tilde{\sigma}_{c}(E)}{{}^{s}\tilde{\sigma}_{c}(E)+{}^{s}\tilde{\sigma}^{*}_{p,eff}}\right\rangle}\qquad(22a)$$

and

$${}^{s}\tilde{\sigma}^{*}_{p,eff}=0.5\left\{{}^{s}\tilde{\sigma}_{p,eff}-\left\langle{}^{s}\tilde{\sigma}_{c}(E)\right\rangle\right\}\qquad(22b)$$

Now the formalism of Froelich can be used yielding the result (14), where ${}^{s}\tilde{\sigma}_{p,eff}$ is replaced by ${}^{s}\tilde{\sigma}^{*}_{p,eff}$.

3. Limits of the approximation

The limits of this approximation are given by condition (21) and the modified condition (15), when ${}^s\tilde{\sigma}_{p,eff}$ is replaced by ${}^s\tilde{\sigma}^*_{p,eff}$. Condition (15) then takes the form

$$\frac{{}^s\tilde{\sigma}_{p,eff} + \langle {}^s\tilde{\sigma}_c(E)\rangle}{2} + {}^s\tilde{\sigma}_c^{\,r}(E)\rangle\rangle \left| \sum_{r' \neq r} {}^s\tilde{\sigma}_c^{\,r'}(E) - \langle {}^s\tilde{\sigma}_c\rangle \right| \qquad (23)$$

Equation (23) is certainly fulfilled for separated resonances, as long as

$${}^s\tilde{\sigma}_{p,eff} > \langle {}^s\tilde{\sigma}_c(E)\rangle \qquad (24)$$

Equation (24) can also be written as

$${}^s\tilde{\sigma}^*_{p,eff} > 0. \qquad (25)$$

This condition is necessary, because (22a) is not defined for negative ${}^s\tilde{\sigma}^*_{p,eff}$. For strong overlapping, condition (23) is more sensible than condition (15).

In the energy range of "statistical resonances" condition (21) cannot be proved. To get some information on the influence of condition (21) on the approximation (22), some calculations in the region of resolved resonance parameters can be done. The flux weighted and the current weighted effective cross sections (10) and (20) may be calculated for a certain energy interval

exactly. In the resolved resonance region it is not necessary to distinguish the single resonance series. Then one gets for the total resonance cross section in the energy group g

$$\sigma_{c,g}(\sigma_o^*) = \frac{\left\langle \dfrac{\sigma_c(E)}{\sigma_c(E) + \sigma^*_{p,eff}} \right\rangle}{\left\langle \dfrac{1}{\sigma_c(E) + \sigma^*_{p,eff}} \right\rangle} \tag{26a}$$

$$_1\sigma_{c,g}(\sigma_o) = \frac{\left\langle \dfrac{\sigma_c(E)}{\{\sigma_c(E) + \sigma_{p,eff}\}^2} \right\rangle}{\left\langle \dfrac{1}{\{\sigma_c(E) + \sigma_{p,eff}\}^2} \right\rangle} \tag{26b}$$

$$\sigma_{p,eff} = \sigma_p + \sigma_o \tag{26c}$$

$$\sigma^*_{p,eff} = 0.5 \cdot \{\sigma_{p,eff} - \langle \sigma_c(E) \rangle\} \tag{26d}$$

$$\sigma_o^* = \sigma^*_{p,eff} - \sigma_p = 0.5\{\sigma_o - (\sigma_p + \langle \sigma_c(E) \rangle)\} \tag{26e}$$

The averages $\langle\ \rangle$ are performed over the energy group g.
For the corresponding resonance self shielding factors one gets

$$f_{t,g}(\sigma_o^*) = \frac{\sigma_{c,g}(\sigma_o^*) + \sigma_p}{\sigma^\infty_{c,g} + \sigma_p} \tag{27a}$$

and

$$ {}_1f_{t,g}(\sigma_o) = \frac{{}_1\sigma_{c,g}(\sigma_o) + \sigma_p}{\sigma_{c,g}^{\infty} + \sigma_p} \qquad (27b) $$

neglecting the macroscopic weighting.

In fig. 1 and fig. 2 the relative errors of the approximated effective resonance cross section and the approximated total resonance self shielding factor for U 235 in the energy range from 50 eV to 100 eV for several temperatures are plotted. As can be seen from these figures, the errors of the total resonance self shielding factors are smaller than those of the effective resonance cross sections because of the contribution of the potential cross section. The lowest σ_o-value, for which the approximation can be used is given by condition (24). The average resonance cross section for this example is $\langle \sigma_c(E) \rangle$ = 49,9 barns; the potential cross section is σ_p = 10,3 barns. So the lowest possible background cross section is = 39,6 barns. This restriction of the approximation to σ_o-values greater than 50 barns is unimportant, because the σ_o-values that correspond to the concentration of U 235 in reactors are in the range of several hundred barns. From fig. 1 one can see that for σ_o-values greater than 500 barns the approximation is better than 1 % for all three temperatures. Since with increasing energy the resonances become smaller and the overlapping becomes more important, one can expect, that in the range of the unresolved resonances, condition (21) is fulfilled better than in the resolved resonance region. Therefore the errors of the approximation should be smaller than in fig. 1.
In fig. 3 and fig. 4 the same results for U 238 in the energy range form 2 keV to 3,3, keV are plotted. In contrast to U 235 the errors of the approximation for the effective resonance cross section (fig. 3) of U 238 are much larger, because of the

higher resonances. On the other hand, the effective resonance cross section U 238 is smaller than the potential cross section, so that the errors in the total resonance self shielding factors are much smaller. In fig. 4 one can see that the errors are smaller than 2 - 3 % in the whole range of $\tilde{\sigma}_o$. The average resonance cross section for this example is $\langle \sigma_c(E) \rangle = 5{,}9$ barns, the potential cross section is $\tilde{\sigma}_p = 10{,}7$ barns, so that condition (24) can be fulfilled for all $\tilde{\sigma}_o$-values.

4. Conclusions

From calculations in the resolved resonance region one can draw the conclusion that the proposed approximation for the current weighted total resonance self shielding factors yields results with relative errors of a few percent. This is sufficient for reactor calculations.

References:

|1| L.P. Abagjan, N.O. Bazazjanc, I.I. Bondarenko, M.N. Nikolaev

Gruppenkonstanten schneller und intermediärer Neutronen für die Berechnung von Kernreaktoren
KFK-tr-144

|2| R. Froelich

Theorie der Dopplerkoeffizienten schneller Reaktoren unter Berücksichtigung der gegenseitigen Abschirmung der Resonanzen
KFK-367, (1965)

|3| H. Huschke

Gruppenkonstanten für dampf- und natriumgekühlte schnelle Reaktoren in einer 26-Gruppendarstellung
KFK-770, (1968)

|4| J.J. Schmidt

Neutron cross sections for fast reactor materials Part I; evaluation.
KFK-120, (1966)

|5| L. Dresner

Resonance absorption in nuclear reactors.
Pergamon Press, (1960)

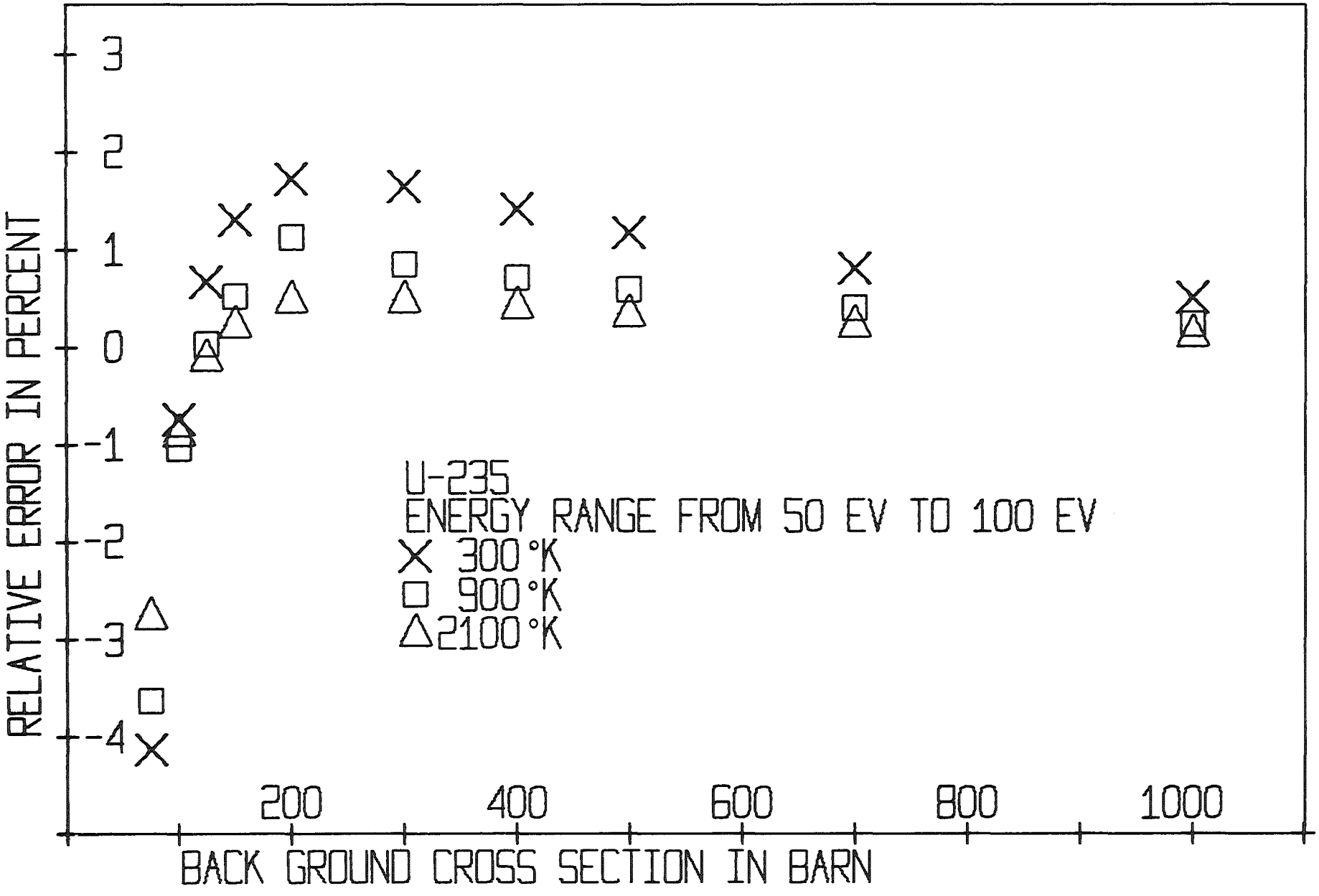


Fig. 1 : $[\sigma_c(\sigma_o^*) - {}_1\sigma_c(\sigma_o)] / [0.01\ {}_1\sigma_c(\sigma_o)]$ over σ_o.

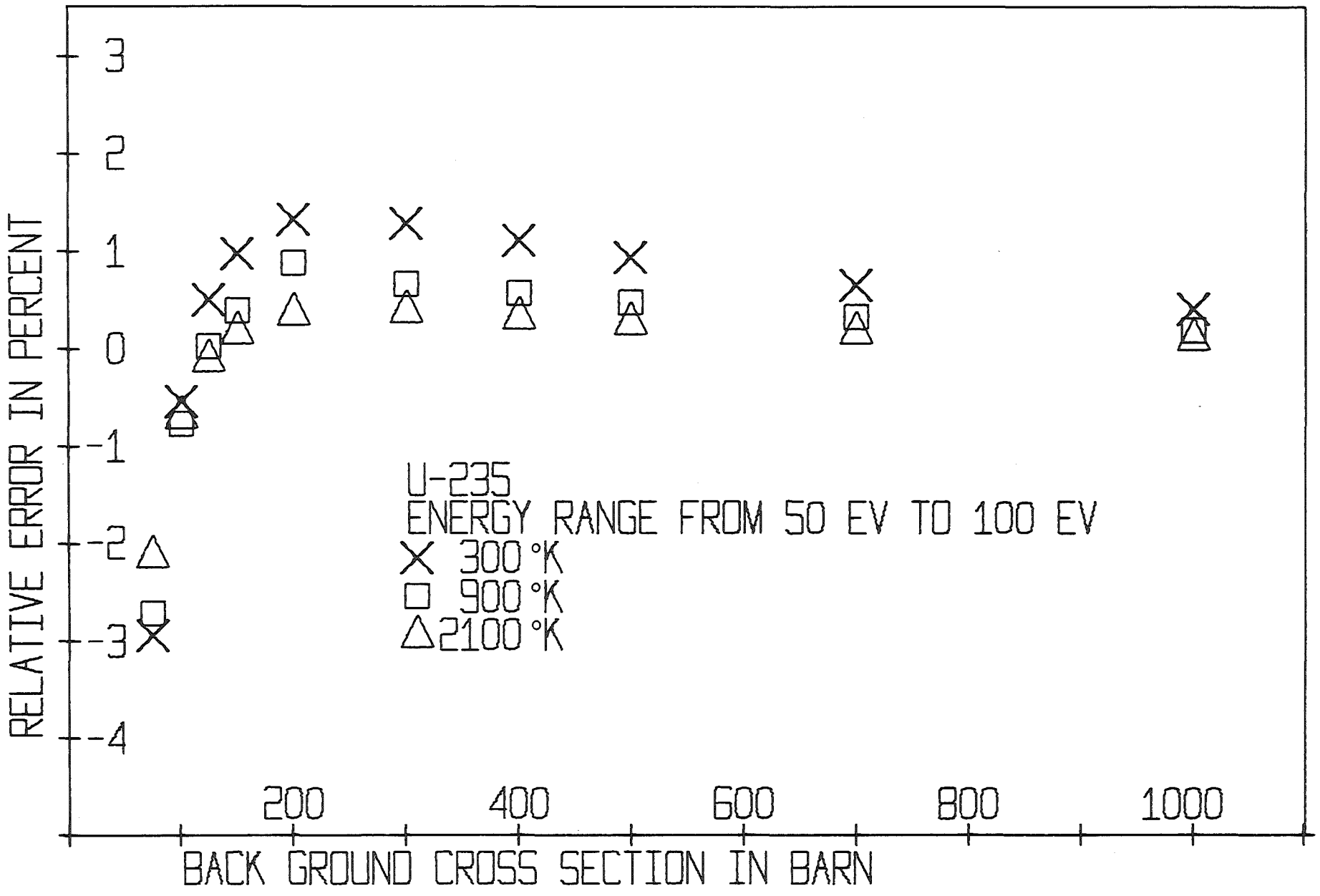


Fig.2 : $[\, f_t(\sigma_o^*) - {}_1f_t(\sigma_o)] / [0.01\ {}_1f_t(\sigma_o)]$ over σ_o.

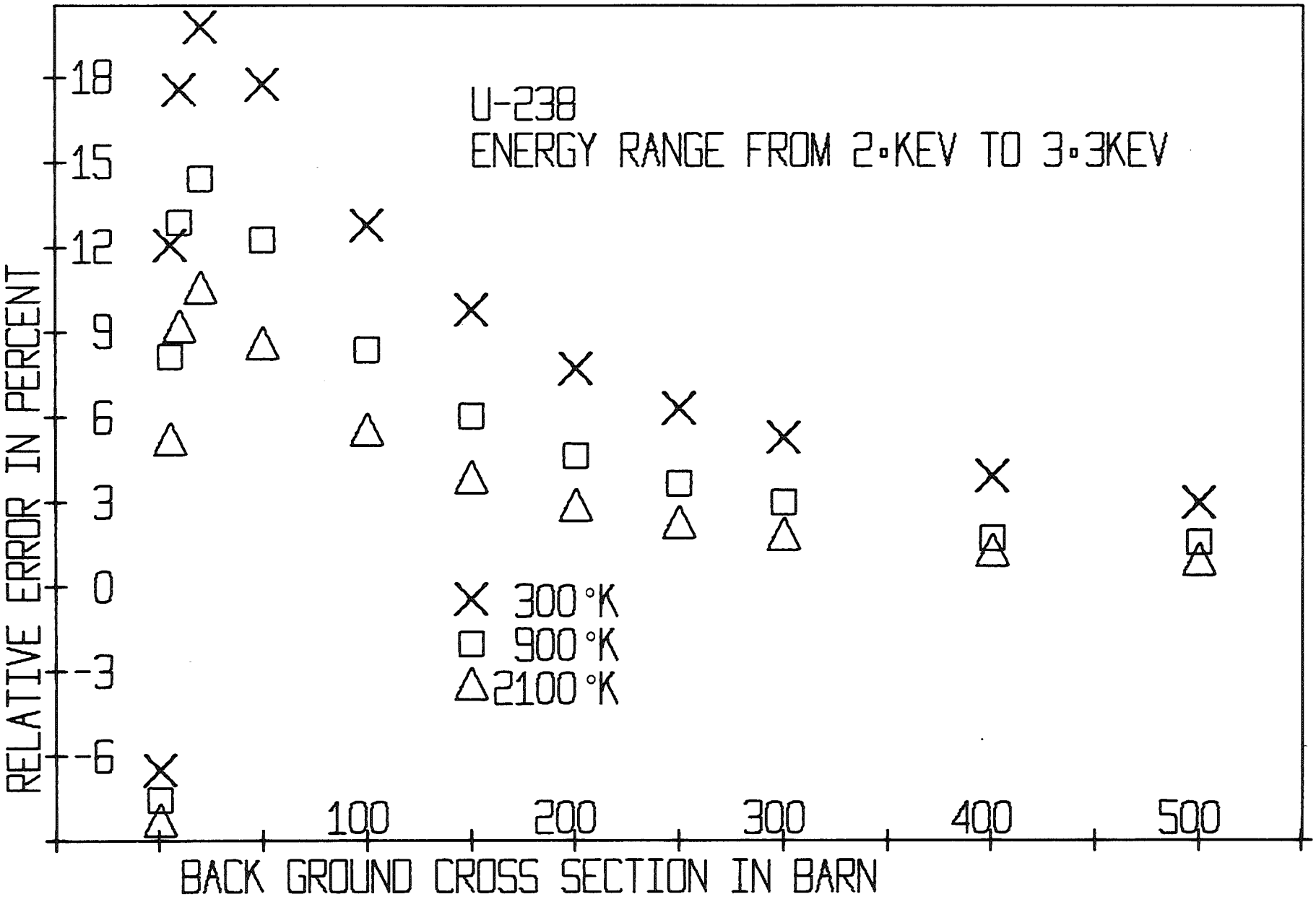


Fig 3.: $[\sigma_c(\sigma_o^*) - {}_1\sigma_c(\sigma_o)] / [0.01\,{}_1\sigma_c(\sigma_o)]$ over σ_o.

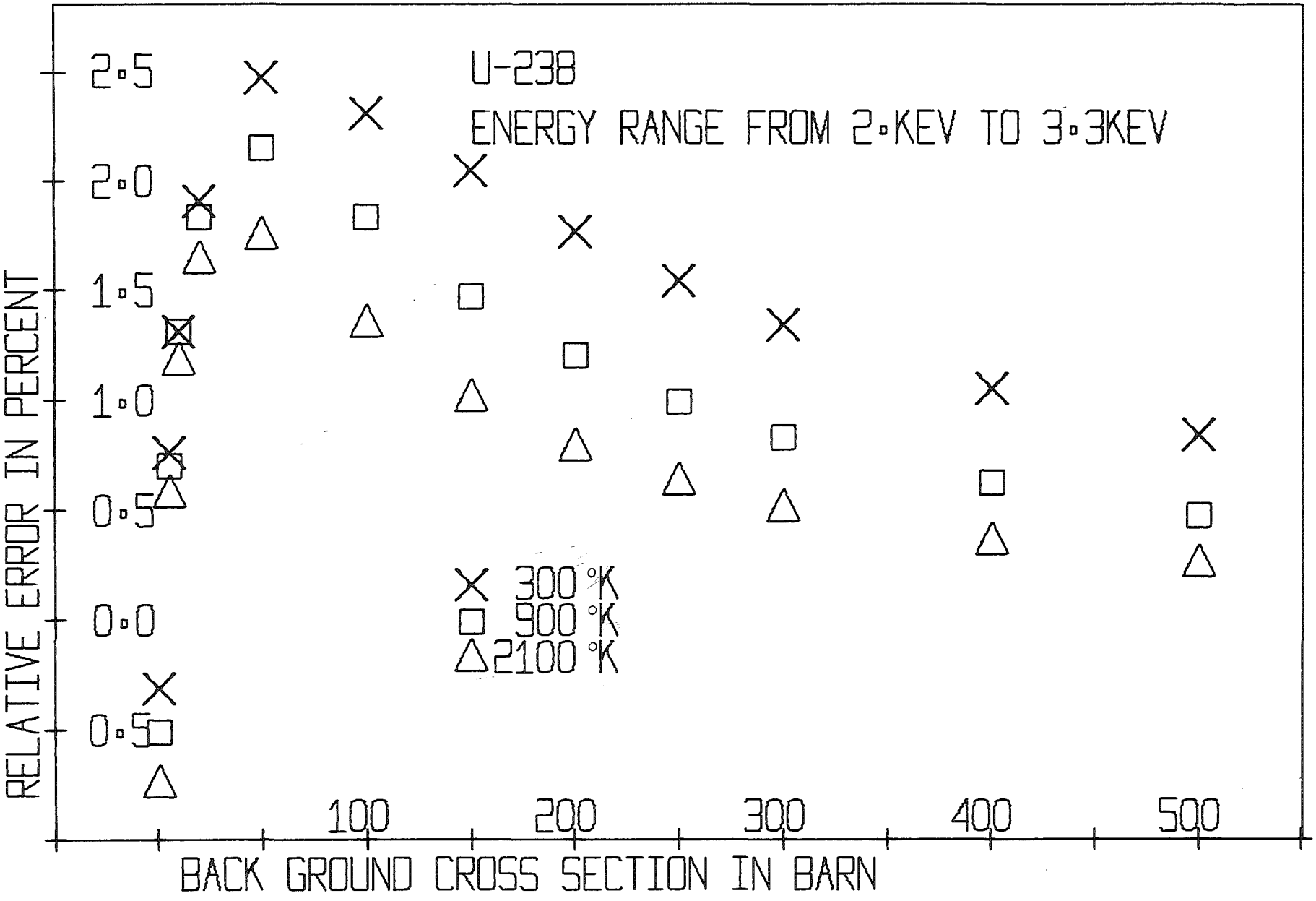


Fig. 4 : $[f_t(\sigma_0^*) - {}_1f_t(\sigma_0)] / [0.01\ {}_1f_t(\sigma_0)]$ over σ_0.

Appendix III Method of integration /Romberg procedure/

The Romberg method which has been used for numerical integration is briefly the following.

Let us have a function f (x) and the integral

$$I = \int_a^b dx\, f(x) \tag{1}$$

is to be calculated.

First an equidistant mesh with 2^n+1 mesh points / including the end points of the interval | a,b |/ are taken and the sum

$$I_{on} = \{0.5\,[f(a)+f(b)] + \sum_{k=1}^{2^n-1} f(X_k^n)\}\,\Delta X_n \tag{2}$$

is calculated, where

$$\Delta X_n = \frac{b-a}{2^n} \quad ; \quad X_k^n = a + k\cdot\Delta X_n \quad (k=1,\ldots 2^n-1)$$

Evidently

$$I_{o,n+1} = 0.5\cdot I_{on} + \Delta X_{n+1} \sum_{k=1,3,\ldots}^{2^{n+1}-1} f(X_k^{n+1}) \tag{3}$$

where

$$\Delta X_{n+1} = 0.5\,\Delta X_n\,, \quad X_k^{n+1} = a + k\,\Delta X_{n+1} \quad (k=1,3,5\ldots)$$

The second summation is taken over the new mesh points of the higher order mesh.

Let us take the expression

$$I_{mn} = \frac{2^{2m}\cdot I_{m-1,n} - I_{m-1,n-1}}{2^{2m}-1} \tag{4}$$

It is easy to prove that the deviation of I_{mn} from I is of the order $(\Delta X_n)^m$ i.e. I_{nn} is the best approximation for the given n.

The I_{mn} form a triangular matrix.

I_{oo}

$I_{o1}\ I_{11}$

.
.
.

$I_{on-1}\ I_{1n-1} \cdots\cdots\ I_{n-1n-1}$

$I_{on}\ \ I_{1n}\ \cdots\cdots\ I_{n-1n}\ \ I_{nn}$

The programming of the method is quite straightforward. A row of the above matrix is always to be stored and by means of the formula (3), (4) the next row can be determined. The process is finished if the quantity

$$\left| \frac{I_{nn} - I_{n-1,n-1}}{I_{nn}} \right| < \varepsilon$$

where ε is the required accuracy.

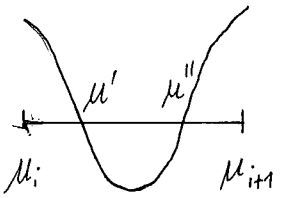
The following should be noted.

1. Only one ε /ERR/ is given. This used for the energy integration. For the angular integration ε/10 is prescribed.
2. Some of the higher moments are very small as far as heavier elements are concerned. In order to avoid a "bad" convergence, the energy integration process for the moment in question is finished when $|I_{nn}| < 10^{-10}$
3. In order to avoid a vaste of computing time the integration will be finished if n reaches a maximal value / for energy integration NUJM, for angle integration NJM /. Reaching these values in the course integration an error message will be generated and the calculation is continued. From the error message the user can decide whether the results are acceptable.

Appendix IV The subintervals in the angular integration

The integrand of (8.5) is a product of two functions. In order to save computing time the actual behaciour of these functions. in the integration interval $[\mu_i, \mu_{i+1}]$ should be taken into account.

a) The polynomial $P_n(t(\mu))$ has n zeros.E.g. let us assume that two zeros are in the interval $|\mu_i, \mu_{i+1}|$ and then the integration interval is divided into three subinterval: $[\mu_i, \mu']$, $[\mu', \mu'']$, $[\mu'', \mu_{i+1}]$. However sometimes it occurs that the intervals (μ_i, μ') or (μ'', μ_{i+1}) are too small. This can give rise to difficulties in the Romberg integration method. Therefore the width of the extreme intervals are investigated and if one of them is less than a given limit (now this limit is $|\mu'' - \mu'|/10$) then it will be joined with the next one.



b) The function $\gamma(\mu)$ has often shown a "nasty" character. This "nasty" character can already be detected at the normalization of angular distribution: N passes beyond NJM. If in a energy group a "nasty" charakter is detected then the integration interval is divided into subintervals defined by the angle point of the angular distribution given in the nuclear data file.

Appendix V. Sample problem

1. Job-Control Cards

```
JOB ORIGIN FROM LOCAL DEVICE=RD2      ,02C.
//INR017MI  JOB  (0017,101,P6M1B),KRIEG,CLASS=A,TIME=15,REGION=340K
// EXEC PGM=MIGROS2,PARM=170000
//STEPLIB DD DSN=LOAD.NUSYS,VOL=SER=NUSICE,UNIT=3330,DISP=SHR
//FT08F001  DD  UNIT=SYSDA,SPACE=(TRK,100)
//FT06F001  DD SYSOUT=A,
// DCB=(RECFM=FBA,LRECL=133,BLKSIZE=931),SPACE=(TRK,25)
//FT01F001  DD  UNIT=2314,VOL=SER=NUSYS0,DSN=KNDF,DISP=SHR
//FT03F001 DD UNIT=SYSDA,SPACE=(TRK,20)
//FT10F001  DD  UNIT=SYSDA,SPACE=(TRK,200)
//FT05F001 DD *
//
```

2. Input

```
**************************
```

```
@U 235@  1
@BLOC@  4
7  1 18 18  2 14 14  4 14 14  5 5 3  7 25 1  8 25 1  10 26 26
@ENDE @  17
@0  16@  0
@BLOC@  4
5  3 4 4  6 3 3  6 12 12  9 3 3  9 12 12
@ENDE@  17
@ENDE@  18
```

On the following pages the output of the results is given. Besides the output of the results for every MIGRØS-2-job, a German input-description with an input sample and the print out of the actual input is provided. It has been omitted here.

STAND DER KERNDATENBIBLIOTHEK VOM 100571

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
0.23[illegible]4425E 02	0.12802895E 02	0.28783478E 02	0.12802895E 02	0.64590790E 02

SIGMA 0	FG	FN	FF	FN1	FT1
0.0	[illegible] 00	0.94163764E 00	0.43603367E 00	0.92344695E 00	0.36389023E 00
0.10000000E 02	[illegible] 00	[illegible] 00	0.50455952E 00	0.92906642E 00	0.41785538E 00
0.10000000E 03	0.71442896E 00	0.96913391E 00	0.72282106E 00	0.95165300E 00	0.62696862E 00
0.10000000E 04	0.93719780E 00	0.99258685E 00	0.93785942E 00	0.98616427E 00	0.90250689E 00
0.10000000E 05	0.99270159E 00	0.99910563E 00	0.99279928E 00	0.99824953E 00	0.98808670E 00
0.10000000E 06	0.99930418E 00	0.99990535E 00	0.99939227E 00	0.99981219E 00	0.99876916E 00
0.10000000E 07	0.99991238E 00	0.99999189E 00	0.99992269E 00	0.99998176E 00	0.99987227E 00

MATERIAL	TEMPERATUR	GRUPPE	GRENZEN	
U 235	900.00	18	0.4650E 02	0.1000E 03

SIGMA G	SIGMA N	SIGMA F	SIGMAN1	SIGMAT1
0.22994293E 02	[illegible]12809570E 02	0.28795914E 02	0.12809570E 02	0.64590775E 02

SIGMA 0	FG	FN	FF	FN1	FT1
0.0	0.51503837E 00	0.95064503E 00	0.52545762E 00	0.92998606E 00	0.41661143E 00
0.10000000E 02	0.58327061E 00	0.95673221E 00	0.59176672E 00	0.93649042E 00	0.48082870E 00
0.10000000E 03	0.78867930E 00	0.97656202E 00	0.78884345E 00	0.96075338E 00	0.70187891E 00
0.10000000E 04	0.95903468E 00	0.99510098E 00	0.95769149E 00	0.99061841E 00	0.93352538E 00
0.10000000E 05	0.99543375E 00	0.99943763E 00	0.99527752E 00	0.99889314E 00	0.99233168E 00
0.10000000E 06	0.99956995E 00	0.99993879E 00	0.99959248E 00	0.99988109E 00	0.99922240E 00
0.10000000E 07	0.99995285E 00	0.99999326E 00	0.99993795E 00	0.99998796E 00	0.99991435E 00

MATERIAL	TEMPERATUR	GRUPPE	GRENZEN	
U 235	2100.00	18	0.4650E 02	0.1000E 03

SIGMA G	SIGMA N	SIGMA F	SIGMAN1	SIGMAT1
0.22947205E 02	0.12792241E 02	0.28690109E 02	0.12792241E 02	0.64429550E 02

SIGMA 0	FG	FN	FF	FN1	FT1
0.0	0.60038620E 00	0.95793915E 00	0.60191047E 00	0.93366927E 00	0.47596300E 00
0.10000000E 02	0.66217357E 00	0.96402717E 00	0.66151232E 00	0.94240171E 00	0.54420239E 00
0.10000000E 03	0.83948672E 00	0.98195404E 00	0.83347678E 00	0.96827495E 00	0.75921273E 00
0.10000000E 04	0.97122353E 00	0.99655139E 00	0.96887636E 00	0.99331534E 00	0.95158803E 00
0.10000000E 05	0.99685490E 00	0.99961168E 00	0.99658918E 00	0.99923521E 00	0.99457383E 00
0.10000000E 06	0.99969882E 00	0.99995881E 00	0.99969935E 00	0.99991757E 00	0.99944764E 00
0.10000000E 07	0.99996769E 00	0.99999511E 00	0.99995691E 00	0.99999112E 00	0.99994034E 00

PROGRAMM KENNZIFFER 2
PROGRAMM ZUR BERECHNUNG VON RESONANZSELBSTABSCHIRMFAKTOREN VON STATISTISCHEN RESONANZPARAMETERN

MATERIAL	TEMPERATUR	GRUPPE	GRENZEN	
U 235	300.00	14	0.1000E 04	0.2150E 04

SIGMA G	SIGMA N	SIGMA F	SIGMAN1	SIGMAT1
0.33934994E 01	0.12306777E 02	0.74021378E 01	0.12306777E 02	0.23102356E 02

SIGMA 0	FG	FN	FF	FN1	FT1
0.0	0.77354968E 00	0.98292530E 00	0.77513117E 00	0.96743643E 00	0.74214095E 00
0.10000000E 02	0.84917933E 00	0.98786384E 00	0.85143816E 00	0.97653657E 00	0.83018833E 00
0.10000000E 03	0.95035458E 00	0.99311745E 00	0.94899106E 00	0.99301809E 00	0.96027339E 00
0.10000000E 04	0.99418187E 00	0.99908733E 00	0.99393761E 00	0.99815631E 00	0.99331576E 00
0.10000000E 05	0.99942076E 00	0.99990880E 00	0.99939656E 00	0.99981672E 00	0.99934429E 00
0.10000000E 06	0.99994653E 00	0.99999177E 00	0.99994475E 00	0.99998331E 00	0.99993974E 00
0.10000000E 07	0.10000000E 01	0.10000000E 01	0.10000000E 01	0.10000000E 01	0.10000000E 01

MATERIAL	TEMPERATUR	GRUPPE	GRENZEN	
U 235	900.00	14	0.1000E 04	0.2150E 04

SIGMA G	SIGMA N	SIGMA F	SIGMAN1	SIGMAT1
0.33934994E 01	0.12306777E 02	0.74021378E 01	0.12306777E 02	0.23102356E 02

SIGMA 0	FG	FN	FF	FN1	FT1
0.0	0.80794090E 00	0.98593742E 00	0.80581999E 00	0.96952617E 00	0.75254667E 00
0.10000000E 02	0.87867934E 00	0.99032903E 00	0.87774932E 00	0.97942162E 00	0.84590864E 00
0.10000000E 03	0.96768624E 00	0.99529058E 00	0.96637660E 00	0.99207813E 00	0.96425921E 00
0.10000000E 04	0.99666643E 00	0.99947429E 00	0.99652636E 00	0.99893630E 00	0.99615276E 00
0.10000000E 05	0.99966973E 00	0.99994755E 00	0.99965602E 00	0.99989378E 00	0.99962395E 00
0.10000000E 06	0.99996924E 00	0.99999493E 00	0.99996859E 00	0.99998987E 00	0.99996555E 00
0.10000000E 07	0.10000000E 01	0.10000000E 01	0.10000000E 01	0.10000000E 01	0.10000000E 01

MATERIAL	TEMPERATUR	GRUPPE	GRENZEN	
U 235	2100.00	14	0.1000E 04	0.2150E 04

SIGMA G	SIGMA N	SIGMA F	SIGMAN1	SIGMAT1
0.33934994E 01	0.12306777E 02	0.74021378E 01	0.12306777E 02	0.23102356E 02

SIGMA 0	FG	FN	FF	FN1	FT1
0.0	0.83612275E 00	0.98812699E 00	0.83280033E 00	0.97210991E 00	0.76919627E 00
0.10000000E 02	0.89682126E 00	0.99082017E 00	0.89438051E 00	0.98215550E 00	0.86282295E 00
0.10000000E 03	0.97812480E 00	0.99687904E 00	0.97724724E 00	0.99318576E 00	0.97129792E 00
0.10000000E 04	0.99780726E 00	0.99965549E 00	0.99771470E 00	0.99930209E 00	0.99746072E 00
0.10000000E 05	0.99978393E 00	0.99996555E 00	0.99977404E 00	0.99993122E 00	0.99975389E 00
0.10000000E 06	0.99997985E 00	0.99999696E 00	0.99997896E 00	0.99999368E 00	0.99997759E 00
0.10000000E 07	0.10000000E 01	0.10000000E 01	0.10000000E 01	0.10000000E 01	0.10000000E 01

PROGRAMM KENNZIFFER 4
PROGRAMM ZUR BERECHNUNG VON GRUPPENWIRKUNGSQUERSCHNITTEN BEI UNENDLICHER VERDUENNUNG

U 235 MUEL GRUPPE 14 BIS 14
0.27999950E-02

U 235 NUE GRUPPE 14 BIS 14
0.24301538E 01

U 235 SGA GRUPPE 14 BIS 14
0.10692280E 02

U 235 SGF GRUPPE 14 BIS 14
0.75102386E 01

U 235 SGC GRUPPE 14 BIS 14
0.31820412E 01

U 235 SGI GRUPPE 14 BIS 14
0.0

U 235 SGN GRUPPE 14 BIS 14
0.12046540E 02

U 235 SG2N GRUPPE 14 BIS 14
0.0

PROGRAMM KENNZIFFER 5
PROGRAMM ZUR BERECHNUNG INELASTISCHER STREUMATRIZEN

PROBSGI

2 U 235 3

	5	6	7	8	9	10	11	12	13	14	15
5	0.279D 00	0.524D 00	0.167D 00	0.223D-01	0.562D-02	0.127D-02	0.276D-03	0.603D-04	0.131D-04	0.281D-05	0.608D-06
	16	17	18	19	20	21	22	23	24	25	26
	0.132D-06	0.281D-07	0.608D-08	0.132D-08	0.281D-09	0.608D-10	0.132D-10	0.281D-11	0.608D-12	0.132D-12	0.359D-13
	4	5	6	7	8	9	10	11	12	13	14
4	0.552D-01	0.382D 00	0.399D 00	0.113D 00	0.366D-01	0.111D-01	0.271D-02	0.597D-03	0.131D-03	0.286D-04	0.612D-05
	15	16	17	18	19	20	21	22	23	24	25
	0.133D-05	0.288D-06	0.615D-07	0.133D-07	0.289D-08	0.615D-09	0.133D-09	0.289D-10	0.615D-11	0.133D-11	0.289D-12
	26										
	0.785D-13										
	3	4	5	6	7	8	9	10	11	12	13
3	0.175D-02	0.453D-01	0.192D 00	0.361D 00	0.248D 00	0.105D 00	0.357D-01	0.891D-02	0.203D-02	0.452D-03	0.987D-04
	14	15	16	17	18	19	20	21	22	23	24
	0.213D-04	0.462D-05	0.100D-05	0.214D-06	0.464D-07	0.101D-07	0.215D-08	0.464D-09	0.101D-09	0.215D-10	0.464D-11
	25	26									
	0.101D-11	0.274D-12									

PROGRAMM KENNZIFFER 7
PROGRAMM ZUR BERECHNUNG DES SPALTSPEKTRUMS

U 235 EINFALLSENERGIE = 0.0 VON GRUPPE 25 BIS 1
CHI 0

0.10703186E-09	0.32318170E-09	0.99962483E-09	0.31642213E-08	0.98985815E-08	0.31139621E-07	0.99362353E-07
0.31199102E-06	0.98313831E-06	0.31392656E-05	0.98584596E-05	0.31055373E-04	0.99062076E-04	0.31036860E-03
0.97276270E-03	0.30689863E-02	0.93898997E-02	0.23881126E-01	0.61028074E-01	0.14057308E 00	0.20230573E 00
0.26991755E 00	0.18339217E 00	0.38322520E-01	0.15635300E-01			

PROGRAMM KENNZIFFER 8
PROGRAMM ZUR BERECHNUNG DES 1/V- GRUPPENMITTELWERTES

GRUPPE	1/V
1	0.25519209E-09
2	0.32105696E-09
3	0.40761239E-09
4	0.53069216E-09
5	0.70539552E-09
6	0.96682840E-09
7	0.13673027E-08
8	0.19336588E-08
9	0.27883824E-08
10	0.40953445E-08
11	0.60131669E-08
12	0.88176435E-08
13	0.12950633E-07
14	0.19015328E-07
15	0.27883853E-07
16	0.40953452E-07
17	0.60131697E-07
18	0.88176307E-07
19	0.12950636E-06
20	0.19015351E-06
21	0.27883834E-06
22	0.40953523E-06
23	0.60131714E-06
24	0.88176398E-06
25	0.12950613E-05
26	0.40279137E-05

PROGRAMM KENNZIFFER 10
PROGRAMM ZUR BERECHNUNG DER THERMISCHEN QUERSCHNITTE

U 235 MUEL 26
0.28400000E-02

U 235 NUE 26
0.24299994E 01

U 235 SGA 26
0.60553198E 03

U 235 SGF 26
0.51578394E 03

U 235 SGC 26
0.89748047E 02

U 235 SGI 26
0.0

U 235 SGN 26
0.16599991E 02

U 235 SG2N 26
0.0

PROGRAMM KENNZIFFER 3
PROGRAMM ZUR BERECHNUNG VON RESONANZSELBSTABSCHIRMFAKTOREN VON PUNKTWEISE GEGEBENEN WIRKUNGSQUERSCHNITTEN

***WARNING 3. 5 : IN THE ENERGY GROUP 4 THE SELFSHIELDING FACTORS ARE SET TO 1, BECAUSE THE CROSS SECTIONS FOUND ON KEDAK FOR THIS GROUP ALL ARE ZERO

0 16 GRUPPE = 4 GRUPPENGRENZEN 0.14000000E 07 0.25000000E 07

	SIGMA A	SIGMA N	SIGMA N01	SIGMA N1	SIGMA T1
	0.0	0.17582741E 01	0.19087684E 00	0.19087684E 00	0.17582703E 01
SIGO	FA	FN	FN01	FN1	FT1
0.0	0.10000000E 01	0.81050962E 00	0.95290893E 00	0.91999471E 00	0.59960687E 00
0.10000000E 02	0.10000000E 01	0.97468221E 00	0.98883152E 00	0.97875798E 00	0.95077115E 00
0.10000000E 03	0.10000000E 01	0.99691004E 00	0.99860436E 00	0.99722087E 00	0.99385238E 00
0.10000000E 04	0.10000000E 01	0.99968928E 00	0.99986470E 00	0.99971133E 00	0.99936974E 00
0.10000000E 05	0.10000000E 01	0.99997497E 00	0.99999422E 00	0.99997669E 00	0.99994141E 00
0.10000000E 06	0.10000000E 01	0.10000029E 01	0.10000010E 01	0.10000048E 01	0.10000029E 01
0.10000000E 07	0.10000000E 01	0.10000000E 01	0.10000000E 01	0.10000000E 01	0.10000000E 01

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

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
0.88370
0.11629

SGNC1 ELASTISCHE STREUMATRIX 1. ORDNUNG FUER 0 16

3.GRUPPE
0.29687
-0.02758

SGNC2 ELASTISCHE STREUMATRIX 2. ORDNUNG FUER 0 16

3.GRUPPE
0.19188
0.00079

SGNC3 ELASTISCHE STREUMATRIX 3. ORDNUNG FUER 0 16

3.GRUPPE
0.08507
-0.00520

SGNC4 ELASTISCHE STREUMATRIX 4. ORDNUNG FUER 0 16

3.GRUPPE
0.01674
-0.00050

SGNC5 ELASTISCHE STREUMATRIX 5. ORDNUNG FUER 0 16

3.GRUPPE
-0.00131
0.00036

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

ALLE MOMENTE WIE DAS 0. MOMENT MIT
F(0,E) (STANDARD F(0,E) = 1/E)

M I K R O W I C H T U N G (FEINSTRUKTUR)

ALLE MOMENTE MIT FS(0,E) = 1
(KEINE FEINSTRUKTURWICHTUNG)

TOTALE ELASTISCHE STREUQUERSCHNITTE SGN UND STREUKOSINUS MUEL FUER 0 16

3.GRUPPE
2.040E 00
2.693E-01

ERLAEUTERUNG
G-TE GRUPPE, 1. ZEILE: TOTALER ELASTISCHER QUERSCHNITT DER G-TEN
GRUPPE
G-TE GRUPPE, 2. ZEILE: MITTLERER STREUKOSINUS DER G-TEN GRUPPE

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
0.84206
0.15793

SGNC1 ELASTISCHE STREUMATRIX 1. ORDNUNG FUER 0 16

12.GRUPPE
0.09014
-0.04811

SGNC2 ELASTISCHE STREUMATRIX 2. ORDNUNG FUER 0 16

12.GRUPPE
0.00343
-0.00263

SGNC3 ELASTISCHE STREUMATRIX 3. ORDNUNG FUER 0 16

12.GRUPPE
0.00004
-0.00004

SGNC4 ELASTISCHE STREUMATRIX 4. ORDNUNG FUER 0 16

12.GRUPPE
0.0
0.0

SGNC5 ELASTISCHE STREUMATRIX 5. ORDNUNG FUER 0 16

12.GRUPPE
-0.00005
0.00005

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

ALLE MOMENTE WIE DAS 0. MOMENT MIT
F(0,E) (STANDARD F(0,E) = 1/E)

M I K R O W I C H T U N G (FEINSTRUKTUR)

ALLE MOMENTE MIT FS(0,E) = 1
(KEINE FEINSTRUKTURWICHTUNG)

TOTALE ELASTISCHE STREUQUERSCHNITTE SGN UND STREUKOSINUS MUEL FUER 0 16

12.GRUPPE
3.700E 00
4.203E-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

PROGRAMM KENNZIFFER 9
PROGRAMM ZUR BERECHNUNG DER ELASTISCHEN STREUMATRIZEN FUER DIE REMO-KORREKTUR

GROUP= 3 NUMBER OF FINE INTERVALS= 70 MATERIAL 0 16

THE VALUES OF SGT

1.0834E 00	1.0891E 00	1.0969E 00	1.1005E 00	1.1038E 00	1.1085E 00
1.1121E 00	1.1146E 00	1.1178E 00	1.1215E 00	1.1260E 00	1.1301E 00
1.1327E 00	1.1357E 00	1.1393E 00	1.1433E 00	1.1482E 00	1.1511E 00
1.1525E 00	1.1542E 00	1.1563E 00	1.1588E 00	1.1616E 00	1.1650E 00
1.1694E 00	1.1731E 00	1.1772E 00	1.2092E 00	1.2685E 00	1.3403E 00
1.4290E 00	1.5346E 00	1.6382E 00	1.7394E 00	1.8771E 00	2.0262E 00
2.1946E 00	2.3595E 00	2.5063E 00	2.6978E 00	2.9278E 00	3.1471E 00
3.1418E 00	3.1065E 00	3.0622E 00	3.0119E 00	3.0118E 00	3.4818E 00
3.3928E 00	3.1109E 00	2.9510E 00	2.9672E 00	2.9898E 00	3.0181E 00
3.0377E 00	3.0173E 00	2.9870E 00	2.9635E 00	2.9481E 00	3.0599E 00
3.8915E 00	4.1098E 00	2.9267E 00	2.6033E 00	2.4405E 00	2.3473E 00
2.2758E 00	2.2157E 00	2.1568E 00	2.0823E 00		

THE VALUES OF SGN

1.0834E 00	1.0891E 00	1.0969E 00	1.1005E 00	1.1038E 00	1.1085E 00
1.1121E 00	1.1146E 00	1.1178E 00	1.1215E 00	1.1260E 00	1.1301E 00
1.1327E 00	1.1357E 00	1.1393E 00	1.1433E 00	1.1482E 00	1.1511E 00
1.1525E 00	1.1542E 00	1.1563E 00	1.1588E 00	1.1616E 00	1.1650E 00
1.1694E 00	1.1731E 00	1.1772E 00	1.2092E 00	1.2685E 00	1.3403E 00
1.4290E 00	1.5346E 00	1.6382E 00	1.7394E 00	1.8771E 00	2.0262E 00
2.1946E 00	2.3595E 00	2.5063E 00	2.6978E 00	2.9278E 00	3.1471E 00
3.1418E 00	3.1065E 00	3.0622E 00	3.0119E 00	3.0118E 00	3.4818E 00
3.3928E 00	3.1109E 00	2.9510E 00	2.9672E 00	2.9898E 00	3.0181E 00
3.0376E 00	3.0164E 00	2.9849E 00	2.9604E 00	2.9440E 00	3.0550E 00
3.8860E 00	4.1035E 00	2.9195E 00	2.5948E 00	2.4295E 00	2.3328E 00
2.2582E 00	2.1959E 00	2.1177E 00	2.0112E 00		

THE VALUES OF MUEL

2.5996E-01	2.5154E-01	2.4003E-01	2.3346E-01	2.3822E-01	2.4620E-01
2.5308E-01	2.5826E-01	2.6471E-01	2.7243E-01	2.8137E-01	2.8979E-01
2.9598E-01	3.0298E-01	3.1088E-01	3.0748E-01	2.9918E-01	2.9230E-01
2.8744E-01	2.8129E-01	2.7386E-01	2.6516E-01	2.5989E-01	2.5777E-01
2.5274E-01	2.2265E-01	1.7932E-01	1.5853E-01	1.7249E-01	1.8829E-01
2.0561E-01	2.2360E-01	2.3239E-01	2.3523E-01	2.3859E-01	2.3798E-01
2.2508E-01	2.0892E-01	1.9457E-01	1.7820E-01	1.6148E-01	1.5731E-01
1.6324E-01	1.7065E-01	1.8022E-01	1.9149E-01	2.0469E-01	2.2036E-01
2.3761E-01	2.6291E-01	2.8662E-01	2.9853E-01	3.1322E-01	3.3129E-01
3.4600E-01	3.5220E-01	3.5739E-01	3.6020E-01	3.6179E-01	3.5162E-01
3.0388E-01	2.6894E-01	2.5509E-01	3.3442E-01	3.7454E-01	3.6963E-01
3.6842E-01	3.7469E-01	3.9465E-01	4.2416E-01		

THE VALUES OF FLUX

1.9998E-01	1.9999E-01	1.9998E-01	1.9998E-01	1.9999E-01	1.9997E-01
1.9997E-01	1.9997E-01	1.9997E-01	1.9997E-01	1.9998E-01	1.9998E-01
1.9999E-01	1.9998E-01	1.9998E-01	1.9998E-01	1.9998E-01	1.9998E-01
1.9998E-01	1.9998E-01	1.9999E-01	1.9999E-01	1.9998E-01	1.9999E-01
1.9998E-01	1.9999E-01	1.9999E-01	1.9998E-01	1.9998E-01	1.9999E-01
1.9999E-01	1.9998E-01	1.9998E-01	1.9998E-01	1.9998E-01	1.9998E-01
1.9998E-01	1.9998E-01	1.9998E-01	1.9998E-01	1.9998E-01	1.9998E-01
1.9998E-01	1.9998E-01	1.9998E-01	1.9998E-01	1.9999E-01	1.9998E-01
1.9999E-01	1.9999E-01	1.9997E-01	1.9997E-01	1.9997E-01	1.9997E-01
1.9997E-01	1.9999E-01	1.9999E-01	1.9999E-01	1.9999E-01	1.9999E-01
1.9999E-01	1.9999E-01	1.9999E-01	1.9999E-01	1.9999E-01	1.9999E-01
1.9999E-01	1.9999E-01	1.9999E-01	1.9999E-01		

```
 ELASTIC SCATTERING MATRIX   SGNC0  FOR O  16     GROUP=   3
FROM GROUP     3 TO GROUP      3
  2.8227E-02  7.8761E-02  1.2239E-01  1.6345E-01  2.1659E-01  2.7287E-01
  3.2734E-01  3.7757E-01  4.2379E-01  4.6571E-01  5.0372E-01  5.3808E-01
  5.6899E-01  5.9703E-01  6.2213E-01  6.3841E-01  6.5196E-01  6.6610E-01
  6.8074E-01  6.9571E-01  7.1089E-01  7.2614E-01  7.4286E-01  7.6173E-01
  7.7919E-01  7.7882E-01  7.7721E-01  7.8409E-01  7.9834E-01  8.1127E-01
  8.2497E-01  8.5349E-01  8.8278E-01  9.0954E-01  9.3579E-01  9.5933E-01
  9.7833E-01  9.9636E-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
  9.7177E-01  9.2124E-01  8.7761E-01  8.3655E-01  7.8341E-01  7.2713E-01
  6.7266E-01  6.2243E-01  5.7621E-01  5.3429E-01  4.9628E-01  4.6192E-01
  4.3101E-01  4.0297E-01  3.7787E-01  3.6159E-01  3.4804E-01  3.3390E-01
  3.1926E-01  3.0429E-01  2.8911E-01  2.7386E-01  2.5714E-01  2.3827E-01
  2.2081E-01  2.2118E-01  2.2279E-01  2.1591E-01  2.0166E-01  1.8873E-01
  1.7503E-01  1.4651E-01  1.1722E-01  9.0457E-02  6.4213E-02  4.0672E-02
  2.1672E-02  3.6398E-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
  2.7734E-02  7.5561E-02  1.1431E-01  1.4845E-01  1.9148E-01  2.3499E-01
  2.7504E-01  3.1030E-01  3.4129E-01  3.6826E-01  3.9177E-01  4.1230E-01
  4.3019E-01  4.4603E-01  4.5948E-01  4.6035E-01  4.5594E-01  4.5095E-01
  4.4530E-01  4.3874E-01  4.3129E-01  4.2293E-01  4.1456E-01  4.0657E-01
  3.9628E-01  3.6824E-01  3.3286E-01  3.1342E-01  3.2575E-01  3.3829E-01
  3.4885E-01  3.4520E-01  3.3349E-01  3.1575E-01  2.9724E-01  2.7649E-01
  2.4648E-01  2.1389E-01  1.9446E-01  1.7864E-01  1.6288E-01  1.5741E-01
  1.6541E-01  1.7411E-01  1.8281E-01  1.9164E-01  2.0459E-01  2.2056E-01
  2.4255E-01  2.6603E-01  2.8650E-01  3.0190E-01  3.1725E-01  3.3260E-01
  3.4599E-01  3.5241E-01  3.5740E-01  3.6040E-01  3.6180E-01  3.5350E-01
  3.0990E-01  2.6659E-01  2.5582E-01  3.3799E-01  3.7447E-01  3.6958E-01
  3.6843E-01  3.7472E-01  3.9501E-01  4.2433E-01
FROM GROUP     3 TO GROUP      4
  2.3338E-01  1.7569E-01  1.2704E-01  8.6316E-02  4.8585E-02  1.2328E-02
 -2.0506E-02 -4.8652E-02 -7.2483E-02 -9.2315E-02 -1.0870E-01 -1.2212E-01
 -1.3295E-01 -1.4172E-01 -1.4866E-01 -1.5337E-01 -1.5682E-01 -1.5903E-01
 -1.6013E-01 -1.6034E-01 -1.5965E-01 -1.5806E-01 -1.5469E-01 -1.4906E-01
 -1.4352E-01 -1.4886E-01 -1.5519E-01 -1.5658E-01 -1.5317E-01 -1.4929E-01
 -1.4343E-01 -1.2335E-01 -1.0140E-01 -8.0464E-02 -5.8776E-02 -3.8308E-02
 -2.0987E-02 -3.6007E-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

2.6766E-02	6.9427E-02	9.9230E-02	1.2126E-01	1.4720E-01	1.7011E-01
1.8788E-01	2.0108E-01	2.1076E-01	2.1789E-01	2.2328E-01	2.2758E-01
2.3134E-01	2.3489E-01	2.3776E-01	2.2621E-01	2.0853E-01	1.9059E-01
1.7245E-01	1.5412E-01	1.3577E-01	1.1762E-01	1.0012E-01	8.3564E-02
6.7289E-02	4.7667E-02	2.6716E-02	2.3535E-02	5.2308E-02	8.3559E-02
1.1489E-01	1.2767E-01	1.3727E-01	1.4783E-01	1.6092E-01	1.7487E-01
1.8748E-01	2.0201E-01	2.0390E-01	2.0228E-01	2.0096E-01	2.3267E-01
2.8650E-01	3.3315E-01	2.9590E-01	2.4299E-01	2.3671E-01	2.5272E-01
2.6846E-01	2.8442E-01	2.8420E-01	2.5902E-01	2.2789E-01	1.8492E-01
1.4501E-01	1.7260E-01	2.1578E-01	2.2436E-01	2.3190E-01	2.4786E-01
2.4956E-01	1.9408E-01	1.4298E-01	1.3944E-01	1.4051E-01	1.4157E-01
1.4177E-01	1.3337E-01	1.2280E-01	1.1221E-01		

FROM GROUP 3 TO GROUP 4

3.0559E-02	-2.2521E-02	-6.2757E-02	-9.2215E-02	-1.0496E-01	-1.1080E-01
-1.1154E-01	-1.0771E-01	-1.0039E-01	-9.0533E-02	-7.8945E-02	-6.6286E-02
-5.3117E-02	-3.9740E-02	-2.6679E-02	-1.8461E-02	-1.1604E-02	-4.4953E-03
2.8189E-03	1.0335E-02	1.7854E-02	2.5172E-02	3.1843E-02	3.7576E-02
4.2971E-02	5.1106E-02	6.0393E-02	7.0159E-02	7.9630E-02	8.7197E-02
9.1914E-02	8.4465E-02	7.4059E-02	6.2687E-02	4.8797E-02	3.3856E-02
1.9663E-02	3.5235E-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 O 16 GROUP= 3

FROM GROUP 3 TO GROUP 3

2.5362E-02	6.0881E-02	7.9167E-02	8.6817E-02	9.3899E-02	9.5909E-02
9.3285E-02	8.8295E-02	8.2518E-02	7.7178E-02	7.3001E-02	7.0453E-02
6.9835E-02	7.1111E-02	7.3614E-02	6.5249E-02	5.3199E-02	4.2406E-02
3.2903E-02	2.4729E-02	1.7893E-02	1.2341E-02	8.0041E-03	4.7971E-03
3.2926E-03	1.1762E-02	2.5130E-02	4.3321E-02	6.5863E-02	8.7285E-02
1.0672E-01	1.1678E-01	1.2388E-01	1.2897E-01	1.3047E-01	1.2671E-01
1.1345E-01	9.5190E-02	8.7900E-02	8.4020E-02	8.0139E-02	7.6330E-02
7.2562E-02	6.8435E-02	6.0340E-02	5.1719E-02	5.2188E-02	5.6995E-02
6.1722E-02	6.6513E-02	7.2391E-02	7.9836E-02	8.4337E-02	8.2694E-02
8.1630E-02	9.7462E-02	1.2062E-01	1.4744E-01	1.6920E-01	1.6948E-01
1.6070E-01	1.2653E-01	9.5032E-02	8.9697E-02	8.6919E-02	8.4150E-02
8.1361E-02	7.8374E-02	7.5339E-02	7.2302E-02		

FROM GROUP 3 TO GROUP 4

-2.1149E-02	-5.8151E-02	-7.7923E-02	-8.5943E-02	-8.5758E-02	-7.9057E-02
-6.7736E-02	-5.4067E-02	-3.9597E-02	-2.5588E-02	-1.2753E-02	-1.5550E-03
7.6880E-03	1.5046E-02	2.0595E-02	2.5728E-02	3.0158E-02	3.3334E-02
3.5209E-02	3.5753E-02	3.4958E-02	3.2880E-02	2.9583E-02	2.5159E-02
1.9983E-02	1.6188E-02	1.0800E-02	6.8687E-04	-1.3722E-02	-2.7010E-02
-3.8428E-02	-4.1735E-02	-4.2329E-02	-4.0933E-02	-3.5941E-02	-2.7825E-02
-1.7787E-02	-3.4100E-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 O 16 GROUP= 3

FROM GROUP 3 TO GROUP 3

2.3577E-02	5.0616E-02	5.6672E-02	5.1047E-02	4.2891E-02	3.0842E-02
1.7509E-02	5.8715E-03	-2.9387E-03	-8.2105E-03	-1.0831E-02	-8.7210E-03
-4.7690E-03	1.2609E-03	8.5238E-03	1.0897E-02	1.2070E-02	1.4060E-02
1.6559E-02	1.9294E-02	2.1858E-02	2.3859E-02	2.4942E-02	2.4802E-02
2.3806E-02	2.7629E-02	3.1281E-02	3.0953E-02	2.6293E-02	2.0377E-02
1.3148E-02	2.4266E-03	-8.9155E-03	-1.9021E-02	-2.6037E-02	-2.8643E-02
-2.5830E-02	-1.6890E-02	-1.5306E-02	-1.7784E-02	-2.0165E-02	-1.1739E-02
3.9115E-03	1.6794E-02	6.4191E-03	-9.0435E-03	-5.3530E-03	7.4612E-03
2.0062E-02	3.2832E-02	3.7516E-02	2.9630E-02	2.2722E-02	1.8113E-02
1.4322E-02	2.2889E-02	3.6789E-02	5.3304E-02	6.6725E-02	6.6888E-02
6.2156E-02	4.4344E-02	2.7793E-02	2.4347E-02	2.2187E-02	2.0034E-02
1.8061E-02	1.7856E-02	1.8101E-02	1.8348E-02		

FROM GROUP 3 TO GROUP 4

-1.9280E-02	-4.7367E-02	-5.4472E-02	-4.9475E-02	-3.9058E-02	-2.4184E-02
-8.0334E-03	6.4495E-03	1.8038E-02	2.6119E-02	3.0737E-02	3.2227E-02
3.1071E-02	2.7838E-02	2.3144E-02	1.8920E-02	1.4174E-02	8.6146E-03
2.5447E-03	-3.7595E-03	-9.8970E-03	-1.5470E-02	-2.0127E-02	-2.3557E-02
-2.5856E-02	-2.9678E-02	-3.2368E-02	-2.9979E-02	-2.1376E-02	-1.1483E-02
-1.0080E-03	6.8100E-03	1.3802E-02	1.9570E-02	2.2244E-02	2.0893E-02
1.5480E-02	3.2629E-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

2.1479E-02	3.9439E-02	3.4446E-02	1.9551E-02	3.5546E-03	-1.2091E-02
-2.4171E-02	-3.0887E-02	-3.2541E-02	-3.0025E-02	-2.4597E-02	-1.7517E-02
-9.9262E-03	-2.5902E-03	3.8581E-03	9.3175E-03	1.3829E-02	1.7008E-02
1.8640E-02	1.8620E-02	1.6962E-02	1.3829E-02	9.4772E-03	4.2549E-03
-1.5461E-03	-9.7245E-03	-1.9033E-02	-2.5900E-02	-2.7145E-02	-2.5613E-02
-2.1620E-02	-1.8142E-02	-1.3216E-02	-7.2960E-03	-2.3016E-03	1.0929E-04
-1.9805E-04	-9.1969E-03	-1.1478E-02	-1.0673E-02	-9.8508E-03	-7.1093E-03
-3.0953E-03	5.7997E-04	1.1216E-03	9.4173E-04	1.1144E-03	1.4553E-03
1.7890E-03	2.1276E-03	1.8221E-03	5.2818E-04	-1.1974E-03	-3.9112E-03
-6.2858E-03	-2.1162E-03	4.1595E-03	9.2182E-03	1.3064E-02	1.2546E-02
1.0472E-02	4.8066E-03	-5.9652E-04	-2.1279E-03	-3.2757E-03	-4.4197E-03
-5.2295E-03	-2.7488E-03	5.6752E-04	3.8876E-03		

FROM GROUP 3 TO GROUP 4

-1.7354E-02	-3.6147E-02	-3.1979E-02	-1.7839E-02	-2.0927E-03	1.3420E-02
2.5361E-02	3.1952E-02	3.3451E-02	3.0795E-02	2.5232E-02	1.8011E-02
1.0282E-02	2.8107E-03	-3.7705E-03	-9.2399E-03	-1.3713E-02	-1.6852E-02
-1.8446E-02	-1.8391E-02	-1.6694E-02	-1.3522E-02	-9.1282E-03	-3.8677E-03
1.8404E-03	8.3427E-03	1.5514E-02	2.1221E-02	2.3019E-02	2.2071E-02
1.8461E-02	1.3109E-02	5.8558E-03	-2.3907E-03	-9.7082E-03	-1.3798E-02
-1.2887E-02	-3.0857E-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		

```
PROGRAMM KENNZIFFER 9
PROGRAMM ZUR BERECHNUNG DER ELASTISCHEN STREUMATRIZEN FUER DIE REMO-KORREKTUR


GROUP= 12 NUMBER OF FINE INTERVALS=   70 MATERIAL  O  16
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
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
   1.9989E-01  1.9989E-01  1.9990E-01  1.9990E-01  1.9990E-01  1.9996E-01
   1.9995E-01  1.9996E-01  1.9997E-01  1.9997E-01  1.9990E-01  1.9989E-01
   1.9990E-01  1.9990E-01  1.9990E-01  1.9990E-01  1.9990E-01  1.9990E-01
   1.9990E-01  1.9990E-01  1.9989E-01  1.9989E-01  1.9990E-01  1.9990E-01
   1.9990E-01  1.9989E-01  1.9990E-01  1.9990E-01  1.9989E-01  1.9990E-01
   1.9990E-01  1.9990E-01  1.9990E-01  1.9990E-01  1.9990E-01  1.9998E-01
   1.9997E-01  1.9997E-01  1.9997E-01  1.9997E-01  1.9990E-01  1.9990E-01
   1.9990E-01  1.9990E-01  1.9990E-01  1.9990E-01  1.9990E-01  1.9990E-01
   1.9990E-01  1.9990E-01  1.9990E-01  1.9990E-01  1.9990E-01  1.9990E-01
   1.9990E-01  1.9990E-01  1.9990E-01  1.9990E-01  1.9990E-01  1.9990E-01
   1.9990E-01  1.9990E-01  1.9990E-01  1.9990E-01  1.9990E-01  1.9990E-01
   1.9990E-01  1.9990E-01  1.9990E-01  1.9990E-01
```

```
 ELASTIC SCATTERING MATRIX   SGNCO  FOR O  16     GROUP=  12
FROM GROUP   12 TO GROUP    12
  2.4398E-02  7.2843E-02  1.2077E-01  1.6817E-01  2.1506E-01  2.6145E-01
  3.0734E-01  3.5274E-01  3.9763E-01  4.4205E-01  4.8600E-01  5.2946E-01
  5.7245E-01  6.1498E-01  6.5705E-01  6.9868E-01  7.3984E-01  7.8057E-01
  8.2085E-01  8.6070E-01  9.0012E-01  9.3912E-01  9.7769E-01  9.9987E-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
  9.7560E-01  9.2716E-01  8.7923E-01  8.3183E-01  7.8494E-01  7.3855E-01
  6.9266E-01  6.4726E-01  6.0237E-01  5.5795E-01  5.1400E-01  4.7054E-01
  4.2755E-01  3.8502E-01  3.4295E-01  3.0132E-01  2.6016E-01  2.1943E-01
  1.7915E-01  1.3930E-01  9.9878E-02  6.0885E-02  2.2314E-02  1.3161E-04
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         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
  2.3694E-02  6.7944E-02  1.0756E-01  1.4264E-01  1.7328E-01  1.9957E-01
  2.2160E-01  2.3946E-01  2.5323E-01  2.6301E-01  2.6889E-01  2.7093E-01
  2.6923E-01  2.6387E-01  2.5492E-01  2.4246E-01  2.2657E-01  2.0733E-01
  1.8481E-01  1.5907E-01  1.3019E-01  9.8251E-02  6.3310E-02  4.1831E-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 GRCUP   12 TO GROUP    13
  1.8007E-02 -2.6244E-02 -6.5862E-02 -1.0094E-01 -1.3158E-01 -1.5787E-01
 -1.7990E-01 -1.9776E-01 -2.1153E-01 -2.2131E-01 -2.2719E-01 -2.2923E-01
 -2.2753E-01 -2.2217E-01 -2.1322E-01 -2.0076E-01 -1.8487E-01 -1.6563E-01
 -1.4311E-01 -1.1737E-01 -8.8494E-02 -5.6551E-02 -2.1610E-02 -1.3129E-04
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         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
  2.2331E-02  5.8828E-02  8.4085E-02  9.9409E-02  1.0608E-01  1.0531E-01
  9.8319E-02  8.6247E-02  7.0222E-02  5.1329E-02  3.0616E-02  9.1103E-03
 -1.2205E-02 -3.2376E-02 -5.0477E-02 -6.5617E-02 -7.6927E-02 -8.3573E-02
 -8.4746E-02 -7.9666E-02 -6.7575E-02 -4.7748E-02 -1.9481E-02  6.6218E-04
  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04
  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04
  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04
  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04
  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04
  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04
  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04
  7.9485E-04  7.9485E-04  7.9485E-04  7.9485E-04
FROM GROUP   12 TO GROUP    13
 -2.1560E-02 -5.8058E-02 -8.3314E-02 -9.8639E-02 -1.0531E-01 -1.0454E-01
 -9.7548E-02 -8.5477E-02 -6.9452E-02 -5.0558E-02 -2.9845E-02 -8.3398E-03
  1.2976E-02  3.3146E-02  5.1247E-02  6.6388E-02  7.7698E-02  8.4343E-02
  8.5516E-02  8.0437E-02  6.8345E-02  4.8518E-02  2.0251E-02  1.3066E-04
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         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
  2.0397E-02  4.6736E-02  5.5371E-02  5.1107E-02  3.8133E-02  2.0051E-02
 -9.3706E-05 -1.9804E-02 -3.7097E-02 -5.0493E-02 -5.8985E-02 -6.2022E-02
 -5.9495E-02 -5.1713E-02 -3.9386E-02 -2.3605E-02 -5.8383E-03  1.2104E-02
  2.8073E-02  3.9599E-02  4.3910E-02  3.7935E-02  1.8332E-02  1.2961E-04
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         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
 -2.0398E-02 -4.6737E-02 -5.5373E-02 -5.1108E-02 -3.8134E-02 -2.0052E-02
  9.2736E-05  1.9803E-02  3.7096E-02  5.0492E-02  5.8983E-02  6.2020E-02
  5.9493E-02  5.1711E-02  3.9385E-02  2.3604E-02  5.8370E-03 -1.2105E-02
 -2.8074E-02 -3.9601E-02 -4.3912E-02 -3.7937E-02 -1.8333E-02 -1.2972E-04
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         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
  1.8015E-02  3.3250E-02  2.7181E-02  1.0437E-02 -9.2209E-03 -2.6488E-02
 -3.8141E-02 -4.2691E-02 -4.0035E-02 -3.1138E-02 -1.7719E-02 -1.9804E-03
  1.3692E-02  2.6975E-02  3.5856E-02  3.8871E-02  3.5321E-02  2.5484E-02
  1.0813E-02 -5.8810E-03 -2.0256E-02 -2.6259E-02 -1.5987E-02 -1.2872E-04
 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07
 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07
 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07
 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07
 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07
 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07
 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07
 -2.5071E-07 -2.5071E-07 -2.5071E-07 -2.5071E-07
FROM GROUP   12 TO GROUP    13
 -1.8015E-02 -3.3250E-02 -2.7182E-02 -1.0438E-02  9.2206E-03  2.6488E-02
  3.8141E-02  4.2691E-02  4.0035E-02  3.1137E-02  1.7719E-02  1.9802E-03
 -1.3692E-02 -2.6975E-02 -3.5856E-02 -3.8872E-02 -3.5321E-02 -2.5485E-02
 -1.0813E-02  5.8808E-03  2.0256E-02  2.6259E-02  1.5987E-02  1.2847E-04
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         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
  1.5329E-02  2.0021E-02  4.4840E-03 -1.4239E-02 -2.6976E-02 -3.0232E-02
 -2.4354E-02 -1.1998E-02  3.1234E-03  1.7222E-02  2.7149E-02  3.0877E-02
  2.7769E-02  1.8614E-02  5.4863E-03 -8.5982E-03 -2.0172E-02 -2.6006E-02
 -2.3915E-02 -1.3722E-02  1.6574E-03  1.4978E-02  1.3366E-02  1.2693E-04
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         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
 -1.5329E-02 -2.0021E-02 -4.4840E-03  1.4239E-02  2.6976E-02  3.0232E-02
  2.4354E-02  1.1998E-02 -3.1235E-03 -1.7222E-02 -2.7149E-02 -3.0877E-02
 -2.7769E-02 -1.8614E-02 -5.4864E-03  8.5979E-03  2.0172E-02  2.6006E-02
  2.3915E-02  1.3722E-02 -1.6574E-03 -1.4978E-02 -1.3366E-02 -1.2692E-04
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0         0.0         0.0
  0.0         0.0         0.0         0.0
```

```
*'DATAMAIN' STELLT FUER EINE FORTRAN-SUBROUTINE 'MAIN' SPEICHERFELDER,
*DEREN LAENGEN IM EXEC-PARM-FELD ANGEGEBEN SIND,BEREIT UND GIBT SIE
*ALS ARGUMENTE AN 'MAIN' NACH FOLGENDEM SCHEMA WEITER.
* // EXEC FHG,PARM.G=(X,Y),REGION.G=RK X,Y SIND 2 FELDLAENGEN
*AUSFUEHRUNG VON 'DATAMAIN' LIEFERT ANFANGSADRESSEN DER ZWEI FELDER IN
*DER TASK-REGION.
* N > 0  GIBT ANZAHL DER FELDER AN (NORMALFALL)
*DURCH 'SUBROUTINE MAIN(N,X,JX,Y,JY)'KOENNEN DIE 2 FELDER IN'MAIN'SO-
*WOHL ALS FESTKOMMA-ALS AUCH ALS GLEITKOMMA-FELDER BENUTZT WERDEN.
*UNTER X(1)=JX(1) BZW. Y(1)=JY(1) KOENNEN DIE LAENGEN XX,YY IN 'MAIN'
*ABGEHOLT WERDEN.
* N = 0  IST FEHLERFALL.HINWEIS AUF FEHLERART UNTER JX(1)-JX(35).
*MAXIMALLAENGE DES PARM-FELDES IST 40 EBCDIC-ZEICHEN.
DATAMAIN  START 0              ANFANG VON 'DATAMAIN'
          EXTRN MAIN
          BC    15,12(0,15)    SPRUNG UM KONSTANTEN
          DC    C'DATAMAIN'    PROG.NAME
          STM   14,12,12(13)   RETTEN DER REGISTER 14,15,0-12
          BALR  10,0           LADE BASIS-REG.10
          USING *,10
          ST    13,AREA+4      SYSTEM SA-ADR. NACH PROG.SA
          LA    4,AREA         PROG.SA-ADRESSE
          ST    4,8(0,13)                    NACH SYSTEM-SA
BEGINN    L     4,0(0,1)       /4/=ADR.DES PARM-FELDS
          LH    3,0(0,4)       /3/=PARM-FELD-LAENGE
          LH    2,=X'0001'     /2/=INKREMENT=1
          AR    4,2            /4/=/4/+1
          AR    3,4            /3/=COMPARAND=ENDADR.DES PARM-FELDES
          LH    5,=X'0000'     /5/=I=PARAMETERZAEHLER=0
PARMLOOP  LR    1,4            /1/=ANFANG DES NEUEN PARAMETERS-1
CHARLOOP  BXH   4,2,LOOPEND    /4/=/4/+1,IF(/4/-/3/)*+1,*+1,LOOPEND
          CLI   0(4),X'6B'     VERGLEICH AUF KOMMA
          BNE   CHARLOOP
CVBLOOP   LR    7,4            /7/=ANZAHL DER
          SR    7,1                    EBCDIC-ZEICHEN
          LPR   7,7
          SH    7,=X'0002'                          -1 OHNE ,
          BL    NOPARM
          LH    6,=X'0005'
          SR    6,7
          BL    ERREXIT
          AH    7,=X'0070'       /7/=7*16+/7/=PACK-LAENGEN
          STC   7,PACK+1         PACK-MODIFIKATION
          BL    PARMLOOP         IF(/7/)PARMLOOP,PACK,PACK
PACK      PACK  X,1(8,1)         /X/=UNSIGNIERTE DEZIMALLAENGE
          NI    X+7,X'FE'        /X/=+/X/
          CVB   6,X              DEZIMAL-BINAER-WANDLUNG
          LTR   6,6
          BNH   NOPARM
          ST    6,LNG(5)         LNG(I)=/6/=BINAERLAENGE
          AH    5,=X'0004'
          SR    4,2
          BXH   4,2,GTMN              KVT02901  P
          B     PARMLOOP         GOTO PARMLOOP
LOOPEND   LR    6,5             /6/=/5/ AND GO TO CVBLOOP
          B     CVBLOOP
GTMN      MVI   AREAS,X'00'      LOESCHEN DES
          MVC   AREAS+1(83),AREAS          AREAS-FELDES
          SH    5,=X'0004'       LETZTER PARAMETER
          IC    6,=X'80'                          FUER
          STC   6,LNG(5)                             GETMAIN
          LA    13,AREA                  ZUORDNUNG DER
          GETMAIN LC,LA=LNG,A=AREAS+4                    FELDER IN SPO
          LTR   6,15             IF(/15/)GTMNCOND,*+2,GTMNCOND
          BNE   GTMNCOND         /15/=0 ODER 4,   COND-CODE NACH GETMAIN
          IC    6,=X'00'
          STC   6,LNG(5)
          AH    5,=X'0004'
          LR    8,5              /8/=K=I
          LR    6,5              /6/=J=I
          AR    5,5              /5/=I=I+I
EPLOOP    SH    6,=X'0004'       J=J-1
          BL    EPILOG           IF(J)EPILOG,*+1,*+1
          SH    5,=X'0004'       I-1
          L     7,AREAS+4(6)     /7/=/AREAS(J+1)/
          ST    7,AREAS+4(5)     AREAS(I)=AREAS(J+1)
          SH    5,=X'0004'       I=I-1
          ST    7,AREAS+4(5)     AREAS(I)=AREAS(J+1)=AREAS(I+1)
          L     9,LNG(6)         /9/=LNG(J)
          ST    9,0(7)           //7//=/9/,/1.WORT DES FELDES/=FELDLAENGE
          B     EPLOOP
EPILOG    SRA   8,2(0)           N=K=/8/*4**-1
          ST    8,N
          LA    8,N
          ST    8,AREAS
RUFIBCOM  L     13,AREA+4        /13/=PROG.SA-ADR
          L     15,=V(IBCOM#)    AUFRUF IBCOM
          BAL    14,64(15)                (OPEN)
RUFMAIN   LA    13,AREA          /13/=PROG.SA-ADR
          LA    1,AREAS          /1/=ARG.LIST-ADR
          L     15,MAINAD        AUFRUF
          BALR  14,15                    MAIN
          CNOP  0,4
RETURNOS  L     13,AREA+4
STOP      L     15,=V(IBCOM#)
          BAL   14,52(15)
          DC    X'0540404040F00000'
GTMNCOND  LA    6,MSG3
          B     ERREX
NOPARM    LA    6,MSG2
          B     ERREX
ERREXIT   LA    6,MSG1
ERREX     ST    6,AREAS+4
          ST    6,AREAS+8
          B     CONDEXIT
CONDEXIT  LH    8,=X'0000'
          B     EPILOG
MAINAD    DC    A(MAIN)
MSG1      DC    C' FELDLAENGE HAT MEHR ALS 6 ZIFFERN. '
MSG2      DC    C' EXEC-PARM-FEHLER,Z.B.NICHT>0.      '
MSG3      DC    C' TASK-REGION IST ZU KLEIN.          '
X         DS    1D
N         DS    1F
AREA      DS    18F
LNG       DS    20F
AREAS     DS    41F
          END   DATAMAIN
```

VL 1

```
      SUBROUTINE FSPIE                                                  10
C   FSPIE IS A SPECIAL ERROR-DETECTING SUBRCUTINE ,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
```

```
C     PROGRAMM ZUR STEUERUNG DES MIGROS-SYSTEMS                         10
C                                                                       20
      SUBROUTINE MAIN (N,XL,NXL)                                        30
      REAL*8 MAT1,N1,N2                                                 40
      DIMENSION XL(1),NXL(1)                                            50
      COMMON MAT1,K(2),NOUT,LIZ                                         60
      DATA N1/'BLOC '/,N2/'ENDE '/,SGC/'SGC '/                          70
      NINP=5                                                            80
      NOUT=6                                                            90
      KDE=1                                                            100
      LIZ=3                                                            110
      NF=8                                                             120
      IF(N.NE.0)  GO TO 18                                             130
      WRITE (NOUT,19) (XL(I),I=1,9)                                    140
   19 FORMAT(1H ,9A4)                                                  150
      STOP                                                             160
   18 CALL FSPIE                                                       170
      IADR=NXL(1)/4                                                    180
      CALL EING(NOUT)                                                  190
      CALL FREEFO (NINP,NF,NOUT,XL,XL,XL)                              200
      CALL NDFOPN (KDE,NXL,NUDAT,0)                                    210
      WRITE (NOUT,1) NUDAT                                             220
    1 FORMAT (1H1/' STAND DER KERNDATENBIBLIOTHEK VOM',I10)            230
      IZI=0                                                            240
    2 READ (NF)                                                        250
   16 READ (NF) MAT1,MAT2                                              260
      IZI=IZI+2                                                        270
      IF(MAT1.EQ.N1.AND.MAT2.LT.2) GO TO 2                             280
      IF(MAT1.EQ.N1.AND.MAT2.EQ.2) GO TO 3                             290
      NE=26                                                            300
      GO TO 4                                                          310
    3 READ (NF) NE                                                     320
      READ (NF) MAT1,MAT2                                              330
      IZI=IZI+2                                                        340
    4 IF(MAT1.EQ.N1.AND.MAT2.EQ.3) GO TO 5                             350
      NFE=1                                                            360
      LSPEC=1                                                          370
      GO TO 6                                                          380
    5 READ (NF) LSPEC,NFE                                              390
      READ (NF) MAT1,MAT2                                              400
      IZI=IZI+2                                                        410
    6 IF(MAT1.EQ.N1.AND.MAT2.NE.4) GO TO 7                             420
      READ (NF) NA                                                     430
      READ (NF) MAT1,MAT2                                              440
      IZI=IZI+2                                                        450
      GO TO 9                                                          460
    7 WRITE (NOUT,8)                                                   470
    8 FORMAT(1HO/' ***ERROR 0. 1 : THE INPUT OF THE MODULE NUMBERS WAS N 480
     1OT FOUND')                                                       490
      STOP                                                             500
    9 IF(MAT1.EQ.N1.AND.MAT2.EQ.5)  GO TO 10                           510
      NT=3                                                             520
      GO TO 11                                                         530
   10 READ (NF) NT                                                     540
      READ (NF) MAT1,MAT2                                              550
      IZI=IZI+2                                                        560
   11 IF(MAT1.EQ.N1.AND.MAT2.EQ.6) GO TO 12                            570
      MI=7                                                             580
      GO TO 13                                                         590
   12 READ (NF) MI                                                     600
      READ (NF) MAT1,MAT2                                              610
      IZI=IZI+2                                                        620
   13 IF(MAT1.EQ.N1.AND.MAT2.EQ.7) GO TO 14                            630
      NTYP=7                                                           640
      GO TO 15                                                         650
   14 READ (NF) NTYP,(XL(I),XL(I+200),I=1,NTYP)                        660
   24 READ (NF) MAT1,MAT2                                              670
      IZI=IZI+2                                                        680
      DO 26 I=1,NTYP                                                   690
      IF(XL(I).EQ.SGC)  NTYP=NTYP+1                                    700
   26 CONTINUE                                                         710
   15 IF(MAT1.EQ.N1.AND.MAT2.LT.12)  GO TO 22                          720
      IF(MAT1.EQ.N1.AND.MAT2.GT.12)  GO TO 23                          730
      IF(MAT1.EQ.N2)  GO TO 23                                         740
      READ (NF) NMAT                                                   750
      IZI=IZI+1                                                        760
      GO TO 25                                                         770
   22 READ (NF)                                                        780
      READ(NF) MAT1,MAT2                                               790
      IZI=IZI+2                                                        800
      GO TO 15                                                         810
   23 NMAT=1                                                           820
   25 DO 17 I=1,IZI                                                    830
   17 BACKSPACE NF                                                     840
      NM  =NTYP*2+1                                                    850
      NZ=NM+NMAT*2                                                     860
      NENG=NZ+NMAT                                                     870
      NSPEC=NENG+NE                                                    880
      NARB=NSPEC+NFE*(LSPEC+1)                                         890
      NTEMP=NARB+NA*3                                                  900
      NSI=NTEMP+NT                                                     910
      NG=NSI+MI+1                                                      920
      NN1=NG+NA                                                        930
      NN2=NN1+NA*NE                                                    940
      NFG=NN2+NA*NE                                                    950
      NFI=NFG+NA*NE                                                    960
      NGG=NFI+NA*NE                                                    970
      NII=NGG+NE                                                       980
      NFR=NII+NE                                                       990
```

```
      I=NFR/2*2                                                          1000
      IF(I.EQ.NFR)  NFR=NFR+1                                            1010
      IF(NFR.LT.IADR)  GO TO 20                                          1020
      WRITE (NOUT,21)                                                    1030
   21 FORMAT(1HO/' ***ERROR 0. 2 : THE PARM.G - FIELD IS ALREADY TOO SHO 1040
     1RT FOR THE CONTROL MODULE')                                        1050
      STOP                                                               1060
   20 NX=NE+1                                                            1070
      CALL INPUT (XL(1),XL(NM),XL(NZ),                                   1080
     1                  XL(NENG),XL(NSPEC),XL(NARB),XL(NTEMP),XL(NSI),  1090
     1XL(NG),XL(NN1),XL(NN2),XL(NFG),XL(NFI),XL(NGG),XL(NII),            1100
     3NMAT,MI,NE,LSPEC+1,NFE,NA,NT,NTYP,NFR,XL,NF,NX,IADR)               1110
      IZI=0                                                              1120
      READ (NF) MAT1                                                     1130
      IF(MAT1.NE.N2)  GO TO 16                                           1140
      I=0                                                                1150
      WRITE (LIZ) I,N2                                                   1160
      RETURN                                                             1170
      END                                                                1180
```

```
C     EINGABEBESCHREIBUNG FUER DAS PROGRAMMSYSTEM MIGROS                10
C                                                                       20
      SUBROUTINE EING(NOUT)                                             30
      WRITE (NOUT,1)                                                    40
    1 FORMAT(1H1/' EINGABEBESCHREIBUNG FUER DAS PROGRAMMSYSTEM MIGROS'//  50
     1' ************************************************'////          60
     2' EINLEITUNG'                                                //    70
     3' DAS PROGRAMMSYSTEM MIGROS ERLAUBT DIE BERECHNUNG VON MIKROS-'  /  80
     4' KOPISCHEN GRUPPENKONSTANTEN VON KERNDATEN. ALS KERNDATEN-'     /  90
     5' BIBLIOTHEK WIRD KEDAK BENOETIGT. DAS PROGRAMMSYSTEM ENTHAELT'  /  100
     6' FOLGENDE PROGRAMME :'                                          //  110
     7' KENNZIFFER   ARBEITSPROGRAMM'                                  //  120
     8'      1       PROGRAMM ZUR BERECHNUNG VON RESONANZSELBSTAB-'    /  130
     9'              SCHIRMFAKTOREN VON AUFGELOESTEN RESONANZPARAME-'  /  140
     A'              TERN (12400)'                                     /  150
     B'      2       PROGRAMM ZUR BERECHNUNG VON RESONANZSELBSTAB- '   /  160
     C'              SCHIRMFAKTOREN VON STATISTISCHEN RESONANZ-'       /  170
     D'              PARAMETERN (01787)'                               /  180
     E'      3       PROGRAMM ZUR BERECHNUNG VON RESONANZSELBSTAB-'    /  190
     F'              SCHIRMFAKTOREN VON PUNKTWEISE GEGEBENEN WIRKUNGS-'/  200
     G'              QUERSCHNITTEN (01700)')                           210
      WRITE (NOUT,14)                                                   220
   14 FORMAT(                                                           230
     1'      4       PROGRAMM ZUR BERECHNUNG VON GRUPPENWIRKUNGSQUER-' /  240
     2'              SCHNITTEN BEI UNENDLICHER VERDUENNUNG (01797)'    /  250
     3'      5       PROGRAMM ZUR BERECHNUNG INELASTISCHER STREU-'     /  260
     4'              MATRIZEN (26640)'                                 /  270
     5'      6       PROGRAMM ZUR BERECHNUNG ELASTISCHER STREUMATRIZEN'/  280
     6'              (23871)'                                          /  290
     7       7       PROGRAMM ZUR BERECHNUNG DES SPALTSPEKTRUMS'       /  300
     8'              (01780)'                                          /  310
     9'      8       PROGRAMM ZUR BERECHNUNG DES 1/V- GRUPPENMITTEL-'  /  320
     A'              WERTES (10242)'                                   /  330
     B'      9       PROGRAMM ZUR BERECHNUNG DER ELASTISCHEN STREU-'   /  340
     C'              MATRIZEN FUER DIE REMO- KORREKTUR'                /  350
     D'     10       PROGRAMM ZUR BERECHNUNG DER THERMISCHEN'          /  360
     E'              QUERSCHNITTE (01722)'                            //  370
     F' DIE NACHFOLGENDE EINGABE IST JEWEILS FUER EIN MATERIAL ZU'     /  380
     G' ERSTELLEN. SOLLEN GRUPPENKONSTANTEN FUER MEHRERE MATERIALIEN'  /  390
     H' IN EINEM LAUF BERECHNET WERDEN, SO IST DIESE EINGABE'          /  400
     G' ENTSPRECHEND OFT ZU WIEDERHOLEN')                                410
      WRITE(NOUT,30)                                                    420
   30 FORMAT(1H ,                                                       430
     1'DIE EINGABE IST DEN FREEFO - KONVENTIONEN ENTSPRECHEND'         /  440
     2' FORMATFREI ZU ERSTELLEN')                                       450
      WRITE (NOUT,13)                                                   460
   13 FORMAT(1H1/1HO/1HO/                                               470
     2' 1. KARTE'                                                      /  480
     3'    MAT        MATERIALNAME IN KEDAK - NOMENKLATUR'            /  490
     4'    ISTRUK  0: DAS MATERIAL WIRD ALS STRUKTURMATERIAL BEHANDELT'/  500
     5'            1: DAS MATERIAL WIRD ALS SCHWERES ISOTOP BEHANDELT'//  510
     6' FALLS DIE INFORMATION DARUEBER, OB ES SICH UM EIN NICHT SPALT-'/  520
     7' BARES ODER UM EIN SPALTBARES MATERIAL HANDELT NICHT DEM'       /  530
     8' LETZTEN ZEICHEN DES MATERIALNAMENS ENTNOMMEN WERDEN SOLL'      /  540
     9' - WOBEI EINE GERADE ZIFFER ALS LETZTES ZEICHEN EIN NICHT'      /  550
     A' SPALTBARES MATERIAL UND EINE UNGERADE ZIFFER ALS LETZTES'      /  560
     B' ZEICHEN EIN SPALTBARES MATERIAL BEZEICHNET - FOLGEN DIE BEIDEN'/  570
     C' NAECHSTEN KARTEN :'/)                                           580
      WRITE (NOUT,2)                                                    590
    2 FORMAT(' 2. KARTE'/                                               600
     1'    @BLOC@  1   KONSTANTE'                                      /  610
     2' 3. KARTE'                                                      /  620
     4'    ISPA  0: DAS MATERIAL IST NICHT SPALTBAR'                   /  630
     5'          1: DAS MATERIAL IST SPALTBAR'                        //  640
     6' FALLS DIE ENERGIEGRUPPENGRENZEN NICHT DIE DES 26-GRUPPEN'      /  650
     7' ABN-SATZES SEIN SOLLEN, FOLGEN DIE BEIDEN NAECHSTEN KARTEN :' //  660
     8' 4. KARTE'                                                      /  670
     9'    @BLOC@  2   KONSTANTE'                                      /  680
     A' 5. KARTE'                                                      /  690
     B'    NE              ANZAHL DER ENERGIEGRUPPENGRENZEN'          /  700
     C'    (ENG(I),I=1,NE)  ENERGIEGRUPPENGRENZEN IN EV IN AUFSTEIGEN-'/  710
     D'                     DER REIHENFOLGE GEORDNET'                  /  720
     E'    DAS PROGRAMMSYSTEM MIGROS KANN EINE BELIEBIGE ANZAHL VON   '/  730
     F'    ENERGIEGRUPPEN BEHANDELN'/)                                 740
      WRITE (NOUT,3)                                                    750
    3 FORMAT(                                                           760
     1' FALLS EIN PUNKTWEISE VORGEGEBENES STOSSDICHTESPEKTRUM VERWEN-' /  770
     2' DET WERDEN SOLL, FOLGEN DIE BEIDEN NAECHSTEN KARTEN :'        //  780
     3' 6. KARTE'                                                      /  790
     4'    @BLOC@  3   KONSTANTE'                                      /  800
     5' 7. KARTE'                                                      /  810
     6'    NSPEC                    ANZAHL DER SPEKTREN'             /  820
     6'    NFE                      ANZAHL DER SPEKTRUMSSTUETZPUNKTE'/  830
     7'    (EF(I),I=1,NFE),((F(I,J),I=1,NFE),J=1,NSPEC)'               /  840
     8'    EF : ENERGIESTUETZPUNKTE DER STOSSDICHTESPEKTREN IN EV'     /  850
     8'    F  : ZUGEHOERIGE WERTE DER STOSSDICHTESPEKTREN'             /  860
     A'    IST DIE ZAHL DER EINGELESENEN SPEKTREN GROESSER 1, SO'      /  870
     B'    WERDEN DIE SPEKTREN 2, 3, ... NUR IM ARBEITSPROGRAMM NR. 6' /  880
```

```
     C'     INTERPRETIERT UND BEDEUTEN DORT DIE MAKROSKOPISCHE WICH-'    /  890
     D'     TUNGSFUNKTION FUER DAS 1., 2.,...MOMENT DER ELASTISCHEN'     /  900
     E'     STREUMATRIX. ES IST DARAUF ZU ACHTEN, DASS DIE ZAHL DER'     /  910
     F'     SPEKTREN MIT DER ZAHL DER ZU BERECHNENDEN MOMENTE UEBEREIN-'/  920
     G'     STIMMT. WIRD NUR EIN SPEKTRUM ANGEGEBEN, SO WIRD DIESES'     /  930
     H'     FUER ALLE MOMENTE DER ELASTISCHEN STREUMATRIX VERWENDET.')       940
      WRITE(NOUT,31)                                                        950
   31 FORMAT(                                                               960
     1'     DIE ANZAHL DER STUETZPUNKTE IST BELIEBIG, ES IST JEDOCH ZU' /  970
     2'     BEACHTEN, DASS DIE SPEKTREN DEN GESAMTEN BETRACHTETEN'       /  980
     3'     ENERGIEBEREICH UEBERSTREICHEN SOLLTEN. WENN DIE KARTEN 6' /  990
     4'     UND 7 NICHT ANGEGEBEN WERDEN, BERECHNET MIGROS DIE SPEK-'  / 1000
     5'     TRUMSWERTE F(I,1) MITTELS DER FUNKTION PHI(E) UND DIE'       / 1010
     6'     SPEKTRUMSWERTE (F(I,L),L=2,NLE+1) MITTELS DER FUNKTION'      / 1020
     7'     PHI1(L,E). NLE SIEHE KARTE 23. STANDARDFUNKTIONEN SIND :'/)      1030
      WRITE(NOUT,43)                                                        1040
   43 FORMAT(1H1/1HO/1HO/                                                   1050
     E'     FUNCTION PHI(E)        FUNCTION PHI1(L,E)'                   / 1060
     F'     PHI=1./E               PHI1=1./E**L'                         / 1070
     1'     RETURN                 RETURN'                               / 1080
     2'     END                    END'                                  / 1090
     3'     VERGL. AUCH DIE KARTE 27 : MAZ(1)'/)                             1100
      WRITE(NOUT,4)                                                         1110
    4 FORMAT(                                                               1120
     1' 8. KARTE'                                                         / 1130
     2'     @BLOC@  4   KONSTANTE'                                        / 1140
     3' 9. KARTE'                                                         / 1150
     4'     NA   ANZAHL DER ANZULAUFENDEN ARBEITSPROGRAMME'               / 1160
     5'     ((NR(I,J),I=1,3),J=1,NA)'                                     / 1170
     6'          HIERBEI BEDEUTET:'                                       / 1180
     7'          NR(1,J)  KENNZIFFER DER ARBEITSPROGRAMME'                / 1190
     8'          NR(2,J)  NUMMER DER ENERGIEGRUPPE, AB DER DAS'           / 1200
     9'                   PROGRAMM NR(1,J) RECHNEN SOLL'                  / 1210
     A'          NR(3,J)  NUMMER DER ENERGIEGRUPPE, BIS ZU DER'           / 1220
     B'                   EINSCHLIESSLICH DAS PROGRAMM NR(1,J)'           / 1230
     C'                   RECHNEN SOLL. DIESE GRUPPENNUMMERN WERDEN'      / 1240
     D'                   IM ENERGETISCH AUFSTEIGENDEN SINNE ANGEGEBEN.'/ 1250
     E'                   NR(2,J).GE.NR(3,J)  DIE NUMERIERUNG DER'        / 1260
     F'                   ENERGIEGRUPPEN ERFOLGT MIT FALLENDER ENERGIE,'/ 1270
     G'                   D.H. DIE ENERGIEGRUPPE, DIE ZU DEN HOECHSTEN' / 1280
     H'                   ENERGIEGRENZEN IN @BLOC @  2  GEHOERT,'       / 1290
     I'                   ERHAELT DIE NUMMER 1.'/)                        1300
      WRITE (NOUT,15)                                                       1310
   15 FORMAT(                                                               1320
     1' KOMMENTAR :'                                                      / 1330
     2' EIN ARBEITSPROGRAMM KANN MEHRFACH AUFGERUFEN WERDEN. DIES IST' / 1340
     3' NOTWENDIG, FALLS MEHRERE NICHT ZUSAMMENHAENGENDE BEREICHE VON' / 1350
     4' ENERGIEGRUPPEN VORGEGEBEN SIND. FUER JEDEN ZUSAMMENHAENGENDEN' / 1360
     5' BEREICH VON ENERGIEGRUPPEN HAT EIN AUFRUF EINES ARBEITSPRO-'   / 1370
     6' GRAMMS ZU ERFOLGEN.'                                           / 1380
     7' NR(2,J), NR(3,J) BEDEUTEN DIE NUMMERN DER AUSSTREUGRUPPEN IM'  / 1390
     8' FALLE VON STREUMATRIZEN. GERECHNET WERDEN ALLE EINSTREUGRUPPEN') 1400
      WRITE(NOUT,5)                                                         1410
    5 FORMAT(                                                               1420
     1' WENN DIE PROGRAMME ZUR BERECHNUNG VON SELBSTABSCHIRMFAKTOREN'  / 1430
     2' AUS RESONANZ- BZW STATISTISCHEN DATEN ANGELAUFEN WERDEN       '/ 1440
     2' (PROGRAMMKENNZIFFER 1 UND 2) UND IM'                           / 1450
     3' FALLE EINES SCHWEREN ISOTOPS (ISTRUK=1) NICHT MIT DEN 3 STAN-' / 1460
     4' DARDTEMPERATUREN 300, 900 UND 2100 GRAD KELVIN UND IM FALLE'   / 1470
     5' EINES STRUKTURMATERIALS (ISTRUK=0) NICHT MIT DER STANDARDTEM-' / 1480
     6' PERATUR 0 GRAD KELVIN GERECHNET WERDEN SOLL, FOLGEN DIE BEIDEN'/ 1490
     7' KARTEN :'                                                     // 1500
     8' 10. KARTE'                                                     / 1510
     9'     @BLOC@ 5   KONSTANTE'                                      / 1520
     A' 11. KARTE'                                                     / 1530
     B'     NT                ANZAHL DER TEMPERATUREN'                 / 1540
     C'     (TEMP(I),I=1,NT)  TEMPERATUREN IN GRAD KELVIN'             / 1550
     D'                       DIE ANZAHL DER TEMPERATUREN IST BELIEBIG') 1560
      WRITE (NOUT,6)                                                    1570
    6 FORMAT(1HO,                                                       1580
     1' WENN EINES DER PROGRAMME ZUR BERECHNUNG VON SELBSTABSCHIRMFAK-'/ 1590
     2' TOREN ANGELAUFEN WIRD (PROGRAMMKENNZIFFER 1 UND 2 UND 3)'      / 1600
     2' UND NICHT MIT DEN 7 STANDARD'                                  / 1610
     3' VERDUENNUNGSGRADEN DES ABN-SATZES ALSO 0, 10, 10**2, 10**3,'   / 1620
     4' 10**4, 10**5, 10**6 GERECHNET WERDEN SOLL, FOLGEN DIE KARTEN:'// 1630
     5' 12. KARTE'                                                     / 1640
     6'     @BLOC@ 6   KONSTANTE'/)                                       1650
      WRITE (NOUT,7)                                                    1660
    7 FORMAT(1H1/1HO/1HO/                                               1670
     7' 13. KARTE'                                                     / 1680
     8'     MI                ANZAHL DER VERDUENNUNGSGRADE'           / 1690
     9'     (SIGO(I),I=1,MI)  VERDUENNUNGSGRADE'                      / 1700
     A'     DIE ANZAHL DER VERDUENNUNGSGRADE IST BELIEBIG'           // 1710
     1' WENN DAS PROGRAMM ZUR BERECHNUNG VON GRUPPENWIRKUNGSQUER-'     / 1720
     2' SCHNITTEN BEI UNENDLICHER VERDUENNUNG ANGELAUFEN WIRD'         / 1730
     2' (PROGRAMMKENNZIFFER 4 UND 10) UND'                             / 1740
     3' NICHT DIE 7 STANDARDTYPEN MUEL,NUE,SGA,SGF,SGI,SGN UND SG2N'/    1750
     4' BERUECKSICHTIGT WERDEN SOLLEN, FOLGEN DIE NAECHSTEN BEIDEN'    / 1760
     5' KARTEN :'                                                     // 1770
     6' 14. KARTE'                                                     / 1780
     7'     @BLOC@ 7   KONSTANTE'                                      / 1790
     8' 15. KARTE'                                                     / 1800
     9'     NTYP                ANZAHL DER WIRKUNGSQUERSCHNITTSTYPEN' / 1810
     A'     (ITYP(I),I=1,NTYP)  WIRKUNGSQUERSCHNITTSTYPEN'            / 1820
     B'     DIE ANZAHL DER QUERSCHNITTSTYPEN IST BELIEBIG'/)              1830
      WRITE (NOUT,20)                                                   1840
   20 FORMAT(                                                           1850
     1' KOMMENTAR: ES KOENNEN FUER BELIEBIGE WIRKUNGSQUERSCHNITTE'     / 1860
     2' GRUPPENMITTELWERTE BERECHNET WERDEN, SOFERN DIESE AUF KEDAK'   / 1870
     3' VORHANDEN SIND. DIES SIND ZUR ZEIT: SGA, SGALP, SGF, SGG, SGI,'/ 1880
     4' SGN, SGP, SGT, SGTR, SGX, SG2N. FERNER WERDEN GEEIGNET '       / 1890
     5' DEFINIERTE GRUPPENMITTELWERTE DER GROESSEN ALPHA, ETA, MUEL,'  / 1900
     6' NUE BERECHNET,SOWIE DER WIRKUNGSQUERSCHNITT SGC = SGA - SGF'   / 1910
     6' (DEFINITION DER OBEN GENANNTEN GROESSEN SIEHE'                 / 1920
     7' KEDAK-NOTIZ NR. 17, INR-NOTIZ NR. 279/71.) FALLS DIE QUER-'    / 1930
     8' SCHNITTSTYPEN SGA UND SGF BERECHNET WERDEN, WIRD AUTOMATISCH'  / 1940
     9' AUCH DER TYP SGC = SGA - SGF BERECHNET'/)                        1950
      WRITE(NOUT,8)                                                     1960
    8 FORMAT(                                                           1970
     1' WENN DAS PROGRAMM ZUR BERECHNUNG DER SELBSTABSCHIRMFAKTOREN'   / 1980
     2' AUS RESONANZDATEN ANGELAUFEN WIRD (PROGRAMMKENNZIFFER 1) UND ' / 1990
     2' DIE ANZAHL DER PRO ENERGIESTUETZSTELLE MITZUNEHMENDEN RESONAN-'/ 2000
```

```
 3' ZEN NICHT 10 BEIDSEITS DER STUETZSTELLE SEIN SOLL, FOLGEN DIE' / 2010
 4' BEIDEN NAECHSTEN KARTEN :'                                    // 2020
 6' 16. KARTE'                                                     / 2030
 7'     @BLOC@ 8   KONSTANTE'                                      / 2040
 8' 17. KARTE'                                                     / 2050
 9'     NRES  ANZAHL DER RESONANZEN'                               // 2060
 A' WENN DAS PROGRAMM ZUR BERECHNUNG VON SELBSTABSCHIRMFAKTOREN'  / 2070
 B' AUS RESONANZDATEN ANGELAUFEN WIRD (PROGRAMMKENNZIFFER 1) '    / 2080
 C' UND DER ZULAESSIGE INTEGRATIONSFEHLER NICHT 0.05 SEIN SOLL,'  / 2090
 D' FOLGEN DIE BEIDEN KARTEN :'                                   // 2100
 D' 18. KARTE'                                                     / 2110
 E'     @BLOC@ 9   KONSTANTE'                                      / 2120
 F' 19. KARTE'                                                     / 2130
 G'     ERROR  ZULAESSIGER INTEGRATIONSFEHLER'/)                    2140
  WRITE (NOUT,9)                                                   2150
 9 FORMAT(                                                         2160
 1' WENN DAS PROGRAMM ZUR BERECHNUNG INELASTISCHER STREUMATRIZEN'  / 2170
 2' ANGELAUFEN WIRD (PROGRAMMKENNZIFFER 5) UND DER PARAMETER XNUE' / 2180
 3' FUER DAS WEISSKOPF''SCHE VERDAMPFUNGSMODELL NICHT 0.16 SEIN '  / 2190
 4' SOLL (KERNTEMPERATUR THETA(E)=SQRT(E/(XNUE*A)), WOBEI A DAS '  / 2200
 5' ATOMGEWICHT IST UND E IN MEV ANGENOMMEN WIRD), FOLGEN DIE'     / 2210
 6' BEIDEN NAECHSTEN KARTEN :'/1H1/1HO/1HO/                        2220
 7' 20. KARTE'                                                     / 2230
 8'     @BLOC@ 10   KONSTANTE'                                     / 2240
 9' 21. KARTE'                                                     / 2250
 A'     XNUE  PARAMETER FUER DAS WEISSKOPF''SCHE'                  / 2260
 B'           VERDAMPFUNGSMODELL'                                 // 2270
 C' WENN DAS PROGRAMM ZUR BERECHNUNG DER ELASTISCHEN STREUMATRIZEN'/ 2280
 D' ANGELAUFEN WIRD (PROGRAMMKENNZIFFER 6) UND NICHT MIT DER'      / 2290
 E' FOLGENDEN STANDARDEINGABE GERECHNET WERDEN SOLL:'              / 2300
 F' ISEL = 2  WENN ISTRUK=0'                                       / 2310
 G' ISEL = 1  WENN ISTRUK=1'                                       / 2320
 H' NLA = 0'                                                       / 2330
 I' NLE = 5'                                                       / 2340
 J' WERDEN DIE FOLGENDEN KARTEN BENOETIGT :'/)                     2350
  WRITE (NOUT,10)                                                  2360
10 FORMAT(                                                        2370
 1' 22. KARTE'                                                     / 2380
 2'     @BLOC@ 11   KONSTANTE'                                     / 2390
 3' 23. KARTE'                                                     / 2400
 4'     ISEL'                                                      / 2410
 5'          |ISEL| =2: FUER LEICHTE UND MITTELSCHWERE ELEMENTE'  / 2420
 5'                     (TOT. ELAST. STREUQUERSCHNITT UNGEAENDERT)'/ 2430
 6'                =1: FUER SCHWERE ELEMENTE'                     / 2440
 6'                    (TOT. ELAST. STREUQUERSCHNITT = 1 GESETZT' / 2450
 7'          ISEL)0:   ZUSAETZLICHER PAPIERAUSDRUCK VON ZWISCHEN-'/ 2460
 5'                    INFORMATIONEN'                             / 2470
 6'     NLA   UNTERER LEGENDRE INDEX'                              / 2480
 7'           NLA GEHT UEBER IN 0 (WEGEN NORMIERUNG)'              / 2490
 8'     NLE   OBERER LEGENDRE INDEX (MAXIMAL 5)'                   / 2500
 8'           NLE GEHT UEBER IN MAX(1,NLE) (WEGEN MUEL-ANPASSUNG)'// 2510
 9' WENN DAS PROGRAMM ZUR BERECHNUNG DER ELASTISCHEN STREUMATRIZEN'/ 2520
 A' ANGELAUFEN WIRD (PROGRAMMKENNZIFFER 6) UND EINE FEINSTRUKTUR-' / 2530
 B' WICHTUNG BERUECKSICHTIGT WERDEN SOLL, FOLGEN DIE KARTEN :'    // 2540
 C' 24. KARTE')                                                    2550
  WRITE (NOUT,32)                                                  2560

32 FORMAT(                                                        2570
  D'     @BLOC@ 12'                                                / 2580
  E' 25. KARTE'                                                    / 2590
  F'     NMAT                        ANZAHL DER MATERIALIEN IN DER' / 2600
  G'                                 MISCHUNG'                     / 2610
  H'     (NAME(I),TZ(I),I=1,NMAT) NAME : MATERIALNAME'             / 2620
  I'                                TZ : TEILCHENDICHTE * 1.E-24'  // 2630
  1' WENN DAS PROGRAMM ZUR BERECHNUNG DER ELASTISCHEN STREUMATRIZEN'/ 2640
  2' ANGELAUFEN WIRD (PROGRAMMKENNZIFFER 6) UND NICHT ALLE MOMENTE' / 2650
  3' MIT DEM SPEKTRUM DES 0. MOMENTES GEWICHTET WERDEN SOLLEN,'     / 2660
  4' FOLGEN DIE KARTEN :'                                          // 2670
  5' 26. KARTE'                                                    / 2680
  6'     @BLOC@ 13'                                                / 2690
  7' 27. KARTE')                                                   2700
  WRITE (NOUT,33)                                                  2710
33 FORMAT(                                                        2720
  8'     MAZ(1)  0 : ALLE MOMENTE WERDEN MIT DEM MAKROSPEKTRUM'    / 2730
  2'                 DES 0. MOMENTES GEWICHTET'                    / 2740
  4'             1 : JEDES MOMENT HAT EIN EIGENES MAKROSPEKTRUM'   / 2750
  3'     MAZ(2)  0 : ALLE MOMENTE WERDEN MIT DEM MIKROSPEKTRUM'    / 2760
  4'                 DES 0. MOMENTES GEWICHTET'                    / 2770
  4'             1 : JEDES MOMENT HAT EIN EIGENES MIKROSPEKTRUM'   / 2780
  5'                 STANDARD : 1/SGT**(L+1) , L=0,...NLE'/)       2790
  WRITE (NOUT,41)                                                  2800
41 FORMAT(1H1/1HO/1HO/                                            2810
  1' WENN DAS PROGRAMM ZUR BERECHNUNG DER ELASTISCHEN STREUMATRIZEN'/ 2820
  2' ANGELAUFEN WIRD (PROGRAMMKENNZIFFER 6) UND DIE MAXIMALE ANZAHL'/ 2830
  3' VON GRUPPEN IN EINER MAKRO - GRUPPE NICHT 4 , DIE ANZAHL DER' / 2840
  4' GRUNDSTUETZPUNKTE IN DEM ENERGIEBEREICH EINER GRUPPE, AUS DEM' / 2850
  5' IN NACHBARGRUPPEN STREUUNG MOEGLICH IST,NICHT GLEICH 70 IST'  / 2860
  6' UND DIE ANZAHL DER GRUNDSTUETZPUNKTE IN DEM ENERGIEBEREICH'   / 2870
  7' EINER GRUPPE, AUS DEM KEINE STREUUNG IN NACHBARGRUPPEN'       / 2880
  8' MOEGLICH IST, NICHT GLEICH 16 IST, FOLGEN DIE KARTEN :'      // 2890
  9' 28. KARTE'                                                    / 2900
  A'     @BLOC@ 14   KONSTANTE'                                    / 2910
  B' 29. KARTE'                                                    / 2920
  C'     NS    MAXIMALE ANZAHL VON GRUPPEN IN EINER MAKRO - GRUPPE' / 2930
  D'     NK    ANZAHL DER GRUNDSTUETZPUNKTE IN DEM ENERGIEBEREICH' / 2940
  E'           EINER GRUPPE, AUS DEM IN NACHBARGRUPPEN STREUUNG'   / 2950
  F'           MOEGLICH IST'                                       / 2960
  G'     NR    ANZAHL DER GRUNDSTUETZPUNKTE IN DEM ENERGIEBEREICH' / 2970
  H'           EINER GRUPPE, AUS DEM KEINE STREUUNG IN NACHBARGRUP-' / 2980
  I'           PEN MOEGLICH IST'/)                                 2990
  WRITE (NOUT,42)                                                  3000
42 FORMAT(                                                        3010
  1' WENN DAS PROGRAMM ZUR BERECHNUNG DER REMO-DATEN ANGELAUFEN'   / 3020
  2' WIRD (PROGRAMMKENNZIFFER 9) UND DER ZULAESSIGE INTEGRATIONS-' / 3030
  3' FEHLER NICHT 0.05, NJM NICHT GLEICH 6 SEIN SOLL, WOBEI'       / 3040
  4' 2**NJM+1 DIE ANZAHL DER WINKELSTUETZPUNKTE FUER DIE WINKEL-'  / 3050
  5' INTEGRATION IST, UND NUJM NICHT GLEICH 10 SEIN SOLL, WOBEI'   / 3060
  6' 2**NUJM+1 DIE MAXIMAL ZULAESSIGE ANZAHL VON ENERGIESTUETZPUNK-'/ 3070
  7' TEN FUER DIE ENERGIEINTEGRATION IST, FOLGEN DIE BEIDEN'       / 3080
  8' KARTEN :'                                                    // 3090
  8' 30. KARTE'                                                    / 3100
  9'     @BLOC@ 15   KONSTANTE'                                    / 3110
  A' 31. KARTE'                                                    / 3120
```

```
  8'      ERR    ZULAESSIGER INTEGRATIONSFEHLER'                          / 3130
  C'      NJM    WOBEI 2**NJM+1 DIE ANZAHL DER WINKELSTUETZPUNKTE'        / 3140
  D'             FUER DIE WINKELINTEGRATION IST'                          / 3150
  E'      NUJM   WOBEI 2**NUJM+1 DIE MAXIMAL ZULAESSIGE ANZAHL VON'       / 3160
  F'             ENERGIESTUETZPUNKTEN FUER DIE ENERGIEINTEGRATION IST'/ 3170
  G)                                                                      3180
   WRITE (NOUT,11)                                                        3190
11 FORMAT(                                                               3200
  1' WENN DAS PROGRAMM ZUR BERECHNUNG DER REMO-DATEN ANGELAUFEN'         / 3210
  2' WIRD (PROGRAMMKENNZIFFER 9) UND NICHT MIT DER FOLGENDEN'            / 3220
  3' STANDARDEINGABE GERECHNET WERDEN SOLL :'                            / 3230
  4' ISELR = 1   WENN ISTRUK=0'                                          / 3240
  4' ISELR = 0   WENN ISTRUK=1                  '                        / 3250
  4' NLRA=0    UNTERER LEGENDRE INDEX'                                   / 3260
  5' NLRE=5    OBERER  LEGENDRE INDEX'                                   / 3270
  6' NCALL=0   ALLE ENERGIEGRUPPEN WERDEN IN ALLEN ANLAEUFEN DES'        / 3280
  7'           PROGRAMMS IN 14 UNTERGRUPPEN ZU JE 5 ENERGIESTUETZ-'      / 3290
  8'           PUNKTEN UNTERTEILT'                                       / 3300
  9' NFG=14    ANZAHL DER UNTERGRUPPEN PRO ENERGIEGRUPPE'                / 3310
  A' NFI=5     ANZAHL DER FEININTERVALLE  PRO UNTERGRUPPE'               / 3320
  B' WERDEN DIE FOLGENDEN KARTEN BENOETIGT :'                           // 3330
  1' 32. KARTE'                                                          / 3340
  2'     @BLOC@ 16   KONSTANTE'/)                                         3350
   WRITE (NOUT,12)                                                       3360
12 FORMAT(1H1/1H0/1H0/                                                   3370
  3' 33. KARTE'                                                          / 3380
  4'     ISELR=1 FUER LEICHTE UND MITTELSCHWERE ELEMENTE'                / 3390
  4'     ISELR=0 FUER SCHWERE ELEMENTE'                                  / 3400
  4'     NLRA   UNTERER LEGENDRE INDEX'                                  / 3410
  5'     NLRE   OBERER LEGENDRE INDEX'                                   / 3420
  6'     NCALL  0: ALLE ENERGIEGRUPPEN WERDEN IN ALLEN ANLAEUFEN'        / 3430
  7'               DES PROGRAMMS IN 14 UNTERGRUPPEN ZU JE 5 ENER-'       / 3440
  8'               GIESTUETZPUNKTEN UNTERTEILT'                          / 3450
  9'            >0: ANZAHL DER PROGRAMMAUFRUFE (MUSS MIT DER ZAHL '      / 3460
  9'               DER AUFRUFE DES ARBEITSPROGRAMMS 9 IN KARTE 9'        / 3470
  9'               UEBEREINSTIMMEN)'                                    // 3480
  A' WENN NCALL.GT.0 , FOLGT NCALL-MAL DIE KARTE :'                     // 3490
  B' 34. KARTE'                                                          / 3500
  C'     NGRE      ANZAHL DER BEREICHE VON ENERGIEGRUPPEN, DIE '        / 3510
  C'               JEWEILS AUF GLEICHE WEISE ZU UNTERTEILEN SIND'       / 3520
  D'     (N1(I),   NUMMER DER ERSTEN ZU UNTERTEILENDEN ENERGIEGRUPPE'/ 3530
  E'      N2(I),   NUMMER DER LETZTEN ZU UNTERTEILENDEN GRUPPE')        3540
   WRITE (NOUT,16)                                                       3550
16 FORMAT(                                                               3560
  F'      NFG(I), ANZAHL DER UNTERGRUPPEN PRO ENERGIEGRUPPE'             / 3570
  G'      NFI(I),I=1,NGRE)  ANZAHL DER ENERGIESTUETZPUNKTE PRO'          / 3580
  H'                        UNTERGRUPPE'                                // 3590
  I' DIE LETZTE KARTE LAUTET :'                                         // 3600
  1' 35. KARTE'                                                          / 3610
  2'     @ENDE@  17   KONSTANTE'                                        // 3620
  3' DIE KARTEN 1 BIS 35 SIND FUER JEDES ZU BEHANDELNDE MATERIAL'        / 3630
  4' ZU WIEDERHOLEN. DIE LETZTE EINGABEKARTE DES JOBS LAUTET :'         // 3640
  5' @ENDE@  18'////)                                                    3650
   WRITE (NOUT,21)                                                       3660
21 FORMAT(                                                               3670
  1' DAS PROGRAMMSYSTEM MIGROS BENOETIGT DD-KARTEN FUER'                 / 3680
  2' FOLGENDE EXTERNE SPEICHER'                                         // 3690
  3'  8  EINHEIT, AUF DIE FREEFO DIE ENTSCHLUESSELTE EINGABE'            / 3700
  4'     SCHREIBT'                                                       / 3710
  5'  1  EINHEIT, AUF DER DIE KERNDATENBIBLIOTHEK STEHT'                 / 3720
  6'  3  EINHEIT, AUF DIE ALLE ARBEITSPROGRAMME IHRE INTERNE'           / 3730
  7'     AUSGABE SCHREIBEN'                                              / 3740
  8' 10  ZWISCHENEINHEIT, DIE NUR VOM PROGRAMM MIT DER KENNZIFFER 6'/ 3750
  9'     BENOETIGT WIRD'                                               /// 3760
  A' AUF DER EXEC - KARTE IST DIE ANGABE DES PARM.G - PARAMETERS'        / 3770
  B' ERFORDERLICH. DIE LAENGE DES BENOETIGTEN PARM.G - FELDES IST'       / 3780
  C' VON DER EINGABE UND DEN GEWUENSCHTEN ARBEITSPROGRAMMEN'             / 3790
  D' ABHAENGIG'                                                          / 3800
  1' IM FOLGENDEN WERDEN DIE SYMBOLE DER EINGABEBESCHREIBUNG'            / 3810
  1' VERWENDET'                                                         // 3820
  1' DIE STEUERPHASE BENOETIGT'                                         // 3830
  2' 2*NTYP+3*NMAT+NFE*(NSPEC+1)+NT+MI+1+3*NE+4*NA*(1+NE) WORTE'/)       3840
   WRITE(NOUT,22)                                                        3850
22 FORMAT(1H1/1H0/1H0/                                                   3860
  2' WOBEI FUER DEN FALL, DASS EINE DIESER GROESSEN NICHT IN DER'        / 3870
  1' EINGABE GESETZT IST, DIE WERTE DER STANDARDEINGABE BENUTZT'         / 3880
  2' WERDEN, ALSO: NTYP=7 , NFE=1 , NSPEC=1 , NT=3 , MI=7 , NMAT=1'// 3890
  3' HIERZU IST DER PLATZBEDARF DES ANGELAUFENEN ARBEITSPROGRAMMS'       / 3900
  4' MIT DEM GROESSTEN PLATZBEDARF ZU ADDIEREN'                         // 3910
  5' PLATZBEDARF DER EINZELNEN ARBEITSPROGRAMME'                        // 3920
  6' KENNZIFFER PLATZBEDARF'                                            // 3930
  7'       1     7*MI+3*NE+7*MAX(300,ANZAHL DER RESONANZENERGIEN'       / 3940
  8'             AUF KEDAK)+5*MAX(400,MAXIMALE ANZAHL DER ENERGIE-'     / 3950
  8'             STUETZPUNKTE, DIE FUER DIE INTEGRATION UEBER EINE'     / 3960
  8'             ENERGIEGRUPPE BENOETIGT WIRD)  WORTE')                 3970
   WRITE (NOUT,24)                                                       3980
24 FORMAT(                                                               3990
  8'             KOMMENTAR:'                                           // 4000
  1'             DIE ANZAHL DER STUETZSTELLEN FUER DIE INTEGRATION'     / 4010
  2'             KANN VOM BENUTZER NICHT IM VORAUS BESTIMMT WERDEN.'    / 4020
  3'             FALLS DIE VORGEGEBENEN 400 SPEICHERWORTE NICHT'        / 4030
  4'             AUSREICHEN, WIRD DIE DIMENSION DES SPEICHERPLATZES'    / 4040
  5'             ERHOEHT, FALLS ES DAS PARM.G-FELD ERLAUBT. WENN DAS'/ 4050
  6'             PARM.G-FELD NICHT AUSREICHEND GROSS IST, WIRD DAS'     / 4060
  8'             ARBEITSPROGRAMM UEBERSPRUNGEN. EMPFOHLEN WIRD IN'      / 4070
  9'             DIESEM FALLE EINE VERDOPPELUNG DES FUER DIE'           / 4080
  A'             INTEGRATION VORGESEHENEN FELDES IM PARM.G-FELD'       // 4090
  A'       2     35*MI  WORTE'                                         // 4100
  B'       3     6*NE+16*MI*NE+2*MAX(1500,ANZAHL DER MUEL-WERTE AUF'    / 4110
  C'             KEDAK IM GEWUENSCHTEN ENERGIEBEREICH)+6*MAX(1500,'     / 4120
  D'             ANZAHL DER SGA-WERTE, ANZAHL DER SGN-WERTE,'           / 4130
  B'             ANZAHL DER SGF-WERTE AUF KEDAK IM GEWUENSCHTEN'        / 4140
  E'             ENERGIEBEREICH)  WORTE'                               // 4150
  F'       4     6*NE+2*MAX(1500,ANZAHL DER SGN-WERTE,ANZAHL DER'       / 4160
  G'             SGF-WERTE AUF KEDAK IM GEWUENSCHTEN ENERGIEBEREICH)'/ 4170
  H'             WORTE'/)                                               4180
   WRITE (NOUT,23)                                                       4190
23 FORMAT(                                                               4200
  1'       5     12*NE+3*(NE+1)+3*MAX(700,ANZAHL DER SGI-WERTE AUF'     / 4210
  2'             KEDAK OBERHALB DER SCHWELLE FUER INELASTISCHE'         / 4220
  3'             STREUUNG)+3*MAX(25,ANZAHL DER INELASTISCHEN ANRE-'     / 4230
  4'             GUNGSNIVEAUS)+MAX(25*400,ANZAHL DER INELASTISCHEN'     / 4240
```

```
     5'            ANREGUNGSNIVEAUS*ANZAHL DER ENERGIESTUETZPUNKTE DES'/ 4250
     6'            ANREGUNGSQUERSCHNITTES ZUM 1. NIVEAU)+MAX(400,'     / 4260
     7'            ANZAHL DER SGI-WERTE AUF KEDAK OBERHALB DER'        / 4270
     8'            SCHWELLE FUER INELASTISCHE STREUUNG)  WORTE'       // 4280
     9'       6    5*MAX(400,ISM)+7*MAX(1000,ISD)+4*(NE+1)+4*NE+'     / 4290
     A'            MAX(400*21,ISM*ICOS)+MAX(400*2,ISM*NECU)+6*MAX(2,' / 4300
     B'            NECU)*NE+2*ICOS+2*MAX(4000,NTT)  WORTE'            / 4310
     C'            DABEI BEDEUTET :'                                  / 4320
     D'            ISM  300+MAXIMALZAHL VON ENERGIESTUETZSTELLEN DER' / 4330
     E'                 SGNC AUF KEDAK IN VIER BENACHBARTEN ENERGIE-' / 4340
     G'            ISD  ISM+MAXIMALZAHL VON ENERGIESTUETZSTELLEN DER' / 4350
     H'                 SGN ODER MUEL AUF KEDAK PRO ENERGIEGRUPPE'    / 4360
     F'                 GRUPPEN'                                      / 4370
     I'            ICOS ANZAHL DER WINKELSTUETZSTELLEN DER SGNC AUF'  / 4380
     J'                 KEDAK')                                        4390
      WRITE (NOUT,25)                                                  4400
   25 FORMAT(1H1/1HO/1HO/                                              4410
     1'            NECU MAXIMALE STREUBREITE IN ENERGIEGRUPPEN (=2'    / 4420
     2'                 FUER EINFACHE UEBERSTREUUNG)'                 // 4430
     1'            NTT  ANZAHL DER SGT - STUETZPUNKTE FUER DIE GEGEBE-'/ 4440
     2'                 NE MISCHUNG IN 4 BENACHBARTEN ENERGIEGRUPPEN'  / 4450
     3'       7    NE   WORTE'                                         // 4460
     4'       8    3*NE+2*MAX(10*NE,NFE)   WORTE'                     // 4470
     5'       9    39+NM1*IMAX*(3+NUJM)+ICOS*(2+NIV)+NIV+IMAX'         / 4480
     6'            +2*NJM+3*NDAT+NE+NFIN*IZV+BUF'                      / 4490
     7'            DABEI BEDEUTET:'                                    / 4500
     8'            NM1=NLRE+1'                                         / 4510
     9'            NFIN  MAXIMALE ANZAHL DER FEININTERVALLE PRO'       / 4520
     A'                  ENERGIEGRUPPE')                               4530
      WRITE (NOUT,28)                                                  4540
   28 FORMAT(                                                          4550
     1'            IZV = MAX(4,IMAX*NM1)'                              / 4560
     8'            NDAT  MAXIMAL MOEGLICHE ANZAHL VON ENERGIESTUETZ-'  / 4570
     C'                  PUNKTEN FUER TOTALE ODER ELASTISCHE QUER-'    / 4580
     D'                  SCHNITTE IN EINER ENERGIEGRUPPE'              / 4590
     E'            NIV   ANZAHL DER ENERGIESTUETZSTELLEN DER SGNC AUF' / 4600
     F'                  KEDAK'                                        / 4610
     G'            ICOS  ANZAHL DER WINKELSTUETZSTELLEN DER SGNC AUF'  / 4620
     H'                  KEDAK'                                        / 4630
     I'            IMAX  MAXIMALE STREUBREITE IN ENERGIEGRUPPEN (=2'   / 4640
     I'                  FUER EINFACHE UEBERSTREUUNG)')                4650
      WRITE(NOUT,29)                                                   4660
   29 FORMAT(                                                          4670
     5'            BUF = MAX(NDAT,2+IMAX*NFIN)'                       // 4680
     J'       10   ES IST KEIN SPEICHERPLATZ ERFORDERLICH'            /// 4690
     K' DIE ANGABE DER REGION AUF DER JOB - KARTE SETZT SICH '          / 4700
     L' ZUSAMMEN AUS DEM PARM.G - FELD UMGERECHNET IN K - BYTES'        / 4710
     M' + 170K - BYTES FUER DAS MIGROS - PROGRAMM UND DIE PUFFER'     //// 4720
     1' EINGABEBEISPIEL'                                               // 4730
     2' //INR017MI  JOB  (0017,101,P6M1B),KRIEG,CLASS=A,TIME=10,'      / 4740
     3' // REGION=340K'                                                / 4750
     4' // EXEC PGM=MIGROS2,PARM=170000'                              / 4760
     4' //STEPLIB  DD DSN=LOAD.NUSYS,UNIT=3330,VOL=SER=NUSICE,DISP=SHR'/ 4770
     5' //FT08F001 DD UNIT=SYSDA,SPACE=(TRK,10)'                      / 4780
     5' //FT06F001 DD SYSOUT=A,DCB=(RECFM=FBA,LRECL=133,BLKSIZE=931),' / 4790
     5' // SPACE=(TRK,80,RLSE)'                                        / 4800
     6' //FT01F001 DD UNIT=2314,VOL=SER=NUSYSC,DSN=KNDF,DISP=SHR'      / 4810
     7' //FT03F001 DD UNIT=3330,VOL=SER=SCRDIC,DISP=(NEW,KEEP),'      / 4820
     8' // SPACE=(TRK,20,RLSE),DSN=GROUP.CONSTANT.OUTPUT,'            / 4830
     7' // DCB=(RECFM=VS,LRECL=32768,BLKSIZE=800)'                    / 4840
     9' //FT10F001 DD UNIT=SYSDA,SPACE=(TRK,100)')                     4850
      WRITE (NOUT,26)                                                  4860
   26 FORMAT(                                                          4870
     1' //FT05F001 DD *'                                              / 4880
     F' @U 235@  1'                                                   / 4890
     G' @BLOC@  4'                                                    / 4900
     1' 7  1 18 18  2 14 14  4 14 14  5 5 3  7 25 1  8 25 1  10 26 26'/ 4910
     3' @ENDE@  17'                                                   / 4920
     2' @D  16@  0'                                                   / 4930
     6' @BLOC@  4'                                                    / 4940
     7' 5  3 4 4  6 3 3  6 12 12  9 3 3  9 12 12'                     / 4950
     E' @ENDE@  17'                                                   / 4960
     4' @ENDE@  18'                                                  /// 4970
     5' ENDE DER EINGABEBESCHREIBUNG'                                // 4980
     6' ***************************'/1H1)                              4990
      RETURN                                                          5000
      END                                                             5010
```

```
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)                                 60
      REAL*8 N9,NV8/5HNLFIN/,VC                                        70
      LOGICAL*1 JF(8),JX(2)                                            80
      INTEGER*2 NFE(80),LV(18),JY(4),LL,JKFE,STERN/2H* /               90
      EQUIVALENCE (JZ(1),JF(1),JY(1),N8),(LL,JX(1))                   100
      DATA LV(1)/1H /,LV(2)/1HO/,LV(3)/1H1/,LV(4)/1H2/,LV(5)/1H3/,    110
     1LV(6)/1H4/,LV(7)/1H5/,LV(8)/1H6/,LV(9)/1H7/,LV(10)/1H8/,        120
     2LV(11)/1H9/,LV(12)/1H+/,LV(13)/1H+/,LV(14)/1H-/,LV(15)/1H./,    130
     3LV(16)/1HE/,LV(17)/1H@/,LV(18)/1H'/,LE/4HHEXA/,LFO/4HFORM/      140
     4,LSPE/4HSPEC/,LNO/4HNORM/                                       150
C                                                                     160
C                                                                     170
C                                                                     180
      IY=80                                                           190
      GOTO 9111                                                       200
C                                                                     210
C                                                                     220
      ENTRY FREE72 (INP,NFI,NFO,LF,F,NF)                              230
      IY=72                                                           240
C                                                                     250
C                                                                     260
 9111 V=1.                                                            270
      MV=1                                                            280
      LPP=0                                                           290
      NF(1)=0                                                         300
```

VI 7

```
      LSU=0
      LS=0
      LP=0
      NS=0
      LO=0
      N=0
      LL=LV(1)/256
      KSPNO=0
      KOUT=0
C
C
C
   33 IF(NF(1).EQ.LE) GOTO 2
      IF(NF(1).EQ.LFO) GOTO 2
      GOTO 201
  200 KOUT=1
      GOTO 12
  201 JZ(1)=NF(1)
      JZ(2)=NF(2)
      IF(N8.EQ.NV8) GOTO 200
      READ (INP,1,END=200,ERR=3) (NFE(I),I=1,80)
    1 FORMAT(80A1)
      GO TO 4
    2 IF(NFI)203,203,202
  202 ENDFILE NFI
      REWIND NFI
  203 RETURN
    3 WRITE (NFO,5)
    5 FORMAT(1HO/48H ERROR-CONDITION IN DATA TRANSFER OR INPUT-ERROR)
      STOP
    4 IF (IY.EQ.80) GOTO 6667
      JKFE=NFE(73)
      NFE(73)=STERN
 6667 WRITE (NFO,6) (NFE(I),I=1,80)
    6 FORMAT(1X,80A1)
      IF (IY.EQ.80) GOTO 6668
      NFE(73)=JKFE
C
C
C
 6668 IF(NF(1).EQ.LNO) GOTO 500
      IF(NF(1).EQ.LSPE) GOTO 501
      GOTO 502
  500 KSPNO=0
      GOTO 11
  501 KSPNO=1
      GOTO 11
  502 IF(NFE(1).EQ.LV(1)) GOTO 10
      IF(N)11,11,12
   12 IF(NFI)13,13,144
  144 IF(KSPNO)145,145,14
   14 WRITE (NFI) N,(NF(I),I=1,N)
  111 IF(KOUT)11,11,2
  145 WRITE (NFI) (NF(I),I=1,N)
      GOTO 111
   13 NS=NS+1
      LF(NS)=N
      N1=NS+1
      N2=NS+N
      N=0
      DO 15  I=N1,N2
      N=N+1
   15 LF(I)=NF(N)
      NS=N2
      GOTO 111
   11 N=0
      J=0
      GO TO 16
   10 J=1
   16 J=J+1
C
C
C
   97 DO 20  K=1,18
      IF(NFE(J).EQ.LV(K)) GO TO 21
   20 CONTINUE
      GO TO 3
C
C
C
   21 IF(K-1)30,30,22
   30 IF(LS)31,31,32
   31 IF(J-IY)16,33,33
C
C
C
   32 IF(LPP)40,40,41
   40 N=N+1
      NF(N)=LSU*MV
   47 LSU=0
      LS=0
      LO=0
      MV=1
      V=1.
      GOTO 31
C
C
C
   41 M=LP-LS
      IF(LS-9)42,43,43
   43 LSU=LSUR
   42 IF(M)44,45,46
   44 IF(78+M)3,3,45
   46 IF(75-M)3,3,45
   45 N=N+1
      VC=V
      F(N)=DFLOAT(LSU)*VC*10.**M
      LP=0
      LPP=0
      GO TO 47
C
C
```

```
C
   22 IF(K-11)50,50,23
   50 LS=LS+1
      LSU=10*LSU+K-2
      IF(LS-9)511,52,511
   52 LSUR=LSU
  511 IF(LPP)51,51,883
  883 LC=-1
      J=J+1
      IF(J-IY)884,884,32
   51 IF(J-IY)16,32,32
C
C
C
   23 IF(K-14)60,60,24
   60 IF(LO)61,61,3
   61 LO=1
      IF(K-14)62,63,63
   63 V=-1.
      MV=-1
   62 IF(J-IY)64,3,3
   64 J=J+1
      DO 65  K=2,11
      IF(NFE(J).EQ.LV(K)) GO TO 50
   65 CONTINUE
      IF(NFE(J).EQ.LV(15)) GO TO 70
      GO TO 3
C
C
C
   24 IF(K-15)70,70,25
   70 IF(LP)71,71,3
   71 LP=LS
      LPP=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
      LC=0
  884 LA=0
      LV1=1
      LP1=0
      IF(J-IY)882,882,3
C
C
C
   25 IF(K-16)80,80,26
   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)86,90,90
   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(1)
  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                                                          2550
  105 IF(NFE(J+1).EQ.LV(1)) GOTO 16                                     2560
      GO TO 3                                                           2570
      END                                                               2580
C     PROGRAMM ZUM LESEN UND PRUEFEN DER EINGABE FUER DAS MIGROS-SYSTEM   10
C                                                                         20
      SUBROUTINE INPUT (ITYP,NAME,TZ,ENG,EF,NR,TEMP,SIGC,NRE,NN1,NN2,     30
     1NFG,NFI,NG,NI,NMAT,MI,NE,NSPEC,NFE,NA,NT,NTYP,NFR,XL,NF,NX,IADR)    40
      REAL*8 MAT1,    MAT,ITYP,N2,NAME,SGC,SGA,SGF                        50
      DIMENSION ENG(NE),EF(NFE,NSPEC),NAME(NMAT),TZ(NMAT),MAZ(2),         60
     1                          NR(3,NA),TEMP(NT),SIGO(MI),ITYP(NTYP),    70
     1INZ(5),IPM(2), NRE(NA),NN1(NA,NE),NN2(NA,NE),NFG(NA,NE),NFI(NA,NE)  80
     2,XL(1),NG(NE),NI(NE)                                                90
      COMMON MAT,ISTRUK,ISPA,NOUT,LIZ,NANF,NEND,KL                       100
      EQUIVALENCE (MAT,IPM(1))                                           110
      DATA              INZ/'0','2','4','6','8'/,N2/'ENDE '/             120
     1,N3/'    '/,SGC/'SGC     '/,SGA/'SGA     '/,SGF/'SGF     '/       130
      CALL FSPIE                                                         140
      MDIM=1500                                                          150
      NER=1500                                                           160
      LDIM=1500                                                          170
      IRE=300                                                            180
      ISTE=400                                                           190
      IWE=400                                                            200
      ISG=400                                                            210
      NET=700                                                            220
      NAE=25                                                             230
      NTT=4000                                                           240
      NMAX=5                                                             250
      ICOS=21                                                            260
      ISM=400                                                            270
      ISD = 1000                                                         280
      NECU = 2                                                           290
      ISCO=ISM*ICOS                                                      300
      ISEC=ISM*NECU                                                      310
      IREMO=0                                                            320
      READ (NF) MAT,ISTRUK                                               330
      READ (NF) MAT1,MAT2                                                340
      IF(MAT2-1)1,2,3                                                    350
    2 READ (NF) ISPA                                                     360
      READ (NF) MAT1,MAT2                                                370
      GO TO 4                                                            380
    3 DO 5 I=1,5                                                         390
      IF(IPM(2).EQ.INZ(I)) GO TO 6                                       400
    5 CONTINUE                                                           410
      ISPA=1                                                             420
      GO TO 4                                                            430
    6 ISPA=0                                                             440
    4 IF(MAT2-2)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
      STOP                                                               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)=0.2E6                                                      660
      ENG(20)=0.4E6                                                      670
      ENG(21)=0.8E6                                                      680
      ENG(22)=1.4E6                                                      690
      ENG(23)=2.5E6                                                      700
      ENG(24)=4.0E6                                                      710
      ENG(25)=6.5E6                                                      720
      ENG(26)=1.0E7                                                      730
   14 IF(MAT2-3)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 0. 4 : THE ENERGY POINTS OF THE MACROSCOPIC  820
     1WEIGHTING FUNCTION ARE NOT GIVEN IN AN INCREASING ORDER')          830
      STOP                                                               840
   17 NFE=1                                                              850
      LSP=0                                                              860
   20 IF(MAT2-4)1,22,23                                                  870
   22 READ (NF) NA,(NR(1,I),NR(2,I),NR(3,I),I=1,NA)                      880
      DO 11 I=1,NA                                                       890
      IF(NR(2,I).GE.NR(3,I).AND.NR(2,I).LE.(NE-1))  GO TO 11             900
      IF(NR(1,I).EQ.10.AND.NR(3,I).LE.NE)  GO TO 11                      910
      WRITE (NOUT,54) NR(1,I)                                            920
   54 FORMAT(1HO/' ***ERROR 0. 5 : THE CHOICE OF ENERGY GROUP BOUNDARIES 930
     1 FOR PROGRAM',I6,' IS NOT VALID')                                  940
      STOP                                                               950
   11 CONTINUE                                                           960
      IF(NFE.EQ.1)  GO TO 114                                            970
      MIN=1                                                              980
      MAX=NE-1                                                           990
      DO 112 I=1,NA                                                     1000
      IF(NR(2,I).GT.MIN)  MIN=NR(2,I)                                   1010
      IF(NR(3,I).LT.MAX)  MAX=NR(3,I)                                   1020
  112 CONTINUE                                                          1030
```

```
      AN=ENG(NE-MIN)                                                    1040
      END=ENG(NE-MAX+1)                                                 1050
      IF(EF(1,1).GE.AN)  GO TO 113                                      1060
      IF(EF(NFE,1).GT.END)  GO TO 114                                   1070
  113 WRITE (NOUT,115)                                                  1080
  115 FORMAT(1HO/' ***ERROR 0. 6 : THE MACROSCOPIC WEIGHTING FUNCTION DO 1090
     1ES NOT INCLUDE ALL ENERGY GROUPS DESIRED')                        1100
      STOP                                                              1110
  114 DO 116 I=1,NA                                                     1120
      IF(NR(1,I).EQ.3.AND.IPM(2).EQ.N3)  GO TO 117                      1130
      GO TO 116                                                         1140
  117 WRITE (NOUT,118) MAT                                              1150
  118 FORMAT(1HO/' ***WARNING 0. 1 : THE SELFSHIELDING FACTORS FOR ',A6, 1160
     1' CAN ONLY BE CALCULATED FROM RESONANCE DATA'/' THE MODULE NUMBER  1170
     2WAS MODIFIED APPROPRIATE')                                        1180
      NR(1,I)=1                                                         1190
  116 CONTINUE                                                          1200
      READ (NF) MAT1,MAT2                                               1210
      GO TO 24                                                          1220
   23 WRITE (NOUT,25)                                                   1230
   25 FORMAT(1HO/' ***ERROR 0. 7 : THE IDENTIFICATION NUMBERS OF MODULES 1240
     1 TO BE CALLED CAN NOT BE FOUND')                                  1250
      STOP                                                              1260
   24 IF(MAT2-5)1,26,27                                                 1270
   26 READ (NF) MT,(TEMP(I),I=1,MT)                                    1280
      READ (NF) MAT1,MAT2                                               1290
      DO 28 I=1,NA                                                      1300
      IF(NR(1,I).EQ.1.OR.NR(1,I).EQ.2) GO TO 29                         1310
   28 CONTINUE                                                          1320
      WRITE (NOUT,30)                                                   1330
   30 FORMAT(1HO/' ***WARNING 0. 2 : THE DECLARATION OF THE TEMPERATURE  1340
     1IS NOT NECESSARY AND IS IGNORED')                                 1350
      GO TO 29                                                          1360
   27 DO 31 I=1,NA                                                      1370
      IF(NR(1,I).EQ.1.OR.NR(1,I).EQ.2) GO TO 32                         1380
   31 CONTINUE                                                          1390
      NT=0                                                              1400
      GO TO 29                                                          1410
   32 IF(ISTRUK.EQ.0) GO TO 34                                          1420
      NT=3                                                              1430
      TEMP(1)=300.                                                      1440
      TEMP(2)=900.                                                      1450
      TEMP(3)=2100.                                                     1460
      GO TO 29                                                          1470
   34 NT=1                                                              1480
      TEMP(1)=0.                                                        1490
   29 IF(MAT2-6)1,33,35                                                 1500
   33 READ (NF) MI,(SIGO(I),I=1,MI)                                    1510
      READ (NF) MAT1,MAT2                                               1520
      DO 36 I=1,NA                                                      1530
      IF(NR(1,I).EQ.1.OR.NR(1,I).EQ.2.OR.NR(1,I).EQ.3) GO TO 37         1540
   36 CONTINUE                                                          1550
      WRITE (NOUT,38)                                                   1560
   38 FORMAT(1HO/' ***WARNING 0. 3 : THE DECLARATION OF THE BACKGROUND C 1570
     1ROSS SECTIONS IS NOT NECESSARY AND IS IGNORED')                   1580
      GO TO 37                                                          1590
   35 DO 39 I=1,NA                                                      1600
      IF(NR(1,I).EQ.1.OR.NR(1,I).EQ.2.OR.NR(1,I).EQ.3) GO TO 40         1610
   39 CONTINUE                                                          1620
      MI=0                                                              1630
      GO TO 37                                                          1640
   40 MI=7                                                              1650
      SIGO(1)=0.                                                        1660
      DO 41 I=1,6                                                       1670
   41 SIGO(I+1)=10.**I                                                  1680
   37 IF(MAT2-7)1,42,43                                                 1690
   42 READ (NF) NTYP,(ITYP(I),I=1,NTYP)                                1700
      READ (NF)MAT1,MAT2                                                1710
      DO 149 I=1,NTYP                                                   1720
      IF(ITYP(I).EQ.SGC)  GO TO 150                                     1730
  149 CONTINUE                                                          1740
      GO TO 151                                                         1750
  150 DO 152 J=1,NTYP                                                   1760
      IF(ITYP(J).EQ.SGA)  GO TO 153                                     1770
  152 CONTINUE                                                          1780
      ITYP(I)=SGA                                                       1790
  153 DO 154 J=1,NTYP                                                   1800
      IF(ITYP(J).EQ.SGF)  GO TO 155                                     1810
  154 CONTINUE                                                          1820
      IF(ITYP(I).EQ.SGA)  GO TO 156                                     1830
      ITYP(I)=SGF                                                       1840
      GO TO 151                                                         1850
  156 NTYP=NTYP+1                                                       1860
      ITYP(NTYP)=SGF                                                    1870
      GO TO 151                                                         1880
  155 IF(ITYP(I).EQ.SGA)  GO TO 151                                     1890
      NTYP=NTYP-1                                                       1900
      DO 157 J=I,NTYP                                                   1910
  157 ITYP(J)=ITYP(J+1)                                                 1920
  151 DO 44 I=1,NA                                                      1930
      IF(NR(1,I).EQ.4) GO TO 45                                         1940
   44 CONTINUE                                                          1950
      WRITE (NOUT,46)                                                   1960
   46 FORMAT(1HO/' ***WARNING 0. 4 : THE DECLARATION OF THE CROSS SECTIO 1970
     1N TYPES IS NOT NECESSARY AND IS IGNORED')                         1980
      GO TO 45                                                          1990
   43 DO 47 I=1,NA                                                      2000
      IF(NR(1,I).EQ.4.OR.NR(1,I).EQ.10)  GO TO 48                       2010
   47 CONTINUE                                                          2020
      NTYP=0                                                            2030
      GO TO 45                                                          2040
   48 NTYP=7                                                            2050
      CALL DOPW (8HMUEL     ,ITYP(1))                                   2060
      CALL DOPW (8HNUE      ,ITYP(2))                                   2070
      CALL DOPW (8HSGA      ,ITYP(3))                                   2080
      CALL DOPW (8HSGF      ,ITYP(4))                                   2090
      CALL DOPW (8HSGI      ,ITYP(5))                                   2100
      CALL DOPW (8HSGN      ,ITYP(6))                                   2110
      CALL DOPW (8HSG2N     ,ITYP(7))                                   2120
   45 IF(MAT2-8)1,49,50                                                 2130
   49 READ (NF) NRES                                                    2140
      READ (NF) MAT1,MAT2                                               2150
```

```
      DO 51 I=1,NA                                                      2160
      IF(NR(1,I).EQ.1) GO TO 52                                         2170
   51 CCNTINUE                                                          2180
      WRITE (NOUT,53)                                                   2190
   53 FORMAT(1HO/' ***WARNING O. 5 : THE DECLARATION OF THE NUMBER OF RE 2200
     1SONANCES IS NOT NECESSARY AND IS IGNCRED')                        2210
      GO TO 52                                                          2220
   50 NRES=10                                                           2230
   52 IF(MAT2-9)1,56,57                                                 2240
   56 READ (NF) ERROR                                                   2250
      READ (NF) MAT1,MAT2                                               2260
      DC 58 I=1,NA                                                      2270
      IF(NR(1,I).EQ.1) GO TO 59                                         2280
   58 CONTINUE                                                          2290
      WRITE (NOUT,60)                                                   2300
   60 FORMAT(1HO/' ***WARNING O. 6 : THE DECLARATION OF THE ALLOWED INTE 2310
     1GRATION ERROR IS NOT NECESSARY AND IS IGNCRED')                   2320
      GO TO 59                                                          2330
   57 ERROR=0.05                                                        2340
   59 IF(MAT2-10)1,63,64                                                2350
   63 READ (NF) XNUE                                                    2360
      READ (NF) MAT1,MAT2                                               2370
      DO 65 I=1,NA                                                      2380
      IF(NR(1,I).EQ.5) GO TO 66                                         2390
   65 CONTINUE                                                          2400
      WRITE (NOUT,67)                                                   2410
   67 FORMAT(1HO/' ***WARNING O. 7 : THE DECLARATION OF THE PARAMETER FO 2420
     1R THE WEISSKOPF EVAPORATION MODEL IS NOT NECESSARY AND IS IGNORED' 2430
     2)                                                                 2440
      GO TO 66                                                          2450
   64 XNUE=0.16                                                         2460
   66 DO 77 I=1,NA                                                      2470
      IF(NR(1,I ).EQ.6) GO TO 78                                        2480
   77 CONTINUE                                                          2490
      IP=0                                                              2500
      GO TO 79                                                          2510
   78 IP=1                                                              2520
      LSPEC=NFE*LSP                                                     2530
   79 IF(MAT2-11)1,80,81                                                2540
   80 IF(IP.EQ.1) GO TO 82                                              2550
      WRITE (NOUT,83)                                                   2560
   83 FORMAT(1HO/' ***WARNING O. 8 : THE INPUT FOR MODULE 6 IS NOT NECES 2570
     1SARY')                                                            2580
   82 READ (NF) ISEL,NLA,NLE                                            2590
      READ (NF) MAT1,MAT2                                               2600
      NLA=0                                                             2610
      IF(NLE.LT.1)  NLE=1                                               2620
      IF(NLE.GT.5)  NLE=5                                               2630
      GO TO 84                                                          2640
   81 NLA=0                                                             2650
      NLE=5                                                             2660
      IF(ISTRUK.EQ.0)  ISEL=2                                           2670
      IF(ISTRUK.EQ.1)  ISEL=1                                           2680
   84 IF(IP.EQ.0)  GO TC 141                                            2690
      IF(NFE.GT.0.AND.EF(1,1).EQ.0) EF(1,1)=1.E-3                       2700
  141 IF(MAT2-12)1,133,134                                              2710
  133 IF(IP.EQ.1)  GO TC 135                                            2720
      WRITE (NOUT,83)                                                   2730
  135 READ (NF) NMAT,(NAME(I),TZ(I),I=1,NMAT)                           2740
      READ (NF) MAT1,MAT2                                               2750
      NTK=1                                                             2760
      GO TO 136                                                         2770
  134 NTK=0                                                             2780
  136 IF(MAT2-13)1,137,140                                              2790
  137 IF(IP.EQ.1)  GO TO 139                                            2800
      WRITE(NOUT,83)                                                    2810
  139 READ (NF) MAZ(1),MAZ(2)                                           2820
      READ (NF) MAT1,MAT2                                               2830
      IF(MAZ(1).EQ.0)  GO TO 138                                        2840
      IF(LSP.EQ.0)  GO TO 138                                           2850
      IF(LSP-(NLE+1))142,138,138                                        2860
  142 LP=NLE+1                                                          2870
      WRITE (NOUT,143) LP                                               2880
  143 FORMAT(1HO/' ***ERROR O. 8 : THE NUMBER CF WEIGHTING FUNCTIONS IS 2890
     'LESS THAN THE NUMBER OF LEGENDRE MOMENTS.'/I5,' NUMBER OF WEIGHTIN 2900
     2G FUNCTIONS ARE NEEDED')                                          2910
      STOP                                                              2920
  140 MAZ(1)=0                                                          2930
      MAZ(2)=0                                                          2940
  138 IF(MAT2-14)1,145,146                                              2950
  145 IF(IP.EQ.1)  GO TO 147                                            2960
      WRITE(NOUT,83)                                                    2970
  147 READ(NF)NS,NK,NRR                                                 2980
      READ(NF)MAT1,MAT2                                                 2990
      GO TO 148                                                         3000
  146 NS=4                                                              3010
      NK=70                                                             3020
      NRR=16                                                            3030
  148 DO 68 I=1,NA                                                      3040
      IF(NR(1,I).EQ.9)  GO TO 69                                        3050
   68 CONTINUE                                                          3060
      IP=0                                                              3070
      GO TO 70                                                          3080
   69 IP=1                                                              3090
   70 IF(MAT2-15)1,71,72                                                3100
   71 IF(IP.EQ.1)  GO TC 73                                             3110
      WRITE (NOUT,74)                                                   3120
   74 FCRMAT(1HO/' ***WARNING O. 9 : THE INPUT FOR MODULE 9 IS NOT NECES 3130
     1SARY')                                                            3140
   73 READ (NF) ERR,NJM,NUJM                                            3150
      READ (NF) MAT1,MAT2                                               3160
      GO TO 75                                                          3170
   72 IF(IP.EQ.0)  GO TO 75                                             3180
      ERR=0.05                                                          3190
      NJM=6                                                             3200
      NUJM=10                                                           3210
   75 IF(MAT2-16)1,76,103                                               3220
   76 IF(IP.EQ.1)  GO TC 104                                            3230
      WRITE (NOUT,74)                                                   3240
  104 READ (NF) ISELR,NLRA,NLRE,NCALL                                   3250
      IF(NCALL.NE.0)  GC TO 158                                         3260
      READ(NF)MAT1,MAT2                                                 3270
```

```
      GO TO 105                                                         3280
  158 IS=0                                                              3290
      DO 109 I=1,NA                                                     3300
      IF(NR(1,I).EQ.9)  IS=IS+1                                         3310
  109 CONTINUE                                                          3320
      IF(IS.EQ.NCALL)  GO TO 110                                        3330
      WRITE (NOUT,111) IS,NCALL                                         3340
  111 FORMAT(1HO/' ***ERROR 0. 9 : MODULE 9 IS CALLED ',I3,' TIMES, IN T 3350
     1HE INPUT BLOC 16 NCALL IS SET TO',I3)                             3360
      STOP                                                              3370
  110 DO 106 I=1,NCALL                                                  3380
      READ (NF)NGRE,(NN1(I,J),NN2(I,J),NFG(I,J),NFI(I,J),J=1,NGRE)      3390
      NRE(I)=NGRE                                                       3400
      DO 106 J=1,NGRE                                                   3410
      IF(NN1(I,J).GE.NN2(I,J))  GO TO 106                               3420
      WRITE (NOUT,107) I                                                3430
  107 FORMAT(1HO/' ***ERROR 0.10 : IN BLOC 16 THE INPUT OF THE ENERGY GR 3440
     1OUPS IS NOT VALID FOR THE ',I3,'. PROGRAM CALL')                  3450
      STOP                                                              3460
  106 CONTINUE                                                          3470
      READ(NF)MAT1,MAT2                                                 3480
      GO TO 108                                                         3490
  103 NLRA=0                                                            3500
      NLRE=5                                                            3510
      ISELR=1                                                           3520
      NCALL=0                                                           3530
  105 NFG( 1,1)=14                                                      3540
      NFI(1,1)=5                                                        3550
      NRE(1)=1                                                          3560
  108 IF(MAT1.EQ.N2)  GO TO 88                                          3570
    1 WRITE (NOUT,89)                                                   3580
   89 FORMAT(1HO/' ***ERROR 0.11 : THE INPUT IS NOT ORDERED IN INCREASIN 3590
     1G ARGUMENTS')                                                     3600
      STOP                                                              3610
   88 NGR=0                                                             3620
      KL=1                                                              3630
  100 NANF=NR(2,KL)                                                     3640
      NEND=NR(3,KL)                                                     3650
      IF(NR(1,KL).EQ.1) GO TO 90                                        3660
      IF(NR(1,KL).EQ.2) GO TO 91                                        3670
      IF(NR(1,KL).EQ.3) GO TO 92                                        3680
      IF(NR(1,KL).EQ.4) GO TO 93                                        3690
      IF(NR(1,KL).EQ.5) GO TO 94                                        3700
      IF(NR(1,KL).EQ.6) GO TO 95                                        3710
      IF(NR(1,KL).EQ.7) GO TO 96                                        3720
      IF(NR(1,KL).EQ.8) GO TO 97                                        3730
      IF(NR(1,KL).EQ.9)  GO TO 119                                      3740
      IF(NR(1,KL).EQ.10)  GO TO 120                                     3750
      WRITE (NOUT,98) NR(1,KL)                                          3760
   98 FORMAT(1HO/' ***ERROR 0.12 : THE DESIRED MODULE',I6,' IS NOT CONTA 3770
     1INED IN MIGROS')                                                  3780
      STOP                                                              3790
  126 IRE=IRE+IREP                                                      3800
      ISTE=ISTE+ISTEP                                                   3810
   90 NGR=0                                                             3820
      IF(NFR+7*MI+3*NE+7*IRE+5*ISTE.GT.IADR)  GO TO 121                 3830
      CALL FGEM(MI,SIGO,NE,ENG,NFE,EF(1,1),EF(1,2),NT,TEMP,ERROR,NRES,  3840
     1NGR,XL(NFR),XL(NFR+7*MI),IRE,IREP,XL(NFR+7*MI+3*NE),XL(NFR+7*MI+  3850
     23*NE+IRE),XL(NFR+7*MI+3*NE+IRE*2),XL(NFR+7*MI+3*NE+3*IRE),        3860
     3XL(NFR+7*MI+3*NE+4*IRE),XL(NFR+7*MI+3*NE+5*IRE),                  3870
     4XL(NFR+7*MI+3*NE+6*IRE),ISTE,ISTEP,XL(NFR+7*MI+3*NE+7*IRE))       3880
      IF(IREP.GT.0.OR.ISTEP.GT.0)  GO TO 126                            3890
      IF(NGR.EQ.0)  GO TO 101                                           3900
      NANF=NE-NGR                                                       3910
      KL=KL-1                                                           3920
      GO TO 91                                                          3930
  101 IF(KL.LE.NA)  GO TO 100                                           3940
      GO TO 102                                                         3950
   91 IF(NFR+35*MI.GT.IADR)  GO TO 121                                  3960
      CALL FSTAT(MI,SIGO,NE,ENG,NFE,EF(1,1),EF(1,2),NT,TEMP,XL(NFR),    3970
     1XL(NFR+15*MI),XL(NFR+30*MI))                                      3980
      NGR=0                                                             3990
      IF(KL.LE.NA)  GO TO 100                                           4000
      GO TO 102                                                         4010
  125 MDIM=MDIM+MDIMP                                                   4020
      NER=NER+NERP                                                      4030
   92 ISIG=0                                                            4040
      IF(SIGO(MI).GE.1.E6)  GO TO 144                                   4050
      ISIG=1                                                            4060
      MI=MI+1                                                           4070
      SIGO(MI)=1.E6                                                     4080
  144 IF(NFR+6*NE+16*MI*NE+2*MDIM+6*NER.GT.IADR)  GO TO 121             4090
      CALL FSTRUK(MI,SIGO,NE,ENG,NFE,EF(1,1),EF(1,2),XL(NFR),XL(NFR+4*NE 4100
     1),XL(NFR+4*NE+5*MI*NE),XL(NFR+4*NE+9*MI*NE),XL(NFR+4*NE+15*MI*NE), 4110
     2XL(NFR+5*NE+15*MI*NE),                                            4120
     3XL(NFR+5*NE+16*MI*NE),MDIM,MDIMP,XL(NFR+6*NE+16*MI*NE),           4130
     4XL(NFR+6*NE+16*MI*NE+MDIM),NER,NERP,XL(NFR+6*NE+16*MI*NE+2*MDIM), 4140
     5XL(NFR+6*NE+16*MI*NE+2*MDIM+3*NER))                               4150
      IF(ISIG.EQ.1)  MI=MI-1                                            4160
      IF(MDIMP.GT.0.OR.NERP.GT.0)  GO TO 125                            4170
      IF(KL.LE.NA)  GO TO 100                                           4180
      GO TO 102                                                         4190
  124 LDIM=LDIM+LDIMP                                                   4200
   93 IF(NFR+6*NE+2*LDIM.GT.IADR)  GO TO 121                            4210
      CALL SUND (NE,ENG,NFE,EF(1,1),EF(1,2),NTYP,ITYP,XL(NFR),          4220
     1XL(NFR+NE),XL(NFR+2*NE),XL(NFR+3*NE),XL(NFR+4*NE),XL(NFR+5*NE),   4230
     2LDIM,LDIMP,XL(NFR+6*NE),XL(NFR+6*NE+LDIM))                        4240
      IF(LDIMP.GT.0)  GO TO 124                                         4250
      IF(KL.LE.NA)  GO TO 100                                           4260
      GO TO 102                                                         4270
  127 NET=NET+NETP                                                      4280
      NAE=NAE+NAEP                                                      4290
      ISG=ISG+ISGP                                                      4300
      IWE=IWE+IWP                                                       4310
   94 L=NFR+8*NE+2*NX+2*NET+2*NAE                                       4320
      IF(L+4*NE+NX+NET+NAE*(ISG+1)+IWE.GT.IADR)  GO TO 121              4330
      CALL SCAT(NE,ENG,     XNUE,NFE,EF(1,1),EF(1,2),NX,XL(NFR),       4340
     1XL(NFR+2*NE),XL(NFR+4*NE),XL(NFR+6*NE),XL(NFR+8*NE),NET,          4350
     2XL(NFR+8*NE+2*NX),NAE,XL(NFR+8*NE+2*NX+2*NET),XL(L),XL(L+NE),     4360
     3XL(L+2*NE),XL(L+3*NE),XL(L+4*NE),NETP,XL(L+4*NE+NX),NAEP,         4370
     4XL(L+4*NE+NX+NET),ISG,ISGP,XL(L+4*NE+NX+NET+NAE),IWE,IWP,         4380
     5XL(L+4*NE+NX+NET+NAE+NAE*ISG))                                    4390
```

```
      IF(NETP.GT.0.OR.NAEP.GT.0.OR.ISGP.GT.C.OR.IWP.GT.0)  GO TO 127     4400
      IF(KL.LE.NA)  GO TO 100                                            4410
      GO TO 102                                                          4420
  123 NECU=NECU+NECUP                                                    4430
      ISM=ISM+ISMP                                                       4440
      ISD=ISD+ISDP                                                       4450
      ICOS=ICOS+ICOSP                                                    4460
      ISCO=MAX0(ISM*ICOS,ISCO+ISCOP)                                     4470
      ISCO=MAX0(ISCO,NECU*ISD)                                           4480
      ISEC=MAX0(ISM*NECU,ISEC+ISECP)                                     4490
      ISEC=MAX0(ISEC,ISD)                                                4500
      NTT=NTT+NTTP                                                       4510
      NANF=NANF-KIM                                                      4520
   95 L=NFR+5*ISM                                                        4530
      M=L+7*ISD                                                          4540
      N=M+2*ICOS                                                         4550
      NN=N+4*NX                                                          4560
      MM=NN+2*NE                                                         4570
      IF(MM+ISCO+ISEC+6*NECU*NE+2*NE+2*NTT.GT.IADR)  GO TO 121           4580
      CALL FLUMMI(XL(NFR),XL(NFR+ISM),XL(NFR+2*ISM),XL(NFR+3*ISM),       4590
     1XL(NFR+4*ISM),XL(NFR+5*ISM),XL(L+ISD),XL(L+2*ISD),                 4600
     2XL(L+3*ISD),XL(L+4*ISD),XL(L+5*ISD),XL(L+6*ISD),XL(L+7*ISD),       4610
     3XL(M+ICOS),XL(M+2*ICOS),XL(N+NX),XL(N+2*NX),XL(N+3*NX),ENG,        4620
     4XL(N+4*NX),XL(NN+NE),                EF(1,1),EF(1,2),XL(NN+2*NE),  4630
     5XL(MM+ISCO),XL(MM+ISCO+ISEC),XL(MM+ISCO+ISEC+6*NECU*NE),           4640
     6XL(MM+ISCO+ISEC+6*NECU*NE+2*NE),                                   4650
     8XL(MM+ISCO+ISEC+6*NECU*NE+2*NE+NTT),NAME,TZ,                       4660
     6NLA,NLE,ISEL,NMAX,NE,NX,NFE,LSPEC,MAZ,NTK,NMAT,NTT,NTTP,           4670
     6                        ICOS,ICOSP,NECU,NECUP,ISM,ISMP,ISD,        4680
     7ISDP,ISCO,ISCOP,ISEC,ISECP,KIM,NS,NK,NRR)                          4690
      IF(NECUP.GT.0.OR.ISMP.GT.0.OR.ISDP.GT.0.OR.ISCOP.GT.0.OR.          4700
     1ICOSP.GT.0.OR.ISECP.GT.0.OR.NTTP.GT.0)  GO TO 123                  4710
      IF(KL.LE.NA)  GO TO 100                                            4720
      GO TO 102                                                          4730
   96 IF(NFR+NE.GT.IADR)  GO TO 121                                      4740
      CALL SPALT (NE,ENG,XL(NFR))                                        4750
      IF(KL.LE.NA)  GO TO 100                                            4760
      GO TO 102                                                          4770
   97 NES=MAX0(10*NE,NFE)                                                4780
      IF(NFR+3*NE+2*NES.GT.IADR)  GO TO 121                              4790
      CALL EDV (NE,ENG,NFE,EF(1,1),EF(1,2),XL(NFR),XL(NFR+NE),XL(NFR+2*  4800
     1NE),NES,XL(NFR+3*NE),XL(NFR+3*NE+NES))                             4810
      IF(KL.LE.NA)  GO TO 100                                            4820
      GO TO 102                                                          4830
  119 IREMO=IREMO+1                                                      4840
      IF(NCALL.EQ.0)  IREMO=1                                            4850
      L=NANF-NEND+1                                                      4860
      M=NRE(IREMO)                                                       4870
      NN=NEND                                                            4880
      IF(NCALL.EQ.0)  NN1(1,1)=NANF                                      4890
      IF(NCALL.EQ.0)  NN2(1,1)=NEND                                      4900
      DO 128 N=1,M                                                       4910
  129 NG(NN)=NFG(IREMO,N)                                                4920
      NI(NN)=NFI(IREMO,N)                                                4930
      NN=NN+1                                                            4940
      IF(NN.LE.NEND+NN1(IREMO,N)-NN2(IREMO,N)+1)  GO TO 129              4950
  128 CONTINUE                                                           4960
      IF(NN-1.EQ.NEND+L)  GO TO 130                                      4970
      WRITE(NOUT,131)                                                    4980
  131 FORMAT(1HO/' ***ERROR 0.13 : FOR MODULE 9 THE INPUT BLOCS 4 AND 16 4990
     1 DO NOT CORRESPOND')                                               5000
      KL=KL+1                                                            5010
      GO TO 132                                                          5020
  130 CALL REMO(NE,ENG,NFE,EF(1,2),EF(1,1),ERR,NLRA,NLRE,L,NG,NI,NJM,    5030
     1NUJM,ISELR,XL(NFR),XL(NFR),IADR-NFR+1)                             5040
  132 IF(KL.LE.NA)  GO TO 100                                            5050
      GO TO 102                                                          5060
  120 CALL THERM (NE,NTYP,ITYP)                                          5070
      IF(KL.LE.NA)  GO TO 100                                            5080
      GO TO 102                                                          5090
  121 WRITE (NOUT,122) NR(1,KL)                                          5100
  122 FORMAT(1HO/' ***ERROR 0.14 : THE PARM.G PARAMETER IN THE EXEC CARD 5110
     1 IS NOT GREAT ENOUGH TO START MODULE',I3)                          5120
      KL=KL+1                                                            5130
      IF(KL.LE.NA)  GO TO 100                                            5140
  102 RETURN                                                             5150
      END                                                                5160
C     SUBROUTINEN ZUM LESEN DER KERNDATENBIBLIOTHEK                        10
C                                                                          20
C     SUBROUTINEN NDFOPN , LDFOPN ZUM ERÖFFNEN DER KERNDATENBIBLIOTHEK     30
C                                                                          40
      SUBROUTINE NDF                                                       50
      DIMENSION IDAT(2),IAD(1003),ISATZ(880),DAT1(60),I(4),IR(3),IW(3),    60
     1NNAM(4),INAM(20),KDAT1(60),MNAM(20),NUNA(2),IWNA(880),XNAM(20),      70
     2XJDAT(880),JDAT(880),NN(4),IBEST(2),DAT2(60),Z(60),XWNA(880)         80
      EQUIVALENCE (I(1),IR(1)),(Z(1),KDAT1(1)),(IWNA(1),XWNA(1)),          90
     1(JDAT(1),XJDAT(1))                                                  100
      DATA I/'KEDA','BIBL','IOTH','    '/,NSZ/1CO/,NOUTP/6/                110
C                                                                         120
      ENTRY NDFOPN (LBN,IDAT,IFD,ISPR)                                    130
      JJ=1                                                                140
      IDAT(1)=I(4)                                                        150
      IDAT(2)=I(4)                                                        160
      GOTO 50                                                             170
C                                                                         180
      ENTRY LDFOPN (LBN,IFD,*)                                            190
      JJ=2                                                                200
   50 NSZ=880                                                             210
      DEFINE FILE 1 (1200,880,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
     1RACTERIZE A VALID KEDAK LIBRARY')
      STOP
    1 CONTINUE
      IFD=ISATZ(4)
      IAD(1)=ISATZ(5)
      IAD(2)=ISATZ(8)
      IAD(3)=ISATZ(11)
      K=4
      IR(1)=ISATZ(6)
      IR(2)=ISATZ(9)
      IR(3)=ISATZ(12)
      IW(1)=ISATZ(7)
      IW(2)=ISATZ(10)
      IW(3)=ISATZ(13)
      DO 3 J=1,3
      N=IR(J)
      IWJ=IW(J)
      IF(IS-N-1)5,6,5
    5 READ (LBN'N) (ISATZ(II),II=1,NSZ)
      IS=N+1
    6 IF(J-3)10,11,11
   10 L=3
      GO TO 326
   11 L=4
  326 IMP=IAD(J)*L+IWJ-1
    8 IF(IMP-NSZ)13,14,15
   14 N=1
      GO TO 16
   15 N=2
   16 DO 12 L=IWJ,NSZ
      IAD(K)=ISATZ(L)
   12 K=K+1
      GO TO (3,17),N
   17 IMP=IMP-NSZ
      IWJ=1
      READ (LBN'IS) (ISATZ(II),II=1,NSZ)
      IS=IS+1
      GO TO 8
   13 DO318 L=IWJ,IMP
      IAD(K)=ISATZ(L)
  318 K=K+1
    3 CONTINUE
      RETURN
C
C
C     SUBROUTINEN NDFLOC , LDFLOC , IDFLOC
C
      ENTRY NDFLOC (KONTR,NNAM,DAT1,ID,KC)
      IF(NSZ.NE.880)  GO TO 1004
      ID=0
      KC=0
      DO 403 LS=1,2
      IF (DAT1(LS).NE.MNAM(LS))  GO TO 104
  403 CONTINUE
      MGL=2
      GOTO 107
  104 MGL=1
  107 J=NNAM(1)*2
      DO 51 N=1,J
   51 Z(N)=DAT1(N)
      L=1
      LS=1
      DO 18 N=1,J
      IF(N-4)19,218,20
   19 IF(N-3)20,218,218
   20 MNAM(L)=KDAT1(N)
      L=L+1
      GOTO 18
  218 IBEST(LS)=KDAT1(N)
      LS=LS+1
   18 CONTINUE
      KK=1
      GOTO427
C
      ENTRY LDFLOC (KONTR,NNAM,INAM,DAT2)
      IF(NSZ.NE.880)  GO TO 1004
      DO 127 LS=1,2
      IF (INAM(LS).NE.MNAM(LS))  GO TO 128
  127 CONTINUE
      MGL=2
      GOTO 129
  128 MGL=1
  129 J=NNAM(1)*2
      DO 21 N=1,J
   21 MNAM(N)=INAM(N)
      KK=2
  427 K=4
      IWJ=0
      DO 22 LS=1,3,2
      IWJ=IWJ+1
      N=IAD(IWJ)*3
      DO 23 M=1,N
      IF (MNAM(LS).NE.IAD(K))  GO TO 23
      IF (MNAM(LS+1).EQ.IAD(K+1))  GO TO 26
   23 K=K+3
      WRITE (NOUTP,2000) (MNAM(M),M=1,4)
 2000 FORMAT(1HO/' ***WARNING NDF. 1 : THE DATA FOR ',2A4,1X,2A4,' ARE N
     1OT INCLUDED IN THE'/' CONVERSIONTABLE OF THE KEDAK LIBRARY')
      MNAM(1)=1
      KONTR=0
      IF(JJ-1)98,98,96
   26 NUNA(IWJ)=IAD(K+2)
   22 K=N+4
      GO TO (227,228),MGL
C
      ENTRY IDFLOC (KONTR,NNAM,INAM,DAT2)
      IF(NSZ.NE.880)  GO TO 1004
      KK=3
      IF(INAM(1)-NUNA(1))130,131,130
  131 MGL=2
      GOTO 132
```

```
      MGL=1
      NUNA(1)=INAM(1)
      NUNA(2)=INAM(2)
      IF(NNAM(1)-2)27,27,52
   52 J=NNAM(1)
      DO 53 LS=3,J
   53 MNAM(2*LS-1)=INAM(LS)
   27 GO TO (227,228),MGL
  227 N=IAD(3)*4
      IWJ=(IAD(1)+IAD(2))*3+4
      DO 28 LS=1,N,4
      IF(NUNA(1)-IAD(IWJ))28,29,28
   28 IWJ=IWJ+4
      KONTR=0
      GO TO 24
   29 NT=IAD(IWJ+1)
      JR=IAD(IWJ+2)
      JW=IAD(IWJ+3)
  228 KR=JR
      KW=JW
      IVY=0
      IF(IS-KR-1)30,31,30
   30 READ (LBN'KR) (ISATZ(II),II=1,NSZ)
      IS=KR+1
   31 DO 32 LS=1,NT
      IF(NUNA(2)-ISATZ(KW))33,34,33
   33 KW=KW+7
      IF(KW-NSZ)32,32,35
   35 READ (LBN'IS) (ISATZ(II),II=1,NSZ)
      IS=IS+1
      KW=KW-NSZ
   32 CONTINUE
      KONTR=0
      GO TO 24
   34 KW=KW+1
      DO 36 LS=1,6
      IF(KW-NSZ)37,37,38
   38 READ (LBN'IS) (ISATZ(II),II=1,NSZ)
      IS=IS+1
      KW=1
   37 GO TO (39,40,40,41,42,43),LS
   39 NWN=ISATZ(KW)
      GOTO 36
   40 NNAM(LS)=ISATZ(KW)
      GOTO 36
   41 NWP=ISATZ(KW)
      GO TO 36
   42 IDR=ISATZ(KW)
      GO TO 36
   43 IDW=ISATZ(KW)
   36 KW=KW+1
      IF(KK-1)46,46,47
   46 NNAM(4)=0
   47 DO 80 LS=1,4
   80 NN(LS)=NNAM(LS)
      IF(NWN)384,384,49
   49 NNK=NWP
      NWR=IDR
      NWW=IDW
      IF(IS-NWR-1)44,45,44
   44 READ (LBN'NWR) (IWNA(II),II=1,NSZ)
      NWR=NWR+1
      GO TO 62
   45 DO 61 LS=1,NSZ
   61 IWNA(LS)=ISATZ(LS)
      NWR=NWR+1
   62 DO 68 N=1,NNK
      NKO=N
      NW=NWW
      KP=5
      JD=3
      DO 54 LS=1,NWN
      IF(IWNA(NWW)-MNAM(KP))58,55,56
   56 KONTR=0
      IVY=1
      IF(KK-2)57,59,859
   59 INAM(KP)=IWNA(NWW)
      GOTO 60
  859 INAM(JD)=IWNA(NWW)
      GO TO 60
   57 DATI(KP+2)=XWNA(NWW)
      GOTO 60
   55 KONTR=1
   60 KP=KP+2
      JD=JD+1
      NWW=NWW+1
      IF(NWW-NSZ)54,54,64
   64 READ (LBN'NWR) (IWNA(II),II=1,NSZ)
      NWR=NWR+1
      NWW=1
   54 CONTINUE
      GO TO 74
   58 NWW=NW+NWN+3
      IF(NWW-NSZ)68,68,70
   70 READ (LBN'NWR) (IWNA(II),II=1,NSZ)
      NWR=NWR+1
   73 NWW=NWW-NSZ
   68 CONTINUE
      KONTR=0
      IF(KK.EQ.3)  GO TO 580
      WRITE (NOUTP,2002) MNAM(5),(MNAM(II),II=1,4)
 2002 FORMAT(1HO/' ***WARNING NDF. 2 : THE FURTHER NAME ',E16.8,' IS GRE
     1ATER THAN THE GREATEST FURTHER NAME '/' INCLUDED IN THE KEDAK LIBR
     2ARY FOR',1X,2A4,1X,2A4)
      GO TO 98
  580 WRITE (NOUTP,581) MNAM(5),(INAM(II),II=1,2)
  581 FORMAT(1HO/' ***WARNING NDF. 2 : THE FURTHER NAME',E16.8,' IS GREA
     1TER THAN THE GREATEST FURTHER NAME'/' INCLUDED IN THE KEDAK LIBRAR
     2Y FOR',2I10)
      GO TO 98
 1004 WRITE (NOUTP,1005)
 1005 FORMAT(1HO/' ***ERROR NDF. 2 : AT FIRST THE --OPN - ROUTINE MUST B
```

```
   1E CALLED')                                                                  2550
      STOP                                                                      2560
   74 NWP=IWNA(NWW)                                                             2570
      DO 75 LS=1,2                                                              2580
      NWW=NWW+1                                                                 2590
      IF(NWW-NSZ)76,76,78                                                       2600
   78 READ (LBN'NWR) (IWNA(II),II=1,NSZ)                                        2610
      NWR=NWR+1                                                                 2620
      NWW=1                                                                     2630
   76 GO TO (81,82),LS                                                          2640
   81 IDR=IWNA(NWW)                                                             2650
      GOTO 75                                                                   2660
   82 IDW=IWNA(NWW)                                                             2670
   75 CONTINUE                                                                  2680
      NWW=NWW+1                                                                 2690
   48 IF(NWN)384,384,383                                                        2700
  384 IF(IS-IDR-1)83,385,83                                                     2710
  383 IF(NWR-IDR-1)83,84,83                                                     2720
  385 DO 386 L=1,NSZ                                                            2730
  386 JDAT(L)=ISATZ(L)                                                          2740
      IDR=IDR+1                                                                 2750
      GO TO 388                                                                 2760
   84 DO 85 L=1,NSZ                                                             2770
   85 JDAT(L)=IWNA(L)                                                           2780
      IDR=IDR+1                                                                 2790
      GO TO 388                                                                 2800
   83 READ (LBN'IDR) (JDAT(II),II=1,NSZ)                                        2810
      IDR=IDR+1                                                                 2820
  388 NPA=1                                                                     2830
   86 JD=NNAM(2)+NNAM(3)                                                        2840
      IF(KK-2)87,88,88                                                          2850
   87 LS=NNAM(1)*2+1                                                            2860
      GO TO 89                                                                  2870
   88 LS=1                                                                      2880
   89 DO 90 L=1,JD                                                              2890
      GO TO (91,92,92),KK                                                       2900
   91 DAT1(LS)=XJDAT(IDW)                                                       2910
      DAT1(LS+1)=0.                                                             2920
      LS=LS+2                                                                   2930
      GO TO 93                                                                  2940
   92 DAT2(LS)=XJDAT(IDW)                                                       2950
      LS=LS+1                                                                   2960
   93 IDW=IDW+1                                                                 2970
      IF(IDW-NSZ) 90,90,94                                                      2980
   94 READ(LBN'IDR) (JDAT(II),II=1,NSZ)                                        2990
      IDR=IDR+1                                                                 3000
      IDW=1                                                                     3010
   90 CONTINUE                                                                  3020
      IF(IVY)1003,1003,98                                                       3030
 1003 KONTR=1                                                                   3040
      GO TO 98                                                                  3050
   24 WRITE(NOUTP,97)NUNA(1),NUNA(2)                                            3060
   97 FORMAT(1HO/' ***WARNING NDF. 3 : THE DATA FOR',2I9,' ARE NOT INCLU        3070
     1DED IN THE KEDAK LIBRARY')                                                3080
      IF(JJ-1)98,98,96                                                          3090
   96 RETURN 1                                                                  3100
      93 RETURN                                                                 3110
C                                                                               3120
C                                                                               3130
C     SUBROUTINEN NDFNXT, LDFNXT , IDFNXT                                       3140
C                                                                               3150
      ENTRY NDFNXT (KONTR,NNAM,DAT1,ID,KC)                                      3160
      ID=0                                                                      3170
      KC=0                                                                      3180
      LL=1                                                                      3190
      GO TO 101                                                                 3200
C                                                                               3210
      ENTRY LDFNXT(KONTR,NNAM,INAM,DAT2)                                        3220
      LL=2                                                                      3230
      GOTO 101                                                                  3240
C                                                                               3250
      ENTRY IDFNXT(KONTR,NNAM,INAM,DAT2)                                        3260
      LL=3                                                                      3270
  101 NPA=NPA+1                                                                 3280
      IVY=0                                                                     3290
      IF(NPA-NWP)102,102,103                                                    3300
  103 KONTR=0                                                                   3310
      IF (NWN)387,387,389                                                       3320
  389 NKO=NKO+1                                                                 3330
      IF(NKO-NNK)391,391,387                                                    3340
  387 RETURN                                                                    3350
  102 KONTR=1                                                                   3360
  391 DO 304 LS=1,3                                                             3370
  304 NNAM(LS)=NN(LS)                                                           3380
      IF(LL-2)105,124,106                                                       3390
  105 NNAM(4)=0                                                                 3400
      KDAT1(1)=MNAM(1)                                                          3410
      KDAT1(2)=MNAM(2)                                                          3420
      KDAT1(3)=IBEST(1)                                                         3430
      KDAT1(4)=IBEST(2)                                                         3440
      KDAT1(5)=MNAM(3)                                                          3450
      KDAT1(6)=MNAM(4)                                                          3460
      DO 401 II=1,6                                                             3470
  401 DAT1(II)=Z(II)                                                            3480
      GO TO 125                                                                 3490
  124 DO 126 LS=1,4                                                             3500
  126 INAM(LS)=MNAM(LS)                                                         3510
      GO TO 125                                                                 3520
  106 DO 327 LS=1,2                                                             3530
  327 INAM(LS)=NUNA(LS)                                                         3540
  125 IF(NWN)86,86,390                                                          3550
  390 IF(KONTR)108,108,86                                                       3560
  108 KP=NWN+3                                                                  3570
      IVY=1                                                                     3580
      L=5                                                                       3590
      DO 109 LS=1,KP                                                            3600
      IF(NWW-NSZ)110,110,111                                                    3610
  111 READ (LBN'NWR) (IWNA(II),II=1,NSZ)                                        3620
      NWR=NWR+1                                                                 3630
      NWW=1                                                                     3640
  110 IF(LS-NWN)112,112,113                                                     3650
  112 IF(LL-2)114,115,116                                                       3660
```

```
114 L=L+2                                                              3670
    KDAT1(L)=IWNA(NWW)                                                 3680
    KDAT1(L+1)=0                                                       3690
    DAT1(L)=Z(L)                                                       3700
    DAT1(L+1)=Z(L+1)                                                   3710
    GO TO 109                                                          3720
115 INAM(L)=IWNA(NWW)                                                  3730
    L=L+2                                                              3740
    GO TO 109                                                          3750
116 L=LS+2                                                             3760
    INAM(L)=IWNA(NWW)                                                  3770
113 L=LS-NWN                                                           3780
    GO TO (119,118,117),L                                              3790
119 NWP=IWNA(NWW)                                                      3800
    GOTO 109                                                           3810
118 IDR=IWNA(NWW)                                                      3820
    GOTO 109                                                           3830
117 IDW=IWNA(NWW)                                                      3840
109 NWW=NWW+1                                                          3850
    GO TO 388                                                          3860
    END                                                                3870
```

```
    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
```

```
    SUBROUTINE FGEM(NS,SIGO,NE,ENG,NEF,ES,F,NT,TEMP,PR,NMR,NFST,SUM,     10
   1SUO,IRE,IREP,ER,L,GJ,GAT,GAN,GAG,GAF,ISTE,ISTEP,STE)                 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),SUO(NE,3),      60
   3ER(IRE),L(IRE),GJ(IRE),GAT(IRE),GAN(IRE),GAG(IRE),GAF(IRE)           70
    COMMON MATN,ISTRUK,ISPA,NOUTP,LZWF,IR(2),KL                          80
    EQUIVALENCE (FEST(1),IFEST(1))                                       90
    WRITE (NOUTP,9000)                                                  100
9000 FORMAT(1H0/1H0/' PROGRAMM KENNZIFFER 1')                           110
```

```
    WRITE (NOUTP,9001)                                                  120
9001 FORMAT(' PROGRAMM ZUR BERECHNUNG VON RESONANZSELBSTABSCHIRMFAKTORE  130
   1N VON AUFGELOESTEN RESONANZPARAMETERN'/)                            140
     CALL FSPIE                                                         150
     CALL DOPW (8HBEST    ,NN(1))                                       160
     CALL DOPW (8HISOT1   ,NN(2))                                       170
     CALL DOPW (8HISOT2   ,NN(3))                                       180
     CALL DOPW (8HRES     ,NN(4))                                       190
     CALL DOPW (8HMIGR    ,MM)                                          200
     IREP=0                                                             210
     IREF=0                                                             220
     ISTEP=0                                                            230
     ISTEF=0                                                            240
     CALL EXPPX(X,X,X,X)                                                250
     NEFE=NEF                                                           260
     IF(NEF.NE.1) GOTO 411                                              270
     NEFE=0                                                             280
 411 PI=3.14159                                                         290
     NE1=NE-1                                                           300
     NMIN=NMR                                                           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
     SIGP=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 DO 63 IE=1,NE1                                                     660
     IF(ENG(IE+1)-ER(NR))63,63,64                                       670
```

```
 63 CONTINUE
    NLAST=NE1
    GOTO 66
 64 NLAST=IE-1
    IF(NLAST)65,65,66
 65 NFST=1
    GCTO 3
 66 NFST    =NLAST+1
  4 NANF=NE-IR(1)
    IF(NANF-NLAST)510,510,3
510 NEND=NE-IR(2)
502 IF(NEND-NLAST)503,503,505
503 NLAST=NEND
    NFST=0
505 DO 60 IT=1,NT
    T=TEMP(IT)
    NR1=1
    DO 10 IE=NANF,NLAST
    DO 36 ISO=1,3
 36 SUMO(ISO)=.0
    DO 37 ISO=1,NS
    DO 37 J1=1,7
 37 SUM(ISO,J1)=.0
    SUME=.0
    K=1
    STE(1,K)=ENG(IE)
    DO 15 INR=NR1,NR
    IF(ENG(IE)-ER(INR))16,15,15
 16 IF(ENG(IE+1)-ER(INR))18,18,17
 17 K=K+1
    IF(K.LE.ISTE)  GO TO 201
    K=1
    ISTEF=ISTEF+1
201 STE(1,K)=ER(INR)
 15 CONTINUE
 18 K=K+1
    IF(K.LE.ISTE)  GO TO 202
    K=1
    ISTEF=ISTEF+1
202 STE(1,K)=ENG(IE+1)
    KMAX=K
    IF(ISTEF.EQ.0)  GO TO 250
    ISTEP=(ISTEF-1)*ISTE+K+50
    RETURN
250 NR1=INR
    DO 19 K=1,KMAX
    CALL WIRQU(NR1,STE(1,K),STE(2,K),STE(3,K),STE(5,K),NR,IRE,ER,GJ,
   1GAN,GAT,GAF,L,GAG,T,A,R,RLA,NMIN)
 19 STE(4,K)=STE(5,K)-STE(3,K)-STE(2,K)
 22 KMX=KMAX+1
    KMX1=KMAX-1
    IF(KMX1)33,34,33
 33 IF(KMX.LE.ISTE)  GO TO 833
    ISTEP=50
    RETURN
833 DO 20 K=1,KMX1
    K1=KMX-K
    DO 20 J1=1,5
 20 STE(J1,K1+1)=STE(J1,K1)
    KMAX=KMAX+1
 35 STE(1,2)=(STE(1,3)+STE(1,1))/2.
    CALL WIRQU(NR1,STE(1,2),STE(2,2),STE(3,2),STE(5,2),NR,IRE,ER,GJ,
   1GAN,
   1GAT,GAF,L,GAG,T,A,R,RLA,NMIN)
    STE(4,2)=STE(5,2)-STE(3,2)-STE(2,2)
    DST=STE(1,2)-STE(1,1)
    CALL STOSS(STE(1,1),STE(1,2),STE(1,3),F1,F2,F3,NEF,ES,F)
    DO 21 J1=2,4
    FLC1=(3.*STE(J1,1)*F1+STE(J1,3)*F3)*DST*.25
    FLC2=(STE(J1,1)*F1+STE(J1,2)*F2)*DST*.5
    IF(FLC1)45,21,45
 45 AFL=ABS((FLC1-FLC2)/FLC1)
    IF(AFL-PR     )21,21,22
 21 CONTINUE
    DO 24 J1=1,3
 24 SUMO(J1)=(STE(J1+1,1)*F1+STE(J1+1,2)*F2)*DST*.5+SUMO(J1)
    SUME=SUME+(F1+F2)*DST*.5
    DO 25 ISO=1,NS
    SIG1=STE(5,1)+SIGO(ISO)
    SIG2=STE(5,2)+SIGO(ISO)
    SIG3=SIG1*SIG1
    SIG4=SIG2*SIG2
    SUM(ISO,5)=(F1/SIG3+F2/SIG4)*DST*.5+SUM(ISO,5)
    SUM(ISO,1)=(F1/SIG1+F2/SIG2)*DST*.5+SUM(ISO,1)
    DO 325 J1=6,7
325 SUM(ISO,J1)=(STE(J1-2,1)*F1/SIG3+STE(J1-2,2)*F2/SIG4)*DST*.5
   1+SUM(ISO,J1)
    DO 25 J1=2,4
 25 SUM(ISO,J1)=(STE(J1,1)*F1/SIG1+STE(J1,2)*F2/SIG2)*DST*.5+SUM(ISO,J
   11)
    DO 27 J1=2,4
    FLC1=(STE(J1,1)*F1+3.*STE(J1,3)*F3)*DST*.25
    FLC2=(STE(J1,2)*F2+STE(J1,3)*F3)*DST*.5
    IF(FLC1)46,27,46
 46 AFL=ABS((FLC1-FLC2)/FLC1)
    IF(AFL-PR     )27,27,28
 27 CONTINUE
    DO 29 J1=1,3
 29 SUMO(J1)=(STE(J1+1,2)*F2+STE(J1+1,3)*F3)*DST*.5+SUMO(J1)
    SUME=SUME+(F2+F3)*DST*.5
    DO 30 ISO=1,NS
    SIG1=STE(5,2)+SIGO(ISO)
    SIG2=STE(5,3)+SIGO(ISO)
    SIG3=SIG1*SIG1
    SIG4=SIG2*SIG2
    SUM(ISO,5)=SUM(ISO,5)+(F2/SIG3+F3/SIG4)*DST*.5
    SUM(ISO,1)=SUM(ISO,1)+(F2/SIG1+F3/SIG2)*.5*DST
    DO 330 J1=6,7
330 SUM(ISO,J1)=SUM(ISO,J1)+(STE(J1-2,2)*F2/SIG3+STE(J1-2,3)*F3/
   1SIG4)*DST*.5
    DO 30 J1=2,4
 30 SUM(ISO,J1)=SUM(ISO,J1)+(STE(J1,2)*F2/SIG1+STE(J1,3)*F3/SIG2)*DST*
```

```
   1.5                                                                  1800
    DO 31 K=3,KMAX                                                      1810
    DO 31 J1=1,5                                                        1820
 31 STE(J1,K-2)=STE(J1,K)                                               1830
    KMAX=KMAX-2                                                         1840
    GOTO 22                                                             1850
 28 DO 32 J1=1,5                                                        1860
 32 STE(J1,1)=STE(J1,2)                                                 1870
    GOTO 35                                                             1880
 34 IF(IT.EQ.1.AND.IE.EQ.NANF)  GO TO 935                               1890
    GO TO 934                                                           1900
935 INDEX=0                                                             1910
    WRITE (LZWF) INDEX,MM                                               1920
934 INDEX=6                                                             1930
    WRITE(LZWF)INDEX,MATN     ,TEMP(IT),IE,ENG(IE),ENG(IE+1)            1940
    DO 38 ISO=1,3                                                       1950
 38 SUMO(ISO)=SUMO(ISO)/SUME                                            1960
    INDEX=5                                                             1970
    SGT1=SUMO(1)+SUMO(2)+SUMO(3)                                        1980
    WRITE(LZWF)INDEX,SUMO(2),SUMO(3),SUMO(1),SUMO(3),SGT1               1990
    INDEX=6                                                             2000
    WRITE(NOUTP,957)                                                    2010
957 FORMAT(1HO,18X,8HMATERIAL,3X,10HTEMPERATUR,2X,6HGRUPPE,7X,7HGRENZE  2020
   1N)                                                                  2030
    IV=NE-IE                                                            2040
    WRITE(NOUTP,958)MATN     ,TEMP(IT),IV,ENG(IE),ENG(IE+1)             2050
958 FORMAT(1H ,18X,A5,F14.2,6X,I2,1X,2E12.4/1X)                         2060
    WRITE(NOUTP,950)                                                    2070
950 FORMAT(1HO,21X,7HSIGMA G,9X,7HSIGMA N,9X,7HSIGMA F,9X,7HSIGMAN1,    2080
   19X,7HSIGMAT1)                                                       2090
    WRITE (NOUTP,951) SUMO(2),SUMO(3),SUMO(1),SUMO(3),SGT1              2100
951 FORMAT(1H ,15X,5E16.8)                                              2110
    WRITE(NOUTP,952)                                                    2120
952 FORMAT(1HO,6X,7HSIGMA 0,11X,2HFG,14X,2HFN,14X,2HFF,14X,3HFN1,       2130
   113X,3HFT1/1X)                                                       2140
    DO 39 ISO=1,NS                                                      2150
    DO 40 J1=2,4                                                        2160
    IF(SUMO(J1-1))420,421,420                                           2170
421 SUM(ISO,J1)=1.                                                      2180
    GOTO 40                                                             2190
420 SUM(ISO,J1)=SUM(ISO,J1)/(SUM(ISO,1)*SUMO(J1-1))                     2200
 40 CONTINUE                                                            2210
    SUM(ISO,6)=SUM(ISO,6)/(SUM(ISO,5)*SUMO(3))                          2220
    SUM(ISO,7)=SUM(ISO,7)/(SUM(ISO,5)*(SUMO(1)+SUMO(2)+SUMO(3)))        2230
    WRITE (NOUTP,953)SIGO(ISO),SUM(ISO,3),SUM(ISO,4),SUM(ISO,2)         2240
   1,SUM(ISO,6),SUM(ISO,7)                                              2250
 39 WRITE(LZWF) INDEX,SIGO(ISO),SUM(ISO,3),SUM(ISO,4),SUM(ISO,2)        2260
   1,SUM(ISO,6),SUM(ISO,7)                                              2270
953 FORMAT(6E16.8)                                                      2280
 10 CONTINUE                                                            2290
 60 CONTINUE                                                            2300
  3 CONTINUE                                                            2310
111 KL=KL+1                                                             2320
    RETURN                                                              2330
    END                                                                 2340
```

```
    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
    XKO=8.6165E-5                                                       80
    ERI=ER(INR)                                                         90
    IF(ERI)20,20,21                                                    100
 20 ERI=1.                                                             110
    GOTO 21                                                            120
 21 ELA=RLA/SQRT(ERI)                                                  130
    SOC=4.*PI*ELA**2*GJ(INR)*GAN(INR)/GAT(INR)                         140
    XLEX=FLOAT(L(INR))-0.5                                             150
    SOC=SOC*(E/ERI)**XLEX                                              160
    X=2.*(E-ER(INR))/GAT(INR)                                          170
    IT=T                                                               180
    IF(IT)4,5,4                                                        190
  5 PSI=1./(1.+X*X)                                                    200
    CHI=X*PSI                                                          210
    GOTO 6                                                             220
  4 DELTA=SQRT(4.*XKO*T*ERI/A)                                         230
    TETA=(DELTA/GAT(INR))**2                                           240
    CALL PSIXI(X,TETA,PSI,CHI)                                         250
  6 IF(L(INR)-1)1,1,2                                                  260
  2 SG=.0                                                              270
    SF=.0                                                              280
    ST=.0                                                              290
    GOTO 3                                                             300
  1 SG=SOC*GAG(INR)*PSI/GAT(INR)                                       310
    SF=SOC*GAF(INR)*PSI/GAT(INR)                                       320
    ELA=RLA/SQRT(E)                                                    330
    DELTA1=2.*(R/ELA-ATAN(R*FLOAT(L(INR))/ELA))                        340
    ST=SOC*(PSI*COS(DELTA1)+CHI*SIN(DELTA1))                           350
    SIGP=4.*PI*R**2                                                    360
    IF(ST+SIGP)10,10,3                                                 370
 10 WRITE(NOUTP,900)ER(INR),E,ST,SIGP                                  380
900 FORMAT(1HO,77H***WARNING 1.01 : THE CONTRIBUTION OF THE RESONANCE  390
   1WITH THE RESONANCE ENERGY,E13.6,3H EV/1H ,18X,13HAT THE ENERGY,E14  400
   2.6,13H IS NEGATIVE,,E14.6,22H BARNS,AND ITS ABSOLUT/1H ,18X,46HVAL  410
   3UE LARGER THAN THE POTENTIAL CROSS SECTION,E14.6,7H BARNS.)         420
  3 RETURN                                                             430
    END                                                                440
```

```
    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
      SIGP=4.*PI*R**2                                                   90
      NR2=NR1+1                                                        100
      DO 1 I=1,NR1                                                     110
      NR3=NR2-I                                                        120
      IF(E-ER(NR3))1,2,2                                               130
    1 CONTINUE                                                         140
    2 SIFG=0.                                                          150
      SIGG=.0                                                          160
      SIGT=SIGP                                                        170
      IA=NR3-NMIN                                                      180
      IF(IA)3,3,4                                                      190
    3 IA=1                                                             200
    4 IE=NR3+NMIN                                                      210
      IF(IE-NR)5,6,6                                                   220
    6 IE=NR                                                            230
    5 DO 7 INR=IA,IE                                                   240
      CALL WIRQ(INR,E,SF,SG,ST,IRE,                                    250
     1                        ER,GJ,GAN,GAT,GAF,L,GAG,T,A,R,RLA)      260
      SIFG=SIFG+SF                                                     270
      SIGG=SIGG+SG                                                     280
      SIGT=SIGT+ST                                                     290
    7 CONTINUE                                                         300
      IF(SIGT)10,10,11                                                 310
   10 WRITE(NOUTP,900)SIGT,E                                           320
   11 CONTINUE                                                         330
  900 FORMAT(1HO,'***WARNING 1.02 : THE TOTAL CROSS SECTION IS NEGATIVE,  340
     1',E14.6,' BARNS, AT THE ENERGY'/19X,E14.8,' EV. THE TOTAL CROSS SE  350
     2CTION HAS BEEN SET EQUAL TO 1. BARN')                            360
      SING=SIGT-SIGG-SIFG                                              370
      IF(SING-1.0)12,13,13                                             380
   12 SING=1.0                                                         390
      SIGT=SING+SIGG+SIFG                                              400
   13 RETURN                                                           410
      END                                                              420
```

```
      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     W 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 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(100),NN(5),NAME(4),X(100),IX(100),CHI(25,4),GF(10,100),         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),XSUG1(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
     X0.544925,0.61641525,0.693415,0.77684375,0.867878,0.968046,         180
     X1.0793867,1.2047147,1.3480617,1.5155082,1.716864,1.9695355,        190
     X2.309333,2.832582,4.2188757,5.9001333E-2,C.1333242,0.19497146,     200
     X0.251645,0.3074142,0.36262126,0.4181491,0.4746072,0.53251576,      210
     X0.5965109,0.65162876,0.7165988,0.78492293,0.86824213,0.94071066,   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
     X0.26520225,0.32682625,0.3842565,0.43967925,0.49512475,0.545537,    250
     X0.6059465,0.659715,0.717307,0.77698,0.83930475,0.90493675,         260
     X0.97467075,1.049486,1.1306795,1.2199627,1.319785,1.4337535,        270
     X1.567579,1.7310672,1.9429085,2.2809085,3.089838/                   280
      WRITE (NOUTP,9000)                                                 290
 9000 FORMAT(1HO/1HO/' PROGRAMM KENNZIFFER 2')                           300
      WRITE (NOUTP,9001)                                                 310
 9001 FORMAT(' PROGRAMM ZUR BERECHNUNG VON RESONANZSELBSTABSCHIRMFAKTORE  320
     1N VON STATISTISCHEN RESONANZPARAMETERN'/)                          330
      NEFE=NFE                                                           340
      IF(NFE.EQ.1)  NEFE=0                                               350
      ISIG=0                                                             360
      IF(SIGO(MI).GE.1.E6)  GO TO 260                                    370
      MI=MI+1                                                            380
      SIGO(MI)=1.E6                                                      390
      ISIG=1                                                             400
  260 CALL DOPW (8HFSTAT   ,MM)                                          410
      CALL DOPW (8HBEST    ,NN(1))                                       420
      CALL DOPW (8HISOT1   ,NN(2))                                       430
      CALL DOPW (8HISOT2   ,NN(3))                                       440
      CALL DOPW (8HST      ,NN(4))                                       450
      CALL DOPW (8HSTGF    ,NN(5))                                       460
      I=0                                                                470
      WRITE (LIZ)I,MM                                                    480
      NGR=J-NANF                                                         490
      NEN=J+1-NEND                                                       500
      IX(1)=MAT                                                          510
      IX(2)=NN(1)                                                        520
      IX(3)=NN(2)                                                        530
      NAME(1)=3                                                          540
      CALL NDFLOC (KONTR,NAME,X,NUDAT,IS)                                550
      IF(KONTR)51,51,62                                                  560
   51 WRITE(NOUTP,153)KONTR                                              570
  153 FORMAT(1HO,3X,7HKONTR =I3)                                         580
      GO TO 1000                                                         590
   62 DEL=344.489/X(4)                                                   600
      SPIN=DABS(X(6))                                                    610
      IX(3)=NN(3)                                                        620
      CALL NDFLOC(KONTR,NAME,X,NUDAT,IS)                                 630
      IF(KONTR)51,51,63                                                  640
   63 XA=X(4)*X(4)                                                       650
      RQU=X(5)*X(5)                                                      660
      EBI=X(6)                                                           670
      IX(3)=NN(4)                                                        680
      IT=1                                                               690
      CALL NDFLOC(KONTR,NAME,X,NUDAT,IS)                                 700
      IF(KONTR)51,51,28                                                  710
   28 GG(IT)=X(6)*1.E3                                                   720
      XL(IT)=IX(4)                                                       730
      IF(XL(IT)-5.E-5.LE.1.)  GO TO 3000                                 740
      WRITE (NOUTP,3001)                                                 750
 3001 FORMAT(1HO,'***ERROR 2.01 : A CALCULATION OF RESONANCE SELFSHIELDI  760
     1NG FACTORS FOR L.GT.1 (L=ANGULAR MOMENTUM) IS NOT POSSIBLE')       770
      GO TO 1000                                                         780
 3000 DN(IT)=X(7)*1.E3                                                   790
      GN(IT)=X(8)*1.E3                                                   800
      GI(IT)=(2.*X(5)+1.)/(4.*SPIN+2.)                                   810
      FXNYN(IT)=IX(10)                                                   820
      XNYN(IT)=IX(11)                                                    830
      CALL NDFNXT(KONTR,NAME,X,NUDAT,IS)                                 840
      IF(KONTR)65,65,66                                                  850
   66 IT=IT+1                                                            860
      GO TO 28                                                           870
   65 IF(ISPA)    1000,201,404                                           880
  404 NAME(1)=3                                                          890
      IX(1)=MAT                                                          900
      IX(2)=NN(1)                                                        910
      IX(3)=NN(5)                                                        920
      IY=1                                                               930
      KI=1                                                               940
      CALL NDFLOC(KONTR,NAME,X,NUDAT,IS)                                 950
```

```
  93 IF(KONTR)51,51,74                                                    960
  74 IF(X(4).LT.ENG(NGR+1))  GO TO 75                                     970
     WRITE(NOUTP,9002)ENG(NGR),ENG(NGR+1)                                 980
9002 FORMAT(1H0,37H***ERROR 2.02 : THE ENERGY GROUP FROM,E16.8,6H EV TO   990
    1,E16.8,22H EV IS NOT POSSIBLE IN/19X,67HTHIS MODULE,BECAUSE NO STA  1000
    2TISTICAL INFORMATION IS AVAILABLE IN THIS/19X,21HENERGYRANGE ON KE  1010
    3DAK.)                                                               1020
     NGR=NGR+1                                                           1030
     IF(NGR-NEN)74,1000,1000                                             1040
  75 IF(X(4).LE.ENG(NGR))  GO TO 76                                      1050
     EY(IY)=ENG(NGR)                                                     1060
     GF(KI,IY)=X(8)*1.E3                                                 1070
     EY(IY+1)=X(4)                                                       1080
     GF(KI,IY+1)=X(8)*1.E3                                               1090
  78 KI=KI+1                                                             1100
     IF(KI.GT.IT)  GO TO 92                                              1110
     CALL NDFNXT(KONTR,NAME,X,NUDAT,IS)                                  1120
     GO TO 93                                                            1130
  92 KI=1                                                                1140
     IY=IY+1                                                             1150
     NEY=IY-1                                                            1160
  79 CALL NDFNXT(KONTR,NAME,X,NUDAT,IS)                                  1170
     IF(KONTR)201,201,91                                                 1180
  76 EY(IY)=X(4)                                                         1190
     GF(KI,IY)=X(8)*1.E3                                                 1200
     GO TO 78                                                            1210
  91 EY(IY)=X(4)                                                         1220
     GF(KI,IY)=X(8)*1.E3                                                 1230
     KI=KI+1                                                             1240
     IF(KI.GT.IT)  GO TO 92                                              1250
     GO TO 79                                                            1260
 201 DO 7  I=1,MT                                                        1270
     TT=TEMP(I)                                                          1280
     IF(TT.EQ.0)  GO TO 700                                              1290
     K=NGR-1                                                             1300
     N=1                                                                 1310
     IF(K+1-NEN)4,1000,1000                                              1320
   4 K=K+1                                                               1330
     E(N)=ENG(K)                                                         1340
  16 CALL QUER(E(N),TT,N,SE        ,SM        ,XNYN,FXNYN,DEL,RQU,CHI,  1350
    1DN,EBI,XA,XL,GN,GG,NEY,EY,GF,GI,IT,MI,SIGO)                         1360
  21 GO TO (23,24,25),N                                                  1370
  23 IF(K+1-NEN)6,6,7                                                    1380
   6 IF(EY(NEY).LT.ENG(K+1))  GO TO 7                                    1390
     N=2                                                                 1400
     E(N)=(ENG(K)+ENG(K+1))*0.5                                          1410
     GO TO 16                                                            1420
  24 N=3                                                                 1430
     GO TO 4                                                             1440
  25 LIJ=5                                                               1450
 128 IF(NEFE)300,301,300                                                 1460
 301 DO 1 IST=1,3                                                        1470
   1 EF(IST)=PHI(E(IST))                                                 1480
     GO TO 27                                                            1490
 300 L=2                                                                 1500
     DO 5 IST=1,3                                                        1510
     DO 12  KK=L,NEFE                                                    1520
     IF(REFE(KK)-E(IST))12,38,213                                        1530
  12 CONTINUE                                                            1540
     KK=NEFE                                                             1550
 213 EF(IST)=EFE(KK-1)+(EFE(KK)-EFE(KK-1))/(REFE(KK)-REFE(KK-1))*(E(IST  1560
    1)-REFE(KK-1))                                                       1570
     GO TO 26                                                            1580
  38 EF(IST)=EFE(KK)                                                     1590
  26 L=KK                                                                1600
   5 CONTINUE                                                            1610
  27 H=(E(3)-E(2))*3.333333E-1                                           1620
     DO 29 KI=1,MI                                                       1630
     DO 29  IS=1,LIJ                                                     1640
     IF(SE(1,IS,KI).NE.-99999..AND.SE(2,IS,KI).NE.-99999..AND.SE(3,IS,   1650
    1KI).NE.-99999.)  GO TO 2000                                         1660
     XEUGZ(IS,KI)=-99999.                                                1670
     GO TO 29                                                            1680
2000 XEUGZ(IS,KI)=H*(SE(1,IS,KI)*EF(1)+4.*SE(2,IS,KI)*EF(2)+SE(3,IS,KI)  1690
    1*EF(3))                                                             1700
  29 CONTINUE                                                            1710
     DO 30  IS=1,LIJ                                                     1720
     IF(SM(1,IS,1).NE.-99999..AND.SM(2,IS,1).NE.-99999..AND.SM(3,IS,1)   1730
    1.NE.-99999.)  GO TO 2001                                            1740
     SU(IS)=-99999.                                                      1750
     GO TO 2002                                                          1760
2001 SU(IS)=H*(SM(1,IS,1)*EF(1)+4.*SM(2,IS,1)*EF(2)+SM(3,IS,1)*EF(3))    1770
2002 IF(SE(1,IS,MI).NE.-99999..AND.SE(2,IS,MI).NE.-99999..AND.SE(3,IS,   1780
    1MI).NE.-99999.)  GO TO 2004                                         1790
     XSUG1(IS)=-99999.                                                   1800
     GO TO 30                                                            1810
2004 XSUG1(IS)=H*(SE(1,IS,MI)*EF(1)+4.*SE(2,IS,MI)*EF(2)+SE(3,IS,MI)*EF  1820
    1(3))                                                                1830
  30 CONTINUE                                                            1840
     XNE=H*(EF(1)+4.*EF(2)+EF(3))                                        1850
     DO 32  KI=1,MI                                                      1860
     DO 32  IS=1,LIJ                                                     1870
     IF(XEUGZ(IS,KI).NE.-99999..AND.XSUG1(IS).NE.-99999.)  GO TO 2003    1880
     XEUGZ(IS,KI)=-99999.                                                1890
     GO TO 32                                                            1900
2003 XEUGZ(IS,KI)=XEUGZ(IS,KI)/XSUG1(IS)                                 1910
  32 CONTINUE                                                            1920
     DO 31  IS=1,LIJ                                                     1930
     IF(SU(IS).EQ.-99999.)  GO TO 31                                     1940
     SU(IS)=SU(IS)/XNE                                                   1950
  31 CONTINUE                                                            1960
     KI=K-1                                                              1970
     IS=J-KI                                                             1980
     WRITE (NOUTP,130) MAT    ,TT,IS,ENG(KI),ENG(K)                      1990
 130 FORMAT(1H0,16X,8HMATERIAL,2X,10HTEMPERATUR,2X,6HGRUPPE,8X,7HGRENZE  2000
    1N/1H ,17X,A5,4X,F8.2,5X,I3,2E12.4)                                  2010
     IN=6                                                                2020
     WRITE (LIZ)IN,MAT    ,TT,KI,ENG(KI),ENG(K)                          2030
 132 WRITE(NOUTP,37)(SU(IS),IS=1,LIJ)                                    2040
  37 FORMAT(1H0,20X,7HSIGMA G,9X,7HSIGMA N,9X,7HSIGMA F,9X,7HSIGMAN1,     2050
    19X,7HSIGMAT1/1H ,14X,5E16.8)                                        2060
     IN=LIJ                                                              2070
```

```
      WRITE(LIZ)IN,(SU(IS),IS=1,LIJ)                                    2080
      WRITE(NOUTP,138)                                                  2090
  138 FORMAT(1HO,5X,7HSIGMA 0,11X,2HFG,14X,2HFN,14X,2HFF,14X,3HFN1,13X, 2100
     13HFT1/1X)                                                         2110
      DO 139  KK=1,MI                                                   2120
      WRITE(NOUTP,36)SIGO(KK),(XEUGZ(IS,KK),IS=1,LIJ)                   2130
   36 FORMAT(1X,E15.8,5E16.8)                                           2140
      IN=LIJ+1                                                          2150
  139 WRITE(LIZ)IN,SIGO(KK),(XEUGZ(IS,KK),IS=1,LIJ)                     2160
   40 DO 70  KK=1,MI                                                    2170
      DO 70  IN=1,LIJ                                                   2180
      SE(1,IN,KK)=SE(3,IN,KK)                                           2190
   70 SM(1,IN,KK)=SM(3,IN,KK)                                           2200
      E(1)=E(3)                                                         2210
      GO TO 23                                                          2220
  700 WRITE (NOUTP,701)                                                 2230
  701 FORMAT(1HO,93H***ERROR 2.03 : A CALCULATION OF RESONANCE SELF SHIE 2240
     1LDING FACTORS AT ZERO TEMPERATURE (DEGREE/17X,39HKELVIN) IS NOT PO 2250
     2SSIBLE IN THIS MODULE,)                                           2260
    7 CONTINUE                                                          2270
 1000 IF(ISIG.EQ.1)  MI=MI-1                                            2280
      BACKSPACE LIZ                                                     2290
      READ(LIZ) I,NN(1)                                                 2300
      IF(I.EQ.0.AND.NN(1).EQ.MM)  BACKSPACE LIZ                         2310
      KL=KL+1                                                           2320
      RETURN                                                            2330
      END                                                               2340
```

```
      SUBROUTINE QUER (E,TT,N,SE,SM,XNYN,FXNY,DEL,RQU,CHI,   DN,EBI,XA,    10
     1XL,GN,GG,NEY,EY,GFA,GI,IT,MI,SIGO)                                  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(100),          60
     3GFA(10,100),GI(10)                                                  70
      COMMON MAT,ISTRUK,ISPA,NOUTP,LIZ,NANF,NENE,KL                       80
      C=0.5                                                               90
      TEST=0.1                                                           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
      ACI(I)=AC(I)*PH(I)                                                 290
    1 ST=ST+ACI(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=DMIT(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)+GAFN(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 2.01 : 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
      IF((ST-ACI(I)).GT.0)  GO TO 23                                     500
      DO 26 L=IJ,5                                                       510
      SE(N,L,K)=-99999.                                                  520
   26 SM(N,L,K)=-99999.                                                  530
      WRITE (NOUTP,42)SIGO(K),I                                          540
   42 FORMAT(1HO,28H***WARNING 2.02 : FOR SIGO =,E12.5,33H SPEFF* IS NEG 550
     1ATIVE IN THE SERIES,I4)                                            560
      GO TO 25                                                           570
   23 A(3)=0.                                                            580
      B(3)=0.                                                            590
      AA=0.398942*ACI(I)*D*EZC/(DL*SPI)                                  600
      IF(AA-TEST)3,3,4                                                   610
    3 BT=(1.-AA)*D*ACI(I)/SPI                                            620
      B(1)=(1.-AA*EZG/EZC)*D*A(1)/SPI                                    630
      IF(ISPA     )5,5,6                                                 640
    6 A(3)=AC(I)*DRFS                                                    650
      B(3)=(1.-AA*EZF/EZC)*D*A(3)/SPI                                    660
    5 A(2)=ACI(I)-A(3)-A(1)                                              670
      B(2)=BT-B(1)-B(3)                                                  680
      QF=1.+ACI(I)/(SPI+ACI(I))                                          690
      BT=QF*BT                                                           700
      B(1)=QF*B(1)                                                       710
      B(2)=QF*B(2)                                                       720
      B(3)=QF*B(3)                                                       730
      IF(ISE.EQ.0)  GO TO 27                                             740
      A(4)=A(2)                                                          750
      A(5)=ACI(I)                                                        760
      B(4)=B(2)                                                          770
      B(5)=BT                                                            780
   27 XNEN=1./(1.-BT/D+XY*ACI(I))                                        790
      IF(XNEN.GT.0)  GO TO 202                                           800
```

```
      WRITE (NOUTP,203)                                                 810
  203 FORMAT(1H0,52H***WARNING 2.03 : INACCURATE CVERLAPPING CORRECTION.  820
     1)                                                                 830
  202 CONTINUE                                                          840
      DO 57 L=IJ,KJ                                                    850
      TERM(L)=(ST-ACI(I))*XNEN*(B(L)/D-XY*A(L))                         860
      SE(N,L,K)=SE(N,L,K)+TERM(L)                                       870
    7 SM(N,L,K)=SM(N,L,K)+A(L)                                          880
   57 CONTINUE                                                          890
      GO TO 20                                                          900
    4 GO=GAMN(E,I,GN,RQU,XL,XA)                                         910
      CI=SPI*GO*1.5707963/(ACI(I)*D)                                    920
      IF(ISPA     )8,8,9                                                930
    8 GF=0.                                                             940
      NF=1                                                              950
      NN=25                                                             960
      GFF(1)=0.                                                         970
      NU=XNYN(I)                                                        980
      DO 10 M=1,NN                                                      990
   10 GNN(M)=GO*CHI(M,NU)                                              1000
   11 GAX=GAMG(E,I,GG)                                                 1010
      BT=0.                                                            1020
      B(1)=0.                                                          1030
      B(2)=0.                                                          1040
      LG=1                                                             1050
      DO 12 M=1,NN                                                     1060
      GNX=GNN(M)                                                       1070
      DO 12 NI=1,NF                                                    1080
      GFX=GFF(NI)                                                      1090
      GTX=GAX+GNX+GFX                                                  1100
      XK=1.442695*ALOG(1.E5*CI*GTX/GNX)                                1110
      XT=GTX/DL                                                        1120
      CALL TAB (XT,XK,LG,DSJ,XABCJ,DJK)                                1130
      B(3)=B(3)+GFX*XABCJ                                              1140
      B(1)=B(1)+XABCJ                                                  1150
   12 BT=BT+GTX*XABCJ                                                  1160
      AZ=NN                                                            1170
      BZ=NF                                                            1180
      FK=AZ*BZ                                                         1190
      B(1)=B(1)*GAX/(PH(I)*FK)                                         1200
      B(3)=B(3)/(PH(I)*FK)                                             1210
      BT=BT/FK                                                         1220
      GO TO 5                                                          1230
    9 NU=XNYN(I)                                                       1240
      A(3)=AC(I)*DRFS                                                  1250
      NN=25                                                            1260
      NF=25                                                            1270
      DO 200 M=1,NN                                                    1280
  200 GNN(M)=GO*CHI(M,NU)                                              1290
      GF=GAFM(E,I,NEY,EY,GFA)                                          1300
      NU=FXNY(I)                                                       1310
      DO 201 M=1,NF                                                    1320
  201 GFF(M)=GF*CHI(M,NU)                                              1330
      GO TO 11                                                         1340
   20 IF(ISE.EQ.1)  GO TO 21                                           1350
      ISE=1                                                            1360
      FT=ST                                                            1370
      ST=ST*0.5                                                        1380
      IJ=4                                                             1390
      KJ=5                                                             1400
      GO TO 22                                                         1410
   21 ST=FT                                                            1420
    2 CONTINUE                                                         1430
   25 CONTINUE                                                         1440
      RETURN                                                           1450
      END                                                              1460
```

```
      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(100),GF(10,100),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
      DO 1 I=1,2                                                        120
      X(I)=.0                                                           130
    1 Y(I)=.0                                                           140
      IF(ISPA     )6,6,5                                                150
    5 NN=25                                                             160
      NF=25                                                             170
      XFN=625.                                                          180
    7 DO 2 I=1,NN                                                       190
      DO 2 J=1,NF                                                       200
      X1=((GNN*CHI(I,NY))**2)/(GNN*CHI(I,NY)+GNG+GNF*CHI(J,NFY))        210
      Y1=GNN*CHI(I,NY)/(GNN*CHI(I,NY)+GNG+GNF*CHI(J,NFY))               220
      X(1)=X(1)+X1                                                      230
      Y(1)=Y(1)+Y1                                                      240
      X(2)=X(2)+X1*GNF*CHI(J,NFY)                                       250
    2 Y(2)=Y(2)+Y1*GNF*CHI(J,NFY)                                       260
      EZG=X(1)/(Y(1)*GNN)                                               270
      EZC=1.+2./XNYN(NS)                                                280
      EZF=X(2)/(Y(2)*GNN)                                               290
      DRSG=Y(1)*GNG/(GNN*XFN)                                           300
      DRFS=Y(2)/(GNN*XFN)                                               310
      GO TO 10                                                          320
    6 NN=25                                                             330
      XFN=25.                                                           340
      DO 3 I=1,NN                                                       350
      X1=((GNN*CHI(I,NY))**2)/(GNN*CHI(I,NY)+GNG)                       360
      Y1=GNN*CHI(I,NY)/(GNN*CHI(I,NY)+GNG)                              370
      X(1)=X(1)+X1                                                      380
    3 Y(1)=Y(1)+Y1                                                      390
      EZG=X(1)/(Y(1)*GNN)                                               400
      EZC=1.+2./XNYN(NS)                                                410
```

```
      EZF=.0                                                            420
      DRSG=Y(1)*GNG/(GNN*XFN)                                           430
      DRFS=.0                                                           440
   10 CONTINUE                                                          450
      RETURN                                                            460
      END                                                               470
```

```
      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
      I1=I+K-2                                                         130
      X1(K)=EP (I1)                                                    140
    5 FX1(K)=EPP(I1)                                                   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(100),GF(10,100),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(100)                                                 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 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
  2T24(20),T25(20),T26(20),T27(20),T28(20),T29(20),T30(20),T31(20),     60
  4T32(20),T33(20)                                                      70
   EQUIVALENCE (XXK(1),R),(XXT(1),T),(XJ(1),U),                         80
  1           (A,C,Y),(B,D,Y1,V0),(T2,Y5,P,EAXG,XKO5,XXXK),             90
  2(T4,Y6,XKO6,J),(DK,RI),(XK1,SJ0),(XK2,SJ1),(DKA,R1,V1),(DKB,R2,V2)   100
  3,(DKC,R3,V3),(SV,N),(AB1,TD,M),(AB2,AXG),(SY1,XXXT,S1),              110
  4(XKO2,XJA2,S2),(SXM,XKO3,XJA3,S3),(XKC4,XJB1),(R1K,XJB2),            120
  5(R2K,XJB3),(R3K,XJC1),(BETA,XJC3),(K,SG,SJ3),(Y2,ZZK,XJ1),(Y3,       130
  6WG),(XJ3,Y4),          (SY,I),(XJC2,SJ2),(XJA1,SJ4)                 140
   EQUIVALENCE (XJ(1),T01(1)),(XJ(21),T02(1)),(XJ(41),T03(1)),          150
  1(XJ(61),T04(1)),(XJ(81),T05(1)),(XJ(101),T06(1)),(XJ(121),T07(1)),   160
  2(XJ(141),T08(1)),(XJ(161),T09(1)),(XJ(181),T10(1)),(XJ(201),T11(1)   170
  3),(XJ(221),T12(1)),(XJ(241),T13(1)),(XJ(261),T14(1)),(XJ(281),T15(   180
  41)),(XJ(301),T16(1)),(XJ(321),T17(1)),(XJ(341),T18(1)),(XJ(361),T1   190
  59(1)),(XJ(381),T20(1)),(XJ(401),T21(1)),(XJ(421),T22(1)),            200
  6(XJ(441),T23(1)),(XJ(461),T24(1)),(XJ(481),T25(1)),(XJ(501),T26(1)   210
  7),(XJ(521),T27(1)),(XJ(541),T28(1)),(XJ(561),T29(1)),(XJ(581),T30(   220
  81)),(XJ(601),T31(1)),(XJ(621),T32(1)),(XJ(641),T33(1))               230
   DATA XXK/ 5.2, 5.6, 6.0, 6.4, 6.8, 7.2, 7.6, 8.0, 8.4, 8.8, 9.2,     240
  X 9.6,10.0,10.4,10.8,11.2,11.6,12.0,12.4,12.8/                        250
   DATA XXT/0.01,0.02,0.03,0.04,0.05,0.06,0.07,0.08,0.09,0.10,0.11,     260
  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,    270
  X0.50,0.56,0.62,0.68,0.74,0.80,0.86,0.92,0.98/                        280
   DATA T01/348.3270,329.0620,309.3460,289.0880,268.2430,246.8240,      290
  X224.91800,202.69300,180.40300,158.38700,137.04200,116.78800,         300
  X 98.01930, 81.05280, 66.09140, 53.20820, 42.35590, 33.39130,         310
  X 26.11050, 20.28100/                                                 320
   DATA T02/205.0000,194.1000,183.5000,173.0000,162.5000,151.9000,      330
  X141.20000,130.20000,119.10000,107.80000, 96.43000, 85.17000,         340
  X 74.17000, 63.64000, 53.78000, 44.78000, 36.74000, 29.75000,         350
  X 23.80000, 18.85000/                                                 360
   DATA T03/154.4000,145.3000,136.9000,128.9000,121.2000,113.7000,      370
  X106.30000, 98.80000, 91.28000, 83.67000, 75.99000, 68.28000,         380
  X 60.61000, 53.09000, 45.83000, 38.98000, 32.65000, 26.95000,         390
  X 21.95000, 17.65000/                                                 400
   DATA T04/129.5430,120.8780,113.1000,105.9960, 99.3851, 93.1199,      410
  X 87.07990, 81.16910, 75.31440, 69.46550, 63.59470, 57.69990,         420
  X 51.80430, 45.95800, 40.23460, 34.72510, 29.52760, 24.73430,         430
  X 20.41850, 16.62540/                                                 440
   DATA T05/115.3000,106.6000, 99.0000, 92.2100, 86.0500, 80.3700,      450
  X 75.03000, 69.93000, 64.97000, 60.10000, 55.26000, 50.43000,         460
  X 45.60000, 40.81000, 36.08000, 31.47000, 27.06000, 22.93000,         470
  X 19.14000, 15.75000/                                                 480
   DATA T06/106.4000, 97.5700, 89.9000, 83.1800, 77.2000, 71.8000,      490
  X 66.84000, 62.19000, 57.76000, 53.47000, 49.27000, 45.13000,         500
  X 41.00000, 36.91000, 32.86000, 28.89000, 25.06000, 21.43000,         510
  X 18.05000, 14.98000/                                                 520
   DATA T07/100.5080, 91.4730, 83.6906, 76.9337, 71.0030, 65.7266,      530
  X 60.95750, 56.57200, 52.46730, 48.56010, 44.78500, 41.09360,         540
  X 37.45480, 33.85470, 30.29690, 26.80240, 23.40750, 20.15950,         550
  X 17.11060, 14.31030/                                                 560
   DATA T08/ 96.4200, 87.1900, 79.2700, 72.4300, 66.4800, 61.2400,      570
  X 56.58000, 52.35000, 48.45000, 44.79000, 41.30000, 37.93000,         580
  X 34.64000, 31.40000, 28.21000, 25.07000, 22.02000, 19.08000,         590
  X 16.29000, 13.72000/                                                 600
   DATA T09/ 93.4900, 84.0900, 76.0200, 69.0800, 63.0800, 57.8400,      610
  X 53.22000, 49.07000, 45.30000, 41.82000, 38.53000, 35.39000,         620
  X 32.36000, 29.39000, 26.48000, 23.62000, 20.83000, 18.14000,         630
  X 15.58000, 13.19000/                                                 640
   DATA T10/ 91.3415, 81.7729, 73.5745, 66.5357, 60.4667, 55.1985,      650
  X 50.58150, 46.48530, 42.79780, 39.42410, 36.28530, 33.31770,         660
  X 30.47200, 27.71280, 25.01900, 22.38310, 19.81150, 17.32270,         670
  X 14.94500, 12.71180/                                                 680
   DATA T11/ 89.7100, 80.0100, 71.6900, 64.5600, 58.4200, 53.1100,      690
  X 48.48000, 44.40000, 40.76000, 37.47000, 34.43000, 31.59000,         700
  X 28.89000, 26.30000, 23.78000, 21.32000, 18.92000, 16.60000,         710
  X 14.38000, 12.28000/                                                 720
   DATA T12/ 88.4600, 78.6400, 70.2200, 62.9900, 56.7800, 51.4200,      730
  X 46.77000, 42.70000, 39.09000, 35.84000, 32.88000, 30.14000,         740
  X 27.55000, 25.09000, 22.70000, 20.39000, 18.14000, 15.97000,         750
  X 13.88000, 11.90000/                                                 760
   DATA T13/ 87.4785, 77.5623, 69.0480, 61.7399, 55.4611, 50.0523,      770
  X 45.37000, 41.28650, 37.68900, 34.47960, 31.57410, 28.90220,         780
  X 26.40610, 24.04060, 21.77230, 19.58010, 17.45450, 15.39730,         790
  X 13.42070, 11.54430/                                                 800
   DATA T14/ 86.7000, 76.7000, 68.1000, 60.7200, 54.3800, 48.9200,      810
  X 44.21000, 40.11000, 36.51000, 33.32000, 30.46000, 27.84000,         820
```

```
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,
X  9.28662,  8.16990/
 DATA T23/ 82.5236, 72.0012, 62.8617, 54.9281, 48.0456, 42.0794,
X 36.91100, 32.43670, 28.56450, 25.21300, 22.30950, 19.78900,
X 17.59340, 15.67080, 13.97510, 12.46640, 11.11010,  9.87782,
X  8.74691,  7.70062/
 DATA T24/ 82.3662, 71.8216, 62.6574, 54.6965, 47.7842, 41.7860,
X 36.58420, 32.07560, 28.16950, 24.78600, 21.85410, 19.31000,
X 17.09880, 15.16850, 13.47470, 11.97790, 10.64360,  9.44274,
X  8.35127,  7.35063/
 DATA T25/ 82.2628, 71.7037, 62.5233, 54.5442, 47.6121, 41.5923,
X 36.36750, 31.83500, 27.90470, 24.49750, 21.54360, 18.98080,
X 16.75420, 14.81430, 13.11730, 11.62440, 10.30150,  9.11911,
X  8.05277,  7.08266/
 DATA T26/ 82.1914, 71.6222, 62.4304, 54.4388, 47.4928, 41.4579,
X 36.21670, 31.66690, 27.71890, 24.29400, 21.32300, 18.74490,
X 16.50530, 14.55600, 12.85400, 11.36100, 10.04360,  8.87225,
X  7.82223,  6.87307/
 DATA T27/ 82.1399, 71.5634, 62.3636, 54.3629, 47.4068, 41.3608,
X 36.10770, 31.54510, 27.58380, 24.14540, 21.16120, 18.57060,
X 16.32020, 14.36230, 12.65480, 11.16000,  9.84471,  8.67993,
X  7.64071,  6.70620/
 DATA T28/ 82.1016, 71.5197, 62.3138, 54.3063, 47.3427, 41.2885,
X 36.02630, 31.45410, 27.48250, 24.03370, 21.03900, 18.43850,
X 16.17910, 14.21370, 12.50080, 11.00330,  9.68843,  8.52743,
X  7.49539,  6.57129/
 DATA T29/ 82.0723, 71.4863, 62.2758, 54.2631, 47.2937, 41.2331,
X 35.96400, 31.38430, 27.40480, 23.94770, 20.94470, 18.33610,
X 16.06920, 14.09740, 12.37950, 10.87900,  9.56356,  8.40460,
X  7.37737,  6.46077/
 DATA T30/ 82.0494, 71.4602, 62.2461, 54.2293, 47.2554, 41.1898,
X 35.91530, 31.32960, 27.34380, 23.88010, 20.87040, 18.25520,
X 15.98200, 14.00470, 12.28240, 10.77890,  9.46232,  8.30433,
X  7.28033,  6.36920/
 DATA T31/ 82.0311, 71.4394, 62.2224, 54.2024, 47.2249, 41.1553,
X 35.87640, 31.28600, 27.29510, 23.82600, 20.81080, 18.19010,
X 15.91170, 13.92970, 12.20340, 10.69720,  9.37921,  8.22151,
X  7.19965,  6.29253/
 DATA T32/ 82.0164, 71.4226, 62.2032, 54.1806, 47.2002, 41.1274,
X 35.84490, 31.25060, 27.25560, 23.78210, 20.76240, 18.13710,
X 15.85430, 13.86820, 12.13850, 10.62960,  9.31019,  8.15236,
X  7.13192,  6.22775/
 DATA T33/ 82.0042, 71.4088, 62.1875, 54.1628, 47.1800, 41.1045,
X 35.81900, 31.22160, 27.22310, 23.74590, 20.72250, 18.09340,
X 15.80680, 13.81720, 12.08440, 10.57320,  9.25227,  8.09408,
X  7.07449,  6.17256/
  N=20
  M=33
  DO 1 I=1,N
  IF(XK-XXK(I))2,3,1
1 CONTINUE
3 IF(I-2)9,33,23
23 IF(I-N+1)33,33,9
33 XXXK=XK
  GO TO 12
2 IF(I-2)9, 5,24
24 IF(I-N+1)32,32,9
32 A=ABS (XK-XXK(I))
  B=XK-XXK(I-1)
  IF(B-A)4,4,5
4 XXXK=XXK(I-1)
  I=I-1
  GO TO 12
5 XXXK=XXK(I)
12 IF(XT-XXT(M-1))499,499,9
499 DO 6 J=1,M
  IF(XT-XXT(J))7,8,6
6 CONTINUE
8 IF(J-2)9,18,28
28 IF(J-M+1)18,18,9
18 XXXT=XT
  GO TO 13
7 IF(J-2)9,11,29
29 IF(J-M+1)17,17,9
17 C=ABS (XT-XXT(J))
  D=XT-XXT(J-1)
  IF(D-C)10,10,11
10 XXXT=XXT(J-1)
  J=J-1
  GO TO 13
```

```
 11 XXXT=XXT(J)                                                                  1950
 13 K=(J-1)*N+I                                                                  1960
    XJB2=XJ(K)                                                                   1970
    XJA2=XJ(K-1)                                                                 1980
    XJC2=XJ(K+1)                                                                 1990
    K=K-N                                                                        2000
    XJB1=XJ(K)                                                                   2010
    XJA1=XJ(K-1)                                                                 2020
    XJC1=XJ(K+1)                                                                 2030
    K=K+2*N                                                                      2040
    XJB3=XJ(K)                                                                   2050
    XJA3=XJ(K-1)                                                                 2060
    XJC3=XJ(K+1)                                                                 2070
    DK=XXXK-XXK(I-1)                                                             2080
    AB1=XXT(J+1)-XXXT                                                            2090
    AB2=XXXT-XXT(J-1)                                                            2100
    AB1=AB1/AB2                                                                  2110
    IF(LG-2)157,800,157                                                          2120
157 IF(XK-XXXK)159,159,70                                                        2130
159 XK1=(XXXK-XK)/DK                                                             2140
    XK2=(XK-XXK(I-1))/DK                                                         2150
    XJ1=XK1*XJA1+XK2*XJB1                                                        2160
    XJ2=XK1*XJA2+XK2*XJB2                                                        2170
    XJ3=XK1*XJA3+XK2*XJB3                                                        2180
    GO TO 71                                                                     2190
 70 XK1=(XXK(I+1)-XK)/DK                                                         2200
    XK2=(XK-XXXK)/DK                                                             2210
    XJ1=XK1*XJB1+XK2*XJC1                                                        2220
    XJ2=XK1*XJB2+XK2*XJC2                                                        2230
    XJ3=XK1*XJB3+XK2*XJC3                                                        2240
 71 DSJ=(AB1+1.)/(AB1*(XT-XXT(J-1))/(XJ3-XJ2)+(XT-XXT(J+1))/(XJ1-XJ2))           2250
    IF(LG)222,111,222                                                            2260
222 XABCJ=XJ2+(XT-XXXT)*DSJ                                                      2270
    IF(LG)800,800,221                                                            2280
221 IF(LG-1)111,111,800                                                          2290
800 XK1=XT-XXT(J-1)                                                              2300
    XK2=XT-XXT(J+1)                                                              2310
    XJ1=AB1/(AB1+1.)                                                             2320
    DKA=XJ1*(XK1/(XJA3-XJA2)+XK2/(XJA1-XJA2))                                    2330
    DKB=XJ1*(XK1/(XJB3-XJB2)+XK2/(XJB1-XJB2))                                    2340
    DKC=XJ1*(XK1/(XJC3-XJC2)+XK2/(XJC1-XJC2))                                    2350
    XK1=XT-XXXT                                                                  2360
    XJ1=XJA2+XK1/DKA                                                             2370
    XJ2=XJB2+XK1/DKB                                                             2380
    XJ3=XJC2+XK1/DKC                                                             2390
    DJK=(0.5*(XJ3-XJ1)+(XK-XXXK)/DK*(XJ3-2.*XJ2+XJ1))/DK                         2400
    GO TO 111                                                                    2410
  9 AXG=XT*XT                                                                    2420
    IF(LG)19,1119,19                                                             2430
 19 IF(XT-6.)1119,2229,2229                                                      2440
1119 TD=1./AXG                                                                   2450
    EAXG=EXP (0.25*AXG)                                                          2460
    XA=XT*0.8862269*(1.-ERF (0.5*XT))*EAXG                                       2470
    XM=1.253314*XT*(1.-ERF(7.071067E-1*XT))*EAXG*EAXG                            2480
    XKO4=SQRT (XA)                                                               2490
    WG=SQRT (((1.+2.*TD)*XA-1.)/(9.*XA*TD*TD))                                   2500

4449 BETA=2.**XK*1.E-5                                                           2510
    Y=XA/BETA                                                                    2520
    IF(LG)995,995,50                                                             2530
  50 IF(LG-1)995,700,995                                                         2540
 995 SV=2.*TD                                                                    2550
    T2=1./SV                                                                     2560
    T4=T2*T2                                                                     2570
    SXA=(-T4-T2)*XA+T4                                                           2580
    SXM=((-2.)*T4-T2)*XM+2.*T4                                                   2590
    DK=SV*XA                                                                     2600
    SG=(0.5*TD*DK*(SXA+2.*XA+SV*SXA)-((1.+SV)*XA-1.)*(DK+TD*TD*SXA))/            2610
   1(SV*DK*DK*TD)                                                                2620
    XKO1=SXA*0.5/XKO4                                                            2630
    XKO2=(XA*SXM-SXA*XM)/(XA*XA)                                                 2640
    XKO3=(SXA*WG-XA*SG*0.5/WG)/(WG*WG)                                           2650
    R1=(-17.)*XKO1-16.*XKO2+XKO3                                                 2660
    R2=5.3333333*(8.*XKO1+11.*XKO2-XKO3)                                         2670
    R3=5.3333333*((-5.)*XKO1-8.*XKO2+XKO3)                                       2680
    XKO5=XM/XA                                                                   2690
    XKO6=XA/WG                                                                   2700
    R1K=32.-17.*XKO4-16.*XKO5+XKO6                                               2710
    R2K=5.3333333*(-18.+8.*XKO4+11.*XKO5-XKO6)                                   2720
    R3K=5.3333333*(12.-5.*XKO4-8.*XKO5+XKO6)                                     2730
    SY=SXA/BETA                                                                  2740
    IF(Y-0.3)900,25,25                                                           2750
  25 SV=1./(1.+Y)                                                                2760
    XJ0=SQRT (SV)                                                                2770
    Y1=1./Y                                                                      2780
    XJ1=(1.-XJ0)*Y1                                                              2790
    XJ2=(0.5-XJ1)*Y1                                                             2800
    XJ3=(0.375-XJ2)*Y1                                                           2810
    XJ4=(0.3125-XJ3)*Y1                                                          2820
    SJC=SY*XJ0*SV*(-0.5)                                                         2830
    SY1=SY*Y1                                                                    2840
    SJ1=(-SJ0)*Y1-XJ1*SY1                                                        2850
    SJ2=(-SJ1)*Y1-XJ2*SY1                                                        2860
    SJ3=(-SJ2)*Y1-XJ3*SY1                                                        2870
    SJ4=(-SJ3)*Y1-XJ4*SY1                                                        2880
    GO TO 1000                                                                   2890
 900 XJ5=(((((((((0.1444644*Y-0.1494459)*Y+0.1549810)*Y-0.1611802)*Y             2900
   1+0.1681880)*Y-0.1761970)*Y+0.1854705)*Y-0.1963806)*Y+0.2094726)*Y            2910
   2-0.2255859)*Y+0.2460937                                                      2920
    XJ4=0.2734375-Y*XJ5                                                          2930
    XJ3=0.3125-Y*XJ4                                                             2940
    XJ2=0.375-Y*XJ3                                                              2950
    XJ1=0.5-Y*XJ2                                                                2960
    XJ0=1.-Y*XJ1                                                                 2970
    SJ5=(((((((((1.444644*Y-1.3450131)*Y+1.239848)*Y-1.1282614)*Y                2980
   1+1.009128)*Y-0.830985)*Y+0.741882)*Y-0.5851418)*Y+0.4189452)*Y-              2990
   20.2255859)*SY                                                                3000
    SJ4=-(SY*XJ5+Y*SJ5)                                                          3010
    SJ3=-(SY*XJ4+Y*SJ4)                                                          3020
    SJ2=-(SY*XJ3+Y*SJ3)                                                          3030
    SJ1=-(SY*XJ2+Y*SJ2)                                                          3040
    SJ0=-(SY*XJ1+Y*SJ1)                                                          3050
1000 DSJ=(-3.1415926)/(BETA*AXG  *XT)*(XKO1*XJC+R1*(-XJ1+2.*XJ2)+XKO4           3060
```

```
     1*SJ0+R1K*(-SJ1+2.*SJ2)+R2*((-3.)*XJ2+4.*XJ3)+R2K*((-3.)*SJ2+4.*    3070
     2SJ3)+R3*((-5.)*XJ3+6.*XJ4)+R3K*((-5.)*SJ3+6.*SJ4))                3080
      IF(LG)60,111,49                                                   3090
   49 IF(LG-1)111,111,60                                                3100
   60 IF(XT-6.)700,220,220                                              3110
  700 ZZK=XM/XA                                                         3120
      S1=1.-XK04                                                        3130
      S2=4.-2.*XK04-2.*ZZK                                              3140
      S3=1.+0.08333333*(XA/WG-5.*XK04-8.*ZZK)                           3150
 6669 RI=1.+Y                                                           3160
      V0=1./SQRT (RI)                                                   3170
      Y2=Y*Y                                                            3180
      Y3=Y2*Y                                                           3190
      Y4=Y2*Y2                                                          3200
      IF(Y-0.2)55,66,66                                                 3210
   55 V1=(-Y+8.)*Y/(16.*RI)+(Y4-8.*Y3)*(Y4-8.*Y3)/(4096.*((Y+2.)*Y+1.)  3220
     1*Y2)                                                              3230
      GO TO 77                                                          3240
   66 V1=(8.-((-Y+4.)*Y+8.)*V0)/Y2                                      3250
   77 IF(Y-2.)88,99,99                                                  3260
   88 SV=RI*RI                                                          3270
      Y5=2.+Y                                                           3280
      Y6=Y5*Y5*Y5                                                       3290
      V2=Y/(2.*Y5*RI)-Y3*Y2/(128.*Y6*SV)                                3300
      P=(3.*Y+16.)*Y+16.                                                3310
      V3=3.*Y2/(RI*P)-3.*Y4*Y4/(16.*SV*P*P*P)                           3320
      GO TO 44                                                          3330
   99 V2=(-8.-4.*Y+((Y+8.)*Y+8.)*V0)*4./Y3                              3340
      V3=(((-6.)*Y-32.)*Y-32.+(((Y+18.)*Y+48.)*Y+32.)*V0)*12./Y4        3350
   44 XABCJ=(V0-S1*V1+S2*V2+S3*V3)*1.5707963/BETA                       3360
      IF(LG)220,111,1111                                                3370
 1111 IF(LG-2)111,220,111                                               3380
  220 DJK=-0.69315*XABCJ-1.088797*Y/SXA*(XKC4*SJ0+R1K*(-SJ1+2.*SJ2)     3390
     1+R2K*(-3.*SJ2+4.*SJ3)+R3K*(-5.*SJ3+6.*SJ4))                       3400
      GO TO 111                                                         3410
 2229 BETA=2.**XK*1.E-5                                                 3420
      XABCJ=1.5707963/(BETA*SQRT (1.+1./BETA-6./AXG))                   3430
      IF(LG)1119,111,34                                                 3440
   34 IF(LG-1)111,111,1119                                              3450
  111 RETURN                                                            3460
      END                                                               3470
```

```
      SUBROUTINE FSTRUK(MI,SIGO,NE,ENG,NFE,REFE,EFE,XINTE,ZA,XN,SE,XII,     10
     1         ZB,XI,MDIM,MDIMP,EMU,XMU,NER,NERP,SN,EN)                    20
      REAL*8 MAT,NTYP,FEST,NFEST,NN                                        30
      DIMENSION ENG(NE),REFE(NFE),EFE(NFE),SIGO(MI),SN(NER ,3),EN(NER ,3   40
     1),FEST(10),ISTM(3)                                                   50
     2,NFEST(10),NADAT(2),NSATZ(4),E(3),FLUSS(2),ST(2),NTYP(6),            60
     3XINTE(NE,4),ZA(MI,NE,5),XN(MI,NE,4),SE(MI,NE,6),XII(NE),             70
     4          EMU(MDIM),XMU(MDIM),        ZB(MI,NE),XI(NE)               80
      COMMON MAT,ISTRUK,ISPA,NOUTP,JA,NANF,NEND,KL                         90
      EQUIVALENCE (FEST(1),NFEST(1))                                      100
      MDIMF=0                                                             110
      MDIMP=0                                                             120
      NERF=0                                                              130
      NERP=0                                                              140
      NEFE=NFE                                                            150
      IF(NFE.EQ.1)  NEFE=0                                                160
      CALL DOPW (8HSTRK     ,NN)                                          170
      CALL DOPW (8HSGA      ,NTYP(1))                                     180
      CALL DOPW (8HSGN      ,NTYP(2))                                     190
      CALL DOPW (8HSGF      ,NTYP(3))                                     200
      CALL DOPW (8HSGT      ,NTYP(4))                                     210
      CALL DOPW (8HBEST     ,NTYP(5))                                     220
      CALL DOPW (8HMUEL     ,NTYP(6))                                     230
      WRITE (NOUTP,9000)                                                  240
 9000 FORMAT(1HO/1HO/' PROGRAMM KENNZIFFER 3')                            250
      WRITE (NOUTP,9001)                                                  260
 9001 FORMAT(' PROGRAMM ZUR BERECHNUNG VON RESONANZSELBSTABSCHIRMFAKTORE  270
     1N VON PUNKTWEISE GEGEBENEN WIRKUNGSQUERSCHNITTEN'/)                 280
      IY=NE-NANF                                                          290
      NEN=NE+1-NEND                                                       300
      NSATZ(1)=3                                                          310
      NFEST(1)=MAT                                                        320
      NFEST(2)=NTYP(5)                                                    330
      JI=NEN-1                                                            340
      DO 3 LI=IY,JI                                                       350
      DO 3 LA=1,MI                                                        360
      ZB(LA,LI)=0.                                                        370
      DO 300 N=1,5                                                        380
  300 ZA(LA,LI,N)=0.                                                      390
      DO 3 N=1,4                                                          400
      XN(LA,LI,N)=0.                                                      410
      IF(ISTRUK.EQ.0.AND.N.EQ.3)  XN(LA,LI,N)=1.                          420
    3 CONTINUE                                                            430
      NFEST(3)=NTYP(6)                                                    440
      CALL NDFLOC(NSUCH1,NSATZ,FEST,NUDAT,NC)                             450
      IF(NSUCH1)85,85,1001                                                460
   85 WRITE(NOUTP,87)(NFEST(K),K=1,3)                                     470
   87 FORMAT(1HO/' ***ERROR 3. 1 : THE DATA FOR ',3A6,' COULD NOT BE FOU  480
     1ND IN THE KEDAK LIBRARY')                                           490
      GO TO 100                                                           500
 1001 EMU(1)=FEST(4)                                                      510
      XMU(1)=FEST(5)                                                      520
      M=2                                                                 530
 1005 IF(EMU(1)-ENG(IY))1002,1002,1004                                    540
 1004 WRITE (NOUTP,11) ENG(IY),(NFEST(K),K=1,3),EMU(1)                    550
      IY=IY+1                                                             560
      IF(IY-JI)1005,1005,1000                                             570
 1002 CALL NDFNXT(NSUCH1,NSATZ,FEST,NUDAT,NC)                             580
      IF(NSUCH1)1010,1010,1006                                            590
 1006 IF(FEST(4)-ENG(IY))1003,1003,1007                                   600
 1003 EMU(1)=FEST(4)                                                      610
      XMU(1)=FEST(5)                                                      620
      GO TO 1002                                                          630
 1007 IF(FEST(4)-ENG(NEN))1008,1014,1014                                  640
 1008 EMU(M)=FEST(4)                                                      650
      XMU(M)=FEST(5)                                                      660
```

```
      M=M+1                                                              670
      IF(M-MDIM)1002,1002,2000                                           680
 2000 M=1                                                                690
      MDIMF=MDIMF+1                                                      700
      GO TO 1002                                                         710
 1014 EMU(M)=FEST(4)                                                     720
      XMU(M)=FEST(5)                                                     730
      GO TO 1009                                                         740
 1010 M=M-1                                                              750
      DO 1011 LI=IY,NEN                                                  760
      IF(EMU(M)-ENG(LI))1013,1012,1011                                   770
 1011 CONTINUE                                                           780
 1012 NEN=LI                                                             790
      LI=NE-NEN+1                                                        800
      IF(NEN-1.LT.JI)  WRITE (NOUTP,1015) LI                             810
 1015 FORMAT(1HO/' ***WARNING 3. 1 : IT IS ONLY POSSIBLE TO CALCULATE UN 820
     1TIL GROUP ',I4,' BECAUSE KEDAK DOES NOT CONTAIN FURTHER MUEL VALUE 830
     2S')                                                                840
      JI=NEN-1                                                           850
      GO TO 1009                                                         860
 1013 NEN=LI-1                                                           870
      LI=NE-NEN+1                                                        880
      WRITE (NOUTP,1015) LI                                              890
      JI=NEN-1                                                           900
 1009 MM=M                                                               910
      IF(MDIMF.EQ.0)  GO TO 2001                                         920
      MDIMP=(MDIMF-1)*MDIM+M+1                                           930
      RETURN                                                             940
 2001 DO 2222 I=1,4                                                      950
      IF(I.EQ.3.AND.ISTRUK.EQ.0)  GO TO 2222                             960
      IF(IY-JI)400,400,1000                                              970
  400 L=IY                                                               980
      LY=2                                                               990
      NFEST(3)=NTYP(I)                                                  1000
      CALL NDFLOC(NSUCH1,NSATZ,FEST,NUDAT,NC)                           1010
      IF(NSUCH1)85,85,86                                                1020
   86 E(1)=FEST(4)                                                      1030
      SIG1=FEST(5)                                                      1040
      IF(I-3)121,121,120                                                1050
  121 EN(1,I)=FEST(4)                                                   1060
      SN(1,I)=FEST(5)                                                   1070
      IST=1                                                             1080
      IF(I.NE.2)  GO TO 120                                             1090
      DO 3012 KK=2,MM                                                   1100
      IF(EMU(KK)-E(1))3012,3013,3014                                    1110
 3012 CONTINUE                                                          1120
      GO TO 3007                                                        1130
 3013 XMU1=XMU(KK)                                                      1140
      GO TO 120                                                         1150
 3014 XMU1=XMU(KK-1)+(XMU(KK)-XMU(KK-1))*(E(1)-EMU(KK-1))/(EMU(KK)-     1160
     1EMU(KK-1))                                                        1170
  120 IX=1                                                              1180
   66 IF(E(1)-ENG(L))8,29,10                                            1190
   10 WRITE(NOUTP,11) ENG(L),(NFEST(K),K=1,3),E(1)                      1200
   11 FORMAT(1HO/' ***WARNING 3. 2 : THE LOWER ENERGY GROUP BOUNDARY ',  1210
     1E16.8,'EV IS NOT IN THE AVAILABLE ENERGY RANGE IN KEDAK FOR ',3A5/ 1220
     2' THE LOWER ENERGY GROUP BOUNDARY HAS BEEN MODYFIED TO ',E16.8,'EV 1230
     3')                                                                1240
      IY=IY+1                                                           1250
      GO TO 201                                                         1260
    8 CALL NDFNXT(NSUCH1,NSATZ,FEST,NUDAT,NC)                           1270
      IF(NSUCH1)12,12,13                                                1280
   12 WRITE(NOUTP,14)NFEST(1),NFEST(2),NTYP(I),E(1)                     1290
   14 FORMAT(1HO/' ***WARNING 3. 3 : THE DESIRED DATA FOR ',3A5,' ARE ON 1300
     1LY AVAILABLE IN KEDAK UNTIL ',E16.8,'EV')                         1310
      JI=L                                                              1320
      IF(NERF.EQ.0)  GO TO 34                                           1330
      NERP=(NERF-1)*NER+IST+1                                           1340
      RETURN                                                            1350
   13 IF(FEST(4)-ENG(L))18,19,15                                        1360
   19 IJ=1                                                              1370
      GO TO 20                                                          1380
   18 IJ=2                                                              1390
   20 E(1)=FEST(4)                                                      1400
      SIG1=FEST(5)                                                      1410
      IF(I-3)123,123,122                                                1420
  123 EN(1,I)=FEST(4)                                                   1430
      SN(1,I)=FEST(5)                                                   1440
      IST=1                                                             1450
      IF(I.NE.2)  GO TO 122                                             1460
      DO 3000 KK=2,MM                                                   1470
      IF(EMU(KK)-E(1))3000,3001,3002                                    1480
 3000 CONTINUE                                                          1490
 3007 WRITE (NOUTP,3003) NTYP(I),NTYP(I)                                1500
 3003 FORMAT(1HO/' ***WARNING 3. 4 : THE TYPE ',A6,' CAN NOT BE CALCULAT 1510
     1ED'/' BECAUSE THE ENERGY POINTS FOR MUEL ARE ALL LESS THAN THE FIR 1520
     2ST ENERGY POINT OF ',A6)                                          1530
      GO TO 2                                                           1540
 3001 XMU1=XMU(KK)                                                      1550
      GO TO 122                                                         1560
 3002 XMU1=XMU(KK-1)+(XMU(KK)-XMU(KK-1))*(E(1)-EMU(KK-1))/(EMU(KK)-     1570
     1EMU(KK-1))                                                        1580
  122 IX=1                                                              1590
      GO TO (29,8),IJ                                                   1600
   15 E(2)=FEST(4)                                                      1610
      SIG2=FEST(5)                                                      1620
      SIG1=SIG1+(SIG2-SIG1)*(ENG(L)-E(1))/(E(2)-E(1))                   1630
      E(1)=ENG(L)                                                       1640
      IF(I-3)125,125,124                                                1650
  125 EN(1,I)=E(1)                                                      1660
      SN(1,I)=SIG1                                                      1670
      EN(2,I)=E(2)                                                      1680
      SN(2,I)=SIG2                                                      1690
      IST=2                                                             1700
      IF(I.NE.2)  GO TO 124                                             1710
      IK=2                                                              1720
      IF(KK.GT.2)  IK=KK-1                                              1730
      DO 3004 KK=IK,MM                                                  1740
      IF(EMU(KK)-E(1))3004,3005,3006                                    1750
 3004 CONTINUE                                                          1760
      GO TO 3007                                                        1770
 3005 XMU1=XMU(KK)                                                      1780
```

```
      GO TO 3008                                                        1790
3006  XMU1=XMU(KK-1)+(XMU(KK)-XMU(KK-1))*(E(1)-EMU(KK-1))/(EMU(KK)-     1800
     1EMU(KK-1))                                                        1810
3008  IF(KK.GT.2)  IK=KK-1                                              1820
      DO 3009 KK=IK,MM                                                  1830
      IF(EMU(KK)-E(2))3009,3010,3011                                    1840
3009  CONTINUE                                                          1850
      GO TO 3007                                                        1860
3010  XMU2=XMU(KK)                                                      1870
      GO TO 124                                                         1880
3011  XMU2=XMU(KK-1)+(XMU(KK)-XMU(KK-1))*(E(2)-EMU(KK-1))/(EMU(KK)-     1890
     1EMU(KK-1))                                                        1900
 124  IX=2                                                              1910
  29  IF(NEFE)210,101,210                                               1920
 101  FLUSS(1)=PHI(E(1))                                                1930
      GO TO (9,16),IX                                                   1940
 210  DO 102 LR=2,NEFE                                                  1950
      IF(REFE(LR)-E(1))102,103,104                                      1960
 102  CONTINUE                                                          1970
 104  FLUSS(1)=EFE(LR-1)+(EFE(LR)-EFE(LR-1))/(REFE(LR)-REFE(LR-1))*(E(1) 1980
     1-REFE(LR-1))                                                      1990
      GO TO (9,16),IX                                                   2000
 103  FLUSS(1)=EFE(LR)                                                  2010
      GO TO (9,16),IX                                                   2020
   9  CALL NDFNXT(NSUCH1,NSATZ,FEST,NUDAT,NC)                           2030
      IF(NSUCH1)12,12,22                                                2040
  22  E(2)=FEST(4)                                                      2050
      SIG2=FEST(5)                                                      2060
      IF(E(2)-ENG(NEN))3015,3015,16                                     2070
3015  IF(I.NE.2)  GO TO 16                                              2080
      IK=KK-1                                                           2090
      DO 3016 KK=IK,MM                                                  2100
      IF(EMU(KK)-E(2))3016,3017,3018                                    2110
3016  CONTINUE                                                          2120
      GO TO 3007                                                        2130
3017  XMU2=XMU(KK)                                                      2140
      GO TO 16                                                          2150
3018  XMU2=XMU(KK-1)+(XMU(KK)-XMU(KK-1))*(E(2)-EMU(KK-1))/(EMU(KK)-     2160
     1EMU(KK-1))                                                        2170
  16  IF(E(2)-ENG(L+1))26,26,25                                         2180
  25  E(3)=E(2)                                                         2190
      SIG3=SIG2                                                         2200
      IX=-1                                                             2210
      SIG2=SIG1+(SIG3-SIG1)*(ENG(L+1)-E(1))/(E(3)-E(1))                 2220
      E(2)=ENG(L+1)                                                     2230
      IF(I-3)127,127,23                                                 2240
 127  IST=IST+1                                                         2250
      ISTM(I)=IST                                                       2260
      IF(IST.LE.NER)  GO TO 2002                                        2270
      IST=1                                                             2280
      NERF=NERF+1                                                       2290
2002  EN(IST,I)=E(2)                                                    2300
      SN(IST,I)=SIG2                                                    2310
      IF(I.NE.2)  GO TO 23                                              2320
      IK=KK-1                                                           2330
      DO 3020 KK=IK,MM                                                  2340
      IF(EMU(KK)-E(2))3020,3021,3022                                    2350
3020  CONTINUE                                                          2360
      GO TO 3007                                                        2370
3021  XMU2=XMU(KK)                                                      2380
      GO TO 23                                                          2390
3022  XMU2=XMU(KK-1)+(XMU(KK)-XMU(KK-1))*(E(2)-EMU(KK-1))/(EMU(KK)-     2400
     1EMU(KK-1))                                                        2410
      GO TO 23                                                          2420
  26  IX=0                                                              2430
 128  IF(I-3)126,126,23                                                 2440
 126  IST=IST+1                                                         2450
      ISTM(I)=IST                                                       2460
      IF(IST.LE.NER)  GO TO 2003                                        2470
      IST=1                                                             2480
      NERF=NERF+1                                                       2490
2003  EN(IST,I)=E(2)                                                    2500
      SN(IST,I)=SIG2                                                    2510
      IF(I.NE.2)  GO TO 23                                              2520
      IK=KK-1                                                           2530
      DO 3024 KK=IK,MM                                                  2540
      IF(EMU(KK)-E(2))3024,3025,3026                                    2550
3024  CONTINUE                                                          2560
      GO TO 3007                                                        2570
3025  XMU2=XMU(KK)                                                      2580
      GO TO 23                                                          2590
3026  XMU2=XMU(KK-1)+(XMU(KK)-XMU(KK-1))*(E(2)-EMU(KK-1))/(EMU(KK)-     2600
     1EMU(KK-1))                                                        2610
  23  IF(NEFE)27,28,27                                                  2620
  28  FLUSS(2)=PHI(E(2))                                                2630
      GO TO 30                                                          2640
  27  DO 31 LR=LY,NEFE                                                  2650
      IF(REFE(LR)-E(2))31,32,33                                         2660
  31  CONTINUE                                                          2670
      LR=NEFE                                                           2680
  33  FLUSS(2)=EFE(LR-1)+(EFE(LR)-EFE(LR-1))/(REFE(LR)-REFE(LR-1))*(E(2) 2690
     1-REFE(LR-1))                                                      2700
      GO TO 36                                                          2710
  32  FLUSS(2)=EFE(LR)                                                  2720
  36  LY=LR                                                             2730
  30  IF(I-4)49,601,49                                                  2740
 601  KK=3                                                              2750
      LRJ=2                                                             2760
      IF(ISTRUK.EQ.1)  LRJ=3                                            2770
      DO 60 JAN=1,LRJ                                                   2780
      IST=ISTM(JAN)                                                     2790
      M=1                                                               2800
  50  DO 51 JJ=2,IST                                                    2810
      IF(EN(JJ,JAN)-E(M))51,52,53                                       2820
  51  CONTINUE                                                          2830
      JJ=IST                                                            2840
  53  ST(M)=SN(JJ-1,JAN)+(SN(JJ,JAN)-SN(JJ-1,JAN))/(EN(JJ,JAN)-         2850
     1EN(JJ-1,JAN))*(E(M)-EN(JJ-1,JAN))                                 2860
      GO TO 54                                                          2870
  52  ST(M)=SN(JJ,JAN)                                                  2880
  54  IF(M-1)57,57,58                                                   2890
  57  M=2                                                               2900
```

```
      GO TO 50                                                          2910
   58 EV=0.5*(E(2)-E(1))                                                2920
      IF(KK.GT.2) IK=KK-1                                               2930
      DO 4000 KK=IK,MM                                                  2940
      IF(EMU(KK)-E(1))4000,4001,4002                                    2950
 4000 CONTINUE                                                          2960
      GO TO 3007                                                        2970
 4001 XMU1=XMU(KK)                                                      2980
      GO TO 4003                                                        2990
 4002 XMU1=XMU(KK-1)+(XMU(KK)-XMU(KK-1))*(E(1)-EMU(KK-1))/(EMU(KK)-     3000
     1EMU(KK-1))                                                        3010
 4003 IF(KK.GT.2) IK=KK-1                                               3020
      DO 4004 KK=IK,MM                                                  3030
      IF(EMU(KK)-E(2))4004,4005,4006                                    3040
 4004 CONTINUE                                                          3050
      GO TO 3007                                                        3060
 4005 XMU2=XMU(KK)                                                      3070
      GO TO 4007                                                        3080
 4006 XMU2=XMU(KK-1)+(XMU(KK)-XMU(KK-1))*(E(2)-EMU(KK-1))/(EMU(KK)-     3090
     1EMU(KK-1))                                                        3100
 4007 DO 60 LI=1,MI                                                     3110
      VA=FLUSS(1)/(SIG1 +SIGO(LI))                                      3120
      VB=FLUSS(2)/(SIG2 +SIGO(LI))                                      3130
      IF(JAN.NE.2)  GO TO 3028                                          3140
      ZB(LI,L     )=ZB(LI,L     )+EV*(ST(1)*XMU1  *VA+ST(2)*XMU2*VB)   3150
 3028 ZA(LI,L,JAN)=ZA(LI,L,JAN)+EV*(ST(1)*VA+ST(2)*VB)                  3160
 3029 XN(LI,L,JAN)=XN(LI,L,JAN)+EV*(VA+VB)                              3170
      IF(JAN.NE.2)  GO TO 60                                            3180
      VA=FLUSS(1)/(SIG1+SIGO(LI))**2                                    3190
      VB=FLUSS(2)/(SIG2+SIGO(LI))**2                                    3200
      ZA(LI,L,4)=ZA(LI,L,4)+EV*(ST(1)*XMU1*VA+ST(2)*XMU2*VB)            3210
 3031 XN(LI,L,4)=XN(LI,L,4)+EV*(VA+VB)                                  3220
      ZA(LI,L,5)=ZA(LI,L,5)+EV*(SIG1*VA+SIG2*VB)                        3230
   60 CONTINUE                                                          3240
      ST(1)=ST(2)                                                       3250
   49 E(1)=E(2)                                                         3260
      SIG1=SIG2                                                         3270
      FLUSS(1)=FLUSS(2)                                                 3280
      IF(I.EQ.2)   XMU1=XMU2                                            3290
      IF(E(2)-ENG(L+1))9,34,34                                          3300
   34 IF(I-3)69,69,62                                                   3310
   62 JFAK=0                                                            3320
      DO 4 LA=1,LRJ                                                     3330
    4 XINTE(L,LA)=ZA(MI,L,LA)/XN(MI,L,LA)                               3340
      XINTE(L,4)=ZA(MI,L,5)/XN(MI,L,4)                                  3350
      XI(L)=ZB(MI,L)/XN(MI,L,2)                                         3360
      XII(L)=ZA(MI,L,4)/XN(MI,L,4)                                      3370
      DO 63 LI=1,MI                                                     3380
      DO 363 LA=1,LRJ                                                   3390
      IF(XINTE(L,LA).EQ.0.OR.XN(LI,L,LA).EQ.0)  GO TO 366               3400
      IF(ISTRUK.EQ.1.AND.LA.EQ.1)  GO TO 5301                           3410
      SE(LI,L,LA)=ZA(LI,L,LA)/(XN(LI,L,LA)*XINTE(L,LA))                 3420
      GO TO 363                                                         3430
 5301 SE(LI,L,LA)=(ZA(LI,L,LA)/XN(LI,L,LA)-ZA(LI,L,3)/XN(LI,L,3))/(     3440
     1XINTE(L,LA)-XINTE(L,3))                                           3450
      GO TO 363                                                         3460
  366 SE(LI,L,LA)=1.                                                    3470
      JFAK=1                                                            3480
  363 CONTINUE                                                          3490
      IF(XI(L).NE.0)  GO TO 367                                         3500
      SE(LI,L,4)=1.                                                     3510
      JFAK=1                                                            3520
      GO TO 900                                                         3530
  367 SE(LI,L,4)=ZB(LI,L)/(XN(LI,L,2)*XI(L))                            3540
  900 IF(XII(L).NE.0)  GO TO 467                                        3550
      SE(LI,L,5)=1.                                                     3560
      JFAK=1                                                            3570
      GO TO 901                                                         3580
  467 SE(LI,L,5)=ZA(LI,L,4)/(XN(LI,L,4)*XII(L))                         3590
  901 IF(XINTE(L,4).EQ.0)  GO TO 368                                    3600
      SE(LI,L,6)=ZA(LI,L,5)/(XN(LI,L,4)*XINTE(L,4))                     3610
      GO TO 63                                                          3620
  368 SE(LI,L,6)=1.                                                     3630
      JFAK=1                                                            3640
   63 CONTINUE                                                          3650
      IF(JFAK.EQ.0)  GO TO 69                                           3660
      LZ=NE-L                                                           3670
      WRITE (NOUTP,5300) LZ                                             3680
 5300 FORMAT(1HO/' ***WARNING 3. 5 : IN THE ENERGY GROUP ',I4,' THE SELF 3690
     1SHIELDING FACTORS ARE SET TO 1, BECAUSE THE CROSS SECTIONS'/' FOUN 3700
     2D ON KEDAK FOR THIS GROUP ALL ARE ZERO')                          3710
   69 L=L+1                                                             3720
      IF(L-JI)64,64,2                                                   3730
   64 IF(IX)166,9,9                                                     3740
  166 IF(E(3)-ENG(L+1))67,67,68                                         3750
   68 E(2)=ENG(L+1)                                                     3760
      SIG2=SIG1+(SIG3-SIG1)*(E(2)-E(1))/(E(3)-E(1))                     3770
      GO TO 128                                                         3780
   67 E(2)=E(3)                                                         3790
      SIG2=SIG3                                                         3800
      GO TO 26                                                          3810
  201 L=L+1                                                             3820
      IF(L-JI)66,66,2                                                   3830
    2 IF(NERF.EQ.0)  GO TO 2222                                         3840
      NERP=(NERF-1)*NER+IST+1                                           3850
      RETURN                                                            3860
 2222 CONTINUE                                                          3870
      N=0                                                               3880
      WRITE (JA) N,NN                                                   3890
      DO 70 LI=IY,JI                                                    3900
      IN=5                                                              3910
      WRITE(JA) IN,MAT     ,LI,ENG(LI),ENG(LI+1)                        3920
      LZ=NE-LI                                                          3930
      WRITE(NOUTP,35) MAT     ,LZ,ENG(LI),ENG(LI+1)                     3940
   35 FORMAT(1HO,A5,9H GRUPPE =I3,3X,15HGRUPPENGRENZEN 2E16.8)          3950
      IF(ISTRUK.EQ.1)  GO TO 5201                                       3960
      WRITE (NOUTP,5200)                                                3970
 5200 FORMAT(1HO,22X,7HSIGMA A,11X,7HSIGMA N,10X,9HSIGMA NO1,9X,        3980
     18HSIGMA N1,10X,8HSIGMA T1/)                                       3990
      GO TO 5203                                                        4000
 5201 WRITE (NOUTP,5202)                                                4010
 5202 FORMAT(1HO,22X,'SIGMA C',11X,'SIGMA N',11X,'SIGMA F',10X,         4020
```

```
     1'SIGMA NO1',9X,'SIGMA N1',10X,'SIGMA T1'/)                                4030
      XINTE(LI,1)=XINTE(LI,1)-XINTE(LI,3)                                       4040
5203  IN=LRJ+3                                                                 4050
      WRITE(JA)IN,(XINTE(LI,LA),LA=1,LRJ),XI(LI),XI(LI),XINTE(LI,4)             4060
      WRITE(NOUTP,37)(XINTE(LI,LA),LA=1,LRJ),XI(LI),XI(LI),XINTE(LI,4)          4070
   37 FORMAT(16X,6E18.8)                                                        4080
      IF(ISTRUK.EQ.1)  GO TO 5204                                               4090
      WRITE (NOUTP,39)                                                          4100
   39 FORMAT(1HO,5X,4HSIGO,15X,2HFA,16X,2HFN,16X,4HFN01,14X,3HFN1,15X,          4110
     13HFT1/)                                                                   4120
      GO TO 5206                                                                4130
5204  WRITE (NOUTP,5205)                                                       4140
5205  FORMAT(1HO,5X,4HSIGO,15X,2HFC,16X,2HFN,16X,2HFF,14X,4HFN01,14X,          4150
     13HFN1,15X,3HFT1/)                                                         4160
5206  IN=LRJ+4                                                                 4170
      DO 70 I=1,MI                                                              4180
      WRITE(JA) IN,SIGO(I),(SE(I,LI,LA),LA=1,LRJ),(SE(I,LI,LA),LA=4,6)          4190
   70 WRITE(NOUTP,38) SIGO(I),(SE(I,LI,LA),LA=1,LRJ),(SE(I,LI,LA),LA=4,6        4200
     1)                                                                         4210
   38 FORMAT(E16.8,6E18.8)                                                      4220
 1000 CONTINUE                                                                  4230
   71 KL=KL+1                                                                   4240
      RETURN                                                                    4250
  100 STOP                                                                      4260
      END                                                                       4270
```

```
      SUBROUTINE SUND (MM,ENG,NFE,REFE,EFE,ITYP,ITNAM,SGC,DUE,XINTE,            10
     1ZINT,XNEN,STREU,LDIM,LDIMP,SE,FSE)                                        20
      INTEGER*2 IHC(2),IMP(2)                                                   30
      REAL*8 MAT,ITNAM,FEST,NFEST,NN,MMM                                        40
      DIMENSION ENG(MM),REFE(NFE),EFE(NFE),ITNAM(ITYP),SGC(MM),E(3),            50
     1FLUSS(2),DUE(MM),XINTE(MM),ZINT(MM),XNEN(MM),STREU(MM),NADAT(2),          60
     2NSATZ(4),FEST(10),NFEST(10),NN(11),SE(LDIM),FSE(LDIM),SFN(2)              70
      COMMON MAT,ISTRUK,ISPA,NOUTP,JA,NANF,NEND,KL                              80
      EQUIVALENCE (FEST(1),NFEST(1)),(IHC(1),HM)                                90
      DATA IMP/'PU','U '/                                                      100
      WRITE (NOUTP,9000)                                                       110
 9000 FORMAT(1HO/1HO/' PROGRAMM KENNZIFFER 4')                                 120
      WRITE (NOUTP,9001)                                                       130
 9001 FORMAT(' PROGRAMM ZUR BERECHNUNG VON GRUPPENWIRKUNGSQUERSCHNITTEN        140
     1BEI UNENDLICHER VERDUENNUNG'/)                                           150
      CALL FSPIE                                                               160
      LDIF=0                                                                   170
      LDIMP=0                                                                  180
      NEFE=NFE                                                                 190
      IF(NFE.EQ.1)  NEFE=0                                                     200
      NGR=MM-NANF                                                              210
      NEN=MM+1-NEND                                                            220
      CALL DOPW (8HBEST    ,NFEST(2))                                          230
      CALL DOPW (8HSGA     ,NN(1))                                             240
      CALL DOPW (8HSGF     ,NN(2))                                             250
      CALL DOPW (8HSGN     ,NN(3))                                             260
      CALL DOPW (8HMUEL    ,NN(4))                                             270
      CALL DOPW (8HNUE     ,NN(5))                                             280
      CALL DOPW (8HSGC     ,NN(6))                                             290
      CALL DOPW (8HSTR     ,NN(7))                                             300
      CALL DOPW (8HH  01   ,NN(8))                                             310
      CALL DOPW (8HALPHA   ,NN(9))                                             320
      CALL DOPW (8HETA     ,NN(10))                                            330
      CALL DOPW (8HSGG     ,NN(11))                                            340
      CALL DOPW (8HSGKE    ,MMM)                                               350
      INR=0                                                                    360
      LL=0                                                                     370
      HM=MAT                                                                   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,ITYP                                                         420
      IF(ITNAM(JJ).EQ.NN(1))  GO TO 805                                        430
      IF(ITNAM(JJ).NE.NN(2))  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 (NOUTP,808) MAT                                                    490
  808 FORMAT(1HO/' ***WARNING 4. 1 : THE GROUP CROSS SECTION SGC CAN NOT       500
     1 BE CALCULATED FOR ',A5/' BECAUSE THE REACTION TYPES SGF AND SGA A       510
     2RE NOT SPECIFIED IN THE INPUT')                                          520
      GO TO 801                                                                530
  822 LAR=0                                                                    540
      DO 821 JJ=1,ITYP                                                         550
      IF(ITNAM(JJ).EQ.NN(1))  GO TO 801                                        560
  821 CONTINUE                                                                 570
      GO TO 807                                                                580
  801 NFEST(1)=MAT                                                             590
      IGRUP=NEN-1                                                              600
      DO 870 JJ=NGR,IGRUP                                                      610
  870 SGC(JJ)=0.                                                               620
      JJJ=1                                                                    630
      DO 3 JJ=1,ITYP                                                           640
      KGRU=0                                                                   650
      NSATZ(1)=3                                                               660
      KSIK=0                                                                   670
      IF(ITNAM(JJ).NE.NN(9).OR.ITNAM(JJ).NE.NN(10))  GO TO 871                 680
      IF(LAR.EQ.0)  GO TO 875                                                  690
      KSIK=1                                                                   700
      NFEST(3)=NN(11)                                                          710
      GO TO 2003                                                               720
  875 WRITE (NOUTP,876)MAT,ITNAM(JJ)                                           730
  876 FORMAT(1HO/' ***WARNING 4. 2 : THE GROUP CROSS SECTION FOR ',2A8,        740
     1' CAN NOT BE CALCULATED'/' BECAUSE THE VALUES OF SGF ARE ZERO')          750
      GO TO 3                                                                  760
  874 KSIK=2                                                                   770
      NFEST(3)=NN(2)                                                           780
      GO TO 2003                                                               790
  879 KSIK=3                                                                   800
      GO TO 2002                                                               810
  871 IF(ITNAM(JJ).EQ.NN(4))  GO TO 2001                                       820
```

```
      IF(ITNAM(JJ).EQ.NN(5))  GO TO 2002                                830
      GO TO 2003                                                        840
 2001 NFEST(3)=NN(3)                                                    850
      GO TO 2004                                                        860
 2002 NFEST(3)=NN(2)                                                    870
 2004 CALL NDFLOC(NSUCH1,NSATZ,FEST,NUDAT,NC)                           880
      IF(NSUCH1)2005,2005,2006                                          890
 2005 SE(1)=ENG(NGR)                                                    900
      FSE(1)=0.                                                         910
      SE(2)=ENG(NEN)                                                    920
      FSE(2)=0.                                                         930
      M=2                                                               940
      WRITE(NOUTP,2070) FEST(3),ITNAM(JJ)                               950
 2070 FORMAT(1HO/' ***WARNING 4. 3 : TYPE ',A6,' IS SET TO ZERO. THIS TY  960
     1PE IS USED TO CALCULATE THE GROUP CROSS SECTION ',A6)             970
      GO TO 2003                                                        980
 2006 SE(1)=FEST(4)                                                     990
      FSE(1)=FEST(5)                                                   1000
      IF(SE(1)-ENG(NGR))2008,2008,2009                                 1010
 2009 WRITE (NOUTP,11) ENG(NGR),(NFEST(K),K=1,3),SE(1)                 1020
 2008 M=2                                                              1030
 2013 CALL NDFNXT (NSUCH1,NSATZ,FEST,NUDAT,NC)                         1040
      IF(NSUCH1)2223,2223,2010                                         1050
 2010 IF(FEST(4)-ENG(NGR))2011,2011,2012                               1060
 2011 SE(1)=FEST(4)                                                    1070
      FSE(1)=FEST(5)                                                   1080
      GO TO 2013                                                       1090
 2012 IF(FEST(4)-ENG(NEN  ))2014,2015,2015                             1100
 2014 SE(M)=FEST(4)                                                    1110
      FSE(M)=FEST(5)                                                   1120
      M=M+1                                                            1130
      IF(M-LDIM)2013,2013,2090                                         1140
 2090 M=1                                                              1150
      LDIF=LDIF+1                                                      1160
      GO TO 2013                                                       1170
 2223 M=M-1                                                            1180
      GO TO 2003                                                       1190
 2015 SE(M)=FEST(4)                                                    1200
      FSE(M)=FEST(5)                                                   1210
 2003 LY=2                                                             1220
      IF(LDIF.EQ.0)  GO TO 2091                                        1230
      LDIMP=(LDIF-1)*LDIM+M+1                                          1240
      RETURN                                                           1250
 2091 MMMM=M                                                           1260
      L=NGR                                                            1270
      M=L                                                              1280
      DO 4 LI=L,IGRUP                                                  1290
      ZINT(LI)=0.                                                      1300
      DUE(LI)=0.                                                       1310
    4 XNEN(LI)=0.                                                      1320
      IF(KSIK.NE.3)  GO TO 971                                         1330
      NFEST(3)=NN(5)                                                   1340
      GO TO 970                                                        1350
  971 IF(KSIK.EQ.0) NFEST(3)=ITNAM(JJ)                                 1360
  970 CALL NDFLOC(NSUCH1,NSATZ,FEST,NUDAT,NC)                          1370
      IF(NSUCH1)5,5,6                                                  1380
    5 WRITE(NOUTP,7) (NFEST(K),K=1,3)                                  1390
    7 FORMAT(1HO/' ***WARNING 4. 4 : DATA FOR ',3A5,' COULD NOT BE FOUND 1400
     1 IN THE KEDAK LIBRARY')                                          1410
      GO TO 300                                                        1420
    6 E(1)=FEST(4)                                                     1430
      SIG1=FEST(5)                                                     1440
      IF(ITNAM(JJ).EQ.NN(4).OR.ITNAM(JJ).EQ.NN(5))  GO TO 2023         1450
      GO TO 66                                                         1460
 2023 DO 2016 KK=2,MMMM                                                1470
      IK=KK                                                            1480
      IF(SE(KK)-E(1))2016,2017,2018                                    1490
 2016 CONTINUE                                                         1500
 2022 WRITE (NOUTP,2019) ITNAM(JJ)                                     1510
 2019 FORMAT(1HO/' ***WARNING 4. 5 : TYPE ',A6,' CAN NOT BE CALCULATED B 1520
     1ECAUSE THE ENERGY SCALE OF'/' THIS TYPE BEGINS AT A HIGHER ENERGY 1530
     2THAN THE HIGHEST ENERGY GROUP BOUNDARY')                         1540
      GO TO 3                                                          1550
 2017 SFN(1)=FSE(KK)                                                   1560
      GO TO 66                                                         1570
 2018 SFN(1)=FSE(KK-1)+(FSE(KK)-FSE(KK-1))*(E(1)-SE(KK-1))/(SE(KK)-SE( 1580
     1KK-1))                                                           1590
   66 IF(E(1)-ENG(L))8,9,10                                            1600
   10 WRITE (NOUTP,11) ENG(L),(NFEST(K),K=1,3),E(1)                    1610
   11 FORMAT(1HO/' ***WARNING 4. 6 : THE LOWER ENERGY GROUP BOUNDARY ',  1620
     1E16.8,'EV IS NOT IN THE AVAILABLE ENERGY RANGE IN KEDAK FOR '/1X,  1630
     23A5,' THE LOWER ENERGY GROUP BOUNDARY HAS BEEN MODYFIED TO ',E16.8 1640
     3,'EV')                                                           1650
      IF(E(1)-ENG(L+1))9,200,200                                       1660
    8 CALL NDFNXT(NSUCH1,NSATZ,FEST,NUDAT,NC)                          1670
      IF(NSUCH1)12,12,13                                               1680
   12 WRITE(NOUTP,14)NFEST(1),NFEST(2),ITNAM(JJ),E(1)                  1690
   14 FORMAT(1HO/' ***WARNING 4. 7 : THE DESIRED DATA FOR ',3A5,' ARE ON 1700
     1LY AVAILABLE IN KEDAK UNTIL ',E16.8,'EV')                        1710
      IZLM=-1                                                          1720
      GO TO 50                                                         1730
   13 IZLM=1                                                           1740
      IF(FEST(4)-ENG(L))18,19,15                                       1750
   19 IJ=1                                                             1760
      GO TO 20                                                         1770
   18 IJ=2                                                             1780
   20 E(1)=FEST(4)                                                     1790
      SIG1=FEST(5)                                                     1800
      IF(ITNAM(JJ).EQ.NN(4).OR.ITNAM(JJ).EQ.NN(5))  GO TO 2024         1810
      GO TO (9,8),IJ                                                   1820
 2024 IF(KK.GT.2)  KK=KK-1                                             1830
      DO 2059 IK=KK,MMMM                                               1840
      IF(SE(IK)-E(1))2059,2020,2021                                    1850
 2059 CONTINUE                                                         1860
      GO TO 2022                                                       1870
 2020 SFN(1)=FSE(IK)                                                   1880
      GO TO (9,8),IJ                                                   1890
 2021 SFN(1)=FSE(IK-1)+(FSE(IK)-FSE(IK-1))*(E(1)-SE(IK-1))/(SE(IK)-SE( 1900
     1IK-1))                                                           1910
      GO TO (9,8),IJ                                                   1920
   15 E(2)=FEST(4)                                                     1930
      SIG2=FEST(5)                                                     1940
```

```
      SIG1=SIG1+(SIG2-SIG1)*(ENG(L)-E(1))/(E(2)-E(1))                    1950
      E(1)=ENG(L)                                                       1960
      IF(ITNAM(JJ).EQ.NN(4).OR.ITNAM(JJ).EQ.NN(5))  GO TO 2037          1970
      GO TO 16                                                          1980
 2037 IF(IK.GT.2) IK=IK-1                                               1990
      KK=IK                                                             2000
      DO 2038 IK=KK,MMMM                                                2010
      IF(SE(IK)-E(1))2038,2039,2040                                     2020
 2038 CONTINUE                                                          2030
      GO TO 2022                                                        2040
 2039 SFN(1)=FSE(IK)                                                    2050
      GO TO 2041                                                        2060
 2040 SFN(1)=FSE(IK-1)+(FSE(IK)-FSE(IK-1))*(E(1)-SE(IK-1))/(SE(IK)-SE(  2070
     1IK-1))                                                            2080
 2041 IF(IK.GT.2) IK=IK-1                                               2090
      KK=IK                                                             2100
      DO 2042 IK=KK,MMMM                                                2110
      IF(SE(IK)-E(2))2042,2043,2044                                     2120
 2042 CONTINUE                                                          2130
      IF(SE(MMMM)-ENG(L+1))2022,2043,2044                               2140
 2043 SFN(2)=FSE(IK)                                                    2150
      GO TO 16                                                          2160
 2044 SFN(2)=FSE(IK-1)+(FSE(IK)-FSE(IK-1))*(E(2)-SE(IK-1))/(SE(IK)-SE(  2170
     1IK-1))                                                            2180
      GO TO 16                                                          2190
    9 CALL NDFNXT(NSUCH1,NSATZ,FEST,NUDAT,NC)                           2200
      IF(NSUCH1)12,12,22                                                2210
   22 E(2)=FEST(4)                                                      2220
      SIG2=FEST(5)                                                      2230
      IF(E(2)-ENG(NEN))2071,2071,16                                     2240
 2071 IZLM=1                                                            2250
      IF(ITNAM(JJ).EQ.NN(4).OR.ITNAM(JJ).EQ.NN(5))  GO TO 2033          2260
      GO TO 16                                                          2270
 2033 IF(IK.GT.2)  IK=IK-1                                              2280
      KK=IK                                                             2290
      DO 2034 IK=KK,MMMM                                                2300
      IF(SE(IK)-E(2))2034,2035,2036                                     2310
 2034 CONTINUE                                                          2320
      GO TO 2022                                                        2330
 2035 SFN(2)=FSE(IK)                                                    2340
      GO TO 16                                                          2350
 2036 SFN(2)=FSE(IK-1)+(FSE(IK)-FSE(IK-1))*(E(2)-SE(IK-1))/(SE(IK)-SE(  2360
     1IK-1))                                                            2370
   16 IF(E(2)-ENG(L+1))26,26,25                                         2380
   25 E(3)=E(2)                                                         2390
      SIG3=SIG2                                                         2400
      IX=-1                                                             2410
      SIG2=SIG1+(SIG3-SIG1)*(ENG(L+1)-E(1))/(E(3)-E(1))                 2420
      E(2)=ENG(L+1)                                                     2430
      IF(ITNAM(JJ).EQ.NN(4).OR.ITNAM(JJ).EQ.NN(5))  GO TO 2029          2440
      GO TO 23                                                          2450
 2029 IF(IK.GT.2)  IK=IK-1                                              2460
      KK=IK                                                             2470
      DO 2030 IK=KK,MMMM                                                2480
      IF(SE(IK)-E(2))2030,2031,2032                                     2490
 2030 CONTINUE                                                          2500
      GO TO 2022                                                        2510
 2031 SFN(2)=FSE(IK)                                                    2520
      GO TO 23                                                          2530
 2032 SFN(2)=FSE(IK-1)+(FSE(IK)-FSE(IK-1))*(E(2)-SE(IK-1))/(SE(IK)-SE(  2540
     1IK-1))                                                            2550
      GO TO 23                                                          2560
   26 IX=0                                                              2570
   23 IF(ITNAM(JJ).EQ.NN(4))  GO TO 72                                  2580
      IF(ITNAM(JJ).NE.NN(5))  GO TO 70                                  2590
   72 IFL=1                                                             2600
      GO TO 573                                                         2610
  972 ZINT(L)=ZINT(L)+0.5*(SIG1*SFN(1)*FLUSS(1)+SIG2*SFN(2)*FLUSS(2))*  2620
     1(E(2)-E(1))                                                       2630
      XNEN(L)=XNEN(L)+0.5*(SFN(1)*FLUSS(1)+SFN(2)*FLUSS(2))*(E(2)-E(1))  2640
      IJ=0                                                              2650
      GO TO 46                                                          2660
   70 IJ=1                                                              2670
      IFL=2                                                             2680
  573 IF (NEFE)27,28,27                                                 2690
   28 FLUSS(1)=PHI(E(1))                                                2700
      FLUSS(2)=PHI(E(2))                                                2710
      GO TO (972,30),IFL                                                2720
   27 J=1                                                               2730
      GO TO 35                                                          2740
   34 J=2                                                               2750
      LY=LR                                                             2760
   35 DO 31 LR=LY,NEFE                                                  2770
      IF(REFE(LR)-E(J))31,32,33                                         2780
   31 CONTINUE                                                          2790
   33 FLUSS(J)=EFE(LR-1)+(EFE(LR)-EFE(LR-1))/(REFE(LR)-REFE(LR-1))*(E(J)  2800
     1-REFE(LR-1))                                                      2810
      GO TO (34,36),J                                                   2820
   32 FLUSS(J)=EFE(LR)                                                  2830
      GO TO (34,36),J                                                   2840
   36 LY=LR                                                             2850
      GO TO (972,30),IFL                                                2860
   30 ZINT(L)=ZINT(L)+0.5*(SIG1*FLUSS(1)+SIG2*FLUSS(2))*(E(2)-E(1))     2870
      IF(MAT    .NE.NN(8))  GO TO 120                                   2880
      IF(ITNAM(JJ).NE.NN(3))  GO TO 120                                 2890
  121 EN=ALOG(E(2)/E(1))                                                2900
      SF1=SIG1*FLUSS(1)                                                 2910
      SF2=SIG2*FLUSS(2)                                                 2920
      DUE(L)=DUE(L)+SF1*EN+SF2-SF1-(SF2-SF1)/(E(2)-E(1))*E(1)*EN        2930
  120 XNEN(L)=XNEN(L)+0.5*(FLUSS(1)+FLUSS(2))*(E(2)-E(1))               2940
   46 IF(E(2)-ENG(L+1))47,50,50                                         2950
   50 IF(ITNAM(JJ).EQ.NN(5).OR.ITNAM(JJ).EQ.NN(9))  GO TO 503           2960
      GO TO 500                                                         2970
  503 IF(XNEN(L).NE.0)  GO TO 500                                       2980
      M=M+1                                                             2990
      KGRU=1                                                            3000
      GO TO 122                                                         3010
  500 XINTE(L)=ZINT(L)/XNEN(L)                                          3020
      IF(MAT    .NE.NN(8))  GO TO 122                                   3030
      IF(ITNAM(JJ).NE.NN(3))  GO TO 122                                 3040
      STREU(L)=DUE(L)/XNEN(L)                                           3050
  122 L=L+1                                                             3060
```

```
      IF(IZLM)300,300,452                                                3070
  452 E(1)=E(2)                                                          3080
      SIG1=SIG2                                                          3090
      SFN(1)=SFN(2)                                                      3100
      IF(L-IGRUP)51,51,52                                                3110
   51 IF(IX)53,9,9                                                       3120
   53 IF(E(3)-ENG(L+1))107,107,108                                       3130
  108 E(2)=ENG(L+1)                                                      3140
      SIG2=SIG1+(SIG3-SIG1)*(E(2)-E(1))/(E(3)-E(1))                      3150
      GO TO 23                                                           3160
  107 E(2)=E(3)                                                          3170
      SIG2=SIG3                                                          3180
      IF(ITNAM(JJ).EQ.NN(4).OR.ITNAM(JJ).EQ.NN(5))  GO TO 2025           3190
      GO TO 26                                                           3200
 2025 IF(IK.GT.2)  IK=IK-1                                               3210
      DO 2026 IK=KK,MMMM                                                 3220
      IF(SE(IK)-E(3))2026,2027,2028                                      3230
 2026 CONTINUE                                                           3240
      IF(SE(MMMM)-ENG(L+1))2022,2027,2028                                3250
 2027 SFN(2)=FSE(IK)                                                     3260
      GO TO 26                                                           3270
 2028 SFN(2)=FSE(IK-1)+(FSE(IK)-FSE(IK-1))*(E(3)-SE(IK-1))/(SE(IK)-SE(   3280
     1IK-1))                                                             3290
      GO TO 26                                                           3300
   47 E(1)=E(2)                                                          3310
      SIG1=SIG2                                                          3320
      SFN(1)=SFN(2)                                                      3330
      GO TO 9                                                            3340
   52 NNN=NEN-1                                                          3350
      IF(KGRU.EQ.0)  GO TO 501                                           3360
      WRITE(NOUTP,502)MAT,ITNAM(JJ)                                      3370
  502 FORMAT(/' ***WARNING 4. 8 : THE GROUP CROSS SECTION FOR',2A9,' CAN  3380
     1NOT BE CALCULATED IN ALL ENERGY GROUPS REQUIRED'/' BECAUSE THE FIS 3390
     2SION CROSS SECTIONS ON KEDAK ARE EQUAL TO ZERO')                   3400
      IF(MM-M.LT.MM-NNN)  GO TO 3                                        3410
  501 IF(JJJ-1)54,56,54                                                  3420
   56 N=0                                                                3430
      WRITE (JA) N,MMM                                                   3440
      JJJ=2                                                              3450
   54 N=2                                                                3460
      WRITE(JA)N,M,NNN                                                   3470
      J=4                                                                3480
      N=NEN-M                                                            3490
      IF(KSIK.EQ.3)  GO TO 881                                           3500
      IF(KSIK.EQ.2)  GO TO 877                                           3510
      IF(KSIK.EQ.0)  GO TO 872                                           3520
      DO 873 J=M,IGRUP                                                   3530
  873 STREU(J)=XINTE(J)                                                  3540
      GO TO 874                                                          3550
  877 DO 878 J=M,IGRUP                                                   3560
  878 STREU(J)=STREU(J)/XINTE(J)                                         3570
      IF(ITNAM(JJ).EQ.NN(10))  GO TO 879                                 3580
      DO 880 J=M,IGRUP                                                   3590
  880 XINTE(J)=STREU(J)                                                  3600
      GO TO 872                                                          3610
  881 DO 882 J=M,IGRUP                                                   3620
```

```
 2045 IF(IK.GT.2)  IK=IK-1
      KK=IK
      DO 2046 IK=KK,MMMM
      IF(SE(IK)-E(2))2046,2047,2048
 2046 CONTINUE
      GO TO 2022
 2047 SFN(2)=FSE(IK)
      GO TO 23
 2048 SFN(2)=FSE(IK-1)+(FSE(IK)-
     1FSE(IK-1))*(E(2)-SE(IK-1))/
     2(SE(IK)-SE(IK-1))
      GO TO 23
```

```
  882 XINTE(J)=XINTE(J)/(1.+STREU(J))                                    3630
  872 WRITE(JA)J,MAT    ,ITNAM(JJ)                                       3640
      WRITE(JA)N,(XINTE(J),J=M,IGRUP)                                    3650
      IST=MM-M                                                           3660
      NI=MM-NNN                                                          3670
      WRITE(NOUTP,910) MAT    ,ITNAM(JJ),IST,NI                          3680
  910 FORMAT(1HO,2A7,9H   GRUPPEI3,4H BISI3)                             3690
      WRITE(NOUTP,909) (XINTE(J),J=M,IGRUP)                              3700
  909 FORMAT(1H ,7E16.8/(1X,7E16.8))                                     3710
      IF(ITNAM(JJ).EQ.NN(1))  GO TO 810                                  3720
      IF(ITNAM(JJ).EQ.NN(2))  GO TO 812                                  3730
      GO TO 816                                                          3740
  810 DO 813 J=M,IGRUP                                                   3750
  813 SGC(J)=SGC(J)+XINTE(J)                                             3760
      IF(INR.EQ.1)  GO TO 818                                            3770
      INR=1                                                              3780
      GO TO 3                                                            3790
  812 DO 814 J=M,IGRUP                                                   3800
  814 SGC(J)=SGC(J)-XINTE(J)                                             3810
      IF(INR.EQ.1)  GO TO 818                                            3820
      INR=1                                                              3830
      GO TO 3                                                            3840
  818 J=2                                                                3850
      WRITE(JA)J,M,NNN                                                   3860
      J=4                                                                3870
      WRITE(JA)J,MAT    ,NN(6)                                           3880
      WRITE(JA)N,(SGC(J),J=M,IGRUP)                                      3890
      WRITE(NOUTP,910) MAT    ,NN(6),IST,NI                              3900
      WRITE(NOUTP,909)(SGC(J),J=M,IGRUP)                                 3910
      GO TO 3                                                            3920
  816 IF(MAT    .NE.NN(8))  GO TO 3                                      3930
      IF(ITNAM(JJ).NE.NN(3))  GO TO 3                                    3940
      J=2                                                                3950
      WRITE(JA)J,M,NNN                                                   3960
      J=4                                                                3970
      WRITE(JA)J,MAT    ,NN(7)                                           3980
      WRITE(JA)N,(STREU(J),J=M,IGRUP)                                    3990
      WRITE (NOUTP,910) MAT,NN(7),IST,NI                                 4000
      WRITE(NOUTP,909)(STREU(J),J=M,IGRUP)                               4010
      GO TO 3                                                            4020
  300 IF(L-IGRUP)600,600,52                                              4030
  600 DO 57 K=L,IGRUP                                                    4040
   57 XINTE(K)=0.                                                        4050
      GO TO 52                                                           4060
  200 XINTE(L)=0.                                                        4070
      L=L+1                                                              4080
      IF(L-IGRUP)66,66,52                                                4090
    3 CONTINUE                                                           4100
  100 KL=KL+1                                                            4110
   63 RETURN                                                             4120
      END                                                                4130
```

```
C      CALCULATION OF THE INELASTIC SCATTERING PROBABILITIES                    10
C                                                                               20
       SUBROUTINE SCAT(NX,EG,    XNUE,NFE,EF,FI,NE27,WAHR,PROB,VW,QUER,         30
      1E,NET,ET,NAE,AE,SU,QUOT,LBA,WEIN,AG,NETP,SGIT,NAEP,KMAX,ISG,ISGP,        40
      2SGIP,IWE,IWP,WERT)                                                       50
       REAL*8 NAM,ISOT,NAM4,EO,EU,DIFF,ET,AE,EMIN,EMAX,E,SUM,QUER,WAHR,         60
      1PROB,WAI,VW,UWA,EH,AB                                                    70
       DIMENSION AE(NAE),KMAX(NAE),ET(NET),SGIP(NAE,ISG),WERT(IWE),             80
      1EG(NX),EF(NFE),FI(NFE),NN(4),SU(NX),QUOT(NX),WAHR(NX),PROB(NX),          90
      2LBA(NX),VW(NX),QUER(NX),E(NE27),WEIN(NX),AG(NE27),SGIT(NET),             100
      3ISOT(2)                                                                  110
       COMMON NAM,ISTRUK,ISPA,NA,LIZ,NANF,NEND,KL                               120
       DATA ISOT/'BEST ','ISOT1'/                                               130
       WRITE (NA    ,9000)                                                      140
 9000  FORMAT(1H0/1H0/' PROGRAMM KENNZIFFER 5')                                 150
       WRITE (NA    ,9001)                                                      160
 9001  FORMAT(' PROGRAMM ZUR BERECHNUNG INELASTISCHER STREUMATRIZEN'/)           170
       WRITE(NA,9002)                                                           180
 9002  FORMAT(1H0/' PROBSGI'/1X)                                                190
       CALL FSPIE                                                               200
       NN(1)=3                                                                  210
       AE(1)=NAM                                                                220
       AE(2)=ISOT(1)                                                            230
       AE(3)=ISOT(2)                                                            240
       CALL NDFLOC (I,NN,AE,K,K)                                                250
       IF(I.EQ.0)  GO TO 1001                                                   260
       A=AE(4)                                                                  270
       NE=NX                                                                    280
       IF(EG(1)-1.E-3)305,301,307                                               290
  305  WRITE (NA,304)                                                           300
  304  FORMAT (' ***ERROR 5.01 : THE LOWER BOUNDARY OF THE LOWEST ENERGY        310
     1GROUP HAS TO BE LARGER OR EQUAL TO 1.E-3 WHICH IS THE LOWEST              320
     2ENERGY ON KEDAK FOR ALL DATA TYPES. THIS IS NOT FULFILLED.')              330
       GO TO 999                                                                340
  307  NE=NE27                                                                  350
       E(1)=0.                                                                  360
       E(1)=1.E-3                                                               370
       AG(1)=1.E-3                                                              380
       DO 302 I=2,NE27                                                          390
       E(I)=0.                                                                  400
       AG(I)=EG(I-1)                                                            410
  302  E(I)=EG(I-1)                                                             420
       GO TO 303                                                                430
  301  DO 300  I=1,NE                                                           440
       E(I)=0.                                                                  450
       AG(I)=EG(I)                                                              460
       E(I)=EG(I)                                                               470
  300  CONTINUE                                                                 480
C      DETERMINATION OF THE EFFECTIVE INITIAL ENERGY GROUP OUT OF WHICH         490
C      INELASTIC SCATTERING OCCURS AND OF THE LAST GROUP UP TO WHICH            500
C      THE TRANSITION PROBABILITIES ARE REQUIRED                                510
  303  NE1=NE-1                                                                 520
       DO 37  IM=1,NE1                                                          530
  37   QUOT(IM)=0.0                                                             540
       IANF=NE-NANF                                                             550
       IE=NE-NEND                                                               560
       KI=2                                                                     570
       CALL AKED(E,    ET,SGIP,JMAT,KMAX,LMAX,SU,QUOT,WERT,AE,EMAX,EMIN,       580
      1IA,NAB,NFE,EF,FI,NE,NX,NET,NETF,NETP,SGIT,NAE,NAEF,NAEP,ISG,ISGF,        590
      2ISGP,IWE,IWF,IWP)                                                        600
       IF(NETF.GT.0.OR.ISGF.GT.0.OR.NAEF.GT.0.OR.IWF.GT.0)  RETURN              610
       IF(IA.GE.IANF)  GOTO 205                                                 620
       NEA=IANF                                                                 630
       GOTO 206                                                                 640
  205  NEA=IA                                                                   650
       IF(IA.LE.IE)   GOTO 206                                                  660
       WRITE(NA,179)                                                            670
  179  FORMAT (' ***ERROR 5.04 : WITH INCIDENT NEUTRON ENERGIES OUT OF          680
      1THE ENRGY GROUPS REQUESTED IN THE INPUT INELASTIC SCATTERING             690
      2CANNOT OCCUR,SINCE THE FIRST ENERGY AT WHICH INELASTIC SCATTERING        700
      3CROSS SECTIONS ARE STORED ON KEDAK IS HIGHER THAN THE UPPER              710
      4ENERGY LIMIT OF THE HIGHEST ENERGY GROUP (LOWEST GROUP NUMBER            720
      5ACCORDING TO THE ABN-SET)')                                              730
       GO TO 999                                                                740
  206  KD=IE-NEA+1                                                              750
       WRITE(NA,172) KI,NAM,KD                                                  760
  172  FORMAT(1H0,3X,I1,3X,A5,3X,I2)                                            770
       MZ=0                                                                     780
       CALL DOUB (8HSMTOT   ,NAM4)                                              790
   26  WRITE(LIZ) MZ,NAM4                                                       800
       IF(ET(1).LT.E(IA+1))  GOTO 39                                            810
  204  KD=KD-1                                                                  820
   39  KZ=KI+1                                                                  830
       WRITE (LIZ) KZ,NAM,KD                                                    840
C      LOOP OVER ALL OUTSCATTERING GROUPS TO BE CONSIDERED                      850
       DO 1  I=NEA,IE                                                           860
       NEI=NE-I                                                                 870
       IF(E(I+1).LE.ET(1))   GOTO 1                                             880
   10  GES=0.                                                                   890
       IF(I-NAB)83,85,1002                                                      900
   85  EH=EMAX                                                                  910
       GO TO 89                                                                 920
   83  EH=E(I+1)                                                                930
   89  NE1=NE-1                                                                 940
C      LOOP OVER ALL INSCATTERING GROUPS                                        950
       DO 2 K=1,I                                                               960
       SUM=DBLE(0.0)                                                            970
C      LOOP OVER ALL INELASTIC EXCITATION LEVELS OF THE MATERIAL CONSIDER        980
       DO 3 J=1,JMAT                                                            990
       IF(J.NE.1)    GOTO 6                                                     1000
    7  KMIN=0                                                                   1010
       GO TO 8                                                                  1020
    6  KMIN=KMAX(1)-KMAX(J)                                                     1030
C      DETERMINATION OF THE LIMITS EU,EO FOR INTEGRATION OVER THE               1040
C      OUTSCATTERING GROUP                                                      1050
    8  IF((E(K)+AE(J)).LT.E(I))  GOTO 9                                         1060
   17  IF((E(K)+AE(J)).GE.EH)    GOTO  88                                       1070
   57  EU=E(K)+AE(J)                                                            1080
       GO TO 44                                                                 1090
    9  IF((E(K+1)+AE(J)).LT.E(I))    GOTO 3                                     1100
   58  EU=E(I)                                                                  1110
   44  IF((E(K+1)+AE(J)).GE.EH)    GOTC 61                                      1120
```

```
   59 EO=E(K+1)+AE(J)                                                    1130
      GO TO 62                                                           1140
   61 EO=EH                                                              1150
C     DETERMINATION OF SIGMA AND THE WEIGHTING FUNCTION AT EU,EO         1160
   62 KJ=KMAX(J)                                                         1170
      IAB=0                                                              1180
      IAF=0                                                              1190
      IF1=IAF+1                                                          1200
      IB=IAB+1                                                           1210
      DO 4 IG=1,KJ                                                       1220
      KM=KMIN+IG                                                         1230
      IF(ET(KM).GE.EU)   GOTO 66                                         1240
   65 IAB=IG                                                             1250
      IAF=IG                                                             1260
      IF(ET(KM+1).LT.EO)    GOTO 4                                       1270
      IF(ET(KM+1).GE.EO)   GOTO 67                                       1280
   66 IF(IG.NE.1)   GOTO 72                                              1290
      SGP1=SGIP(J,1)                                                     1300
      CALL TRA(EU,FI1,NFE,EF,FI)                                         1310
      IAF=1                                                              1320
      IF(ET(KM).LT.EO)  GOTO 4                                           1330
  164 SGP2=SGIP(J,1)                                                     1340
      CALL TRA(EO,FI2,NFE,EF,FI)                                         1350
      GO TO 80                                                           1360
   72 IF(IAB.NE.0)    GOTO 70                                            1370
   73 IF(ET(KM).GE.EO)   GOTO 75                                         1380
   76 IAF=IG                                                             1390
      GO TO 4                                                            1400
   70 IF(ET(KM).LT.EO)   GOTO 74                                         1410
   75 IF1=IAF+1                                                          1420
      KMF=KMIN+IF1                                                       1430
      KMAF=KMIN+IAF                                                      1440
      SGP2=SGIP(J,IAF)+(SGIP(J,IF1)-SGIP(J,IAF))*(EO-ET(KMAF))/(ET(KMF)- 1450
     1ET(KMAF))                                                          1460
      CALL TRA(EO,FI2,NFE,EF,FI)                                         1470
      GO TO 80                                                           1480
   74 IAF=IG                                                             1490
   67 IB=IAB+1                                                           1500
      KMB=KMIN+IB                                                        1510
      KMAB=KMIN+IAB                                                      1520
      SGP1=SGIP(J,IAB)+(SGIP(J,IB)-SGIP(J,IAB))*(EU-ET(KMAB))/(ET(KMB)-E 1530
     1T(KMAB))                                                           1540
      CALL TRA(EU,FI1,NFE,EF,FI)                                         1550
      GO TO 4                                                            1560
    4 CONTINUE                                                           1570
C     CALCULATION OF THE INTEGRAL BETWEEN EU AND EO BY TRAPEZOIDAL RULE  1580
   80 IF(IAB.EQ.0)   GOTO 79                                             1590
   78 KMB=KMIN+IB                                                        1600
      IF(ET(KMB).NE.EU)  GOTO 82                                         1610
   81 IB1=IB                                                             1620
      LIE=IAF                                                            1630
      GO TO 77                                                           1640
   82 IB1=IAB                                                            1650
      LIE=IAF                                                            1660
      GO TO 77                                                           1670
   79 IB1=1                                                              1680
      IF(IF1.EQ.IAF)  GOTO 185                                           1690
      LIE=IF1                                                            1700
      KMB1=KMIN                                                          1710
      GOTO 182                                                           1720
  185 LIE=IAF                                                            1730
   77 KMB1=KMIN+IB1                                                      1740
  182 KMAF=KMIN+IAF                                                      1750
      DO 60  L=IB1,LIE                                                   1760
      IF(IAB.NE.0)     GOTO 183                                          1770
      IF(IF1.EQ.IAF)    GOTO 183                                         1780
      KML=KMIN+L-1                                                       1790
      GOTO 184                                                           1800
  183 KML=KMIN+L                                                         1810
  184 IF(IB1.LT.LIE)  GOTO 63                                            1820
   64 F1=SGP1*FI1                                                        1830
      F2=SGP2*FI2                                                        1840
      DIFF=EO-EU                                                         1850
      GO TO 45                                                           1860
   63 IF(L.NE.IB1)   GOTO 49                                             1870
   48 F1=SGP1*FI1                                                        1880
      DIFF=ET(KMB1+1)-EU                                                 1890
      GO TO 43                                                           1900
   49 IF(L.NE.LIE)  GOTO 46                                              1910
   47 F1=F2                                                              1920
      DIFF=EO-ET(KMAF)                                                   1930
      F2=SGP2*FI2                                                        1940
      GO TO 45                                                           1950
   46 F1=F2                                                              1960
      DIFF=ET(KML+1)-ET(KML)                                             1970
   43 IF(IAB.EQ.0)     GOTO 181                                          1980
      F2=SGIP(J,L+1)*WERT(KML+1)                                         1990
      GOTO 45                                                            2000
  181 F2=SGIP(J,L)*WERT(KML+1)                                           2010
   45 SUM=SUM+DIFF*(DBLE(F1)+DBLE(F2))/2.                                2020
   60 CONTINUE                                                           2030
C     SUMMATION LOOP FOR INTEGRAL CLOSED                                 2040
    3 CONTINUE                                                           2050
C     LOOP OVER EXCITAION LEVELS J CLOSED                                2060
   88 IF(SU(I).EQ.0.0)     GOTO 42                                       2070
   51 QUER(K)=SUM/DBLE(SU(I))                                            2080
      GO TO 52                                                           2090
   42 QUER(K)=DBLE(0.0)                                                  2100
   52 GES=GES+SNGL(QUER(K))                                              2110
    2 CONTINUE                                                           2120
C     LOOP OVER ALL INSCATTERING GROUPS K CLOSED                         2130
 1002 IF(I-NAB)111,115,131                                               2140
  115 IF(EMAX     .EQ.ET(LMAX))  GOTO 111                                2150
  110 IF(EMAX     .EQ.E(NAB+1))  GOTO 111                                2160
      IF(EMAX     .LT.E(NAB+1))   GOTO 133                               2170
  131 DI=0.                                                              2180
      GO TO 134                                                          2190
  133 DI=1.0-GES/QUOT(NAB)                                               2200
      IF(DI.LE.0.0)   GOTO 111                                           2210
C     CALCULATION OF THE SCATTERING PROBABILITIES IN THE CONTINUUM RANGE 2220
  134 CALL XKON(NAB,I,DI,    EMAX,PROB,A,NE,AG,NFE,EF,FI,XNUE,NX)        2230
  111 QUO=0.                                                             2240
```

```
      KE=0                                                                2250
      DO 55 LK=1,I                                                        2260
      LB=I+1-LK                                                           2270
      IF(I-NAB)130,139,135                                                2280
  135 WAHR(LK)=PROB(LK)                                                   2290
      GO TO 56                                                            2300
  139 IF(EMAX     .EQ.ET(LMAX))  GOTO 130                                 2310
      IF(EMAX     .EQ.E(NAB+1))  GOTO 130                                 2320
      IF(EMAX     .LT.E(NAB+1))   GOTO 141                                2330
  141 KE=1                                                                2340
      IF(DI.LE.0.0)  GOTO 130                                             2350
   27 IF(QUOT(NAB).NE.0.0)     GOTO 143                                   2360
  142 WAHR(LK)=DBLE(0.0)                                                  2370
      GO TO 144                                                           2380
  143 WAHR(LK)=QUER(LK)/DBLE(QUOT(NAB))                                   2390
  144 WAI=WAHR(LK)+PROB(LK)                                               2400
      WAHR(LK)=WAI                                                        2410
      GO TO 56                                                            2420
  130 IF(GES.EQ.0.0)     GOTO 54                                          2430
   53 WAHR(LK)=QUER(LK)/DBLE(GES)                                         2440
      GO TO 56                                                            2450
   54 WAHR(LK)=DBLE(0.0)                                                  2460
   56 QUO=QUO+SNGL(WAHR(LK))                                              2470
      VW(LB)=WAHR(LK)                                                     2480
   55 CONTINUE                                                            2490
      NZ=1                                                                2500
      DO 170 KV=1,I                                                       2510
      WAHR(KV)=VW(KV)                                                     2520
      AB=DBLE(0.0)                                                        2530
      IF(WAHR(KV).LE.AB)  GOTO 170                                        2540
  171 NZ=KV                                                               2550
  170 CONTINUE                                                            2560
      IF(KE.NE.1)    GOTO 136                                             2570
C     CONCERNS ONLY THE SCATTERING PROBABILITIES IN THE DISCRETE REGION   2580
  145 DO 137 KO=1,I                                                       2590
      IF(QUO.NE.0.0)     GOTO 161                                         2600
  162 UWA=DBLE(0.0)                                                       2610
      GOTO 163                                                            2620
  161 UWA=WAHR(KO)/DBLE(QUO)                                              2630
  163 WAHR(KO)=UWA                                                        2640
  137 CONTINUE                                                            2650
C     ORGANIZATION OF THE OUTPUT ON LISTING IN THE FORM OF MAXIMUM 11     2660
C     SCATTERING PROBABILITIES PER LINE STARTING WITH THE OUTSCATTERING   2670
C     GROUP OF LOWEST ENERGY(LARGEST GROUP NUMBER ACCORDING TO ABN-SET)   2680
  136 DO 126 LN=1,NZ                                                      2690
      LBA(LN)=NEI+LN-1                                                    2700
  126 CONTINUE                                                            2710
      KI=NZ/11                                                            2720
      KII=KI*11                                                           2730
      IF(NZ.NE.KII)  GOTO 168                                             2740
  167 KI1=KI                                                              2750
      GOTO 169                                                            2760
  168 KI1=KI+1                                                            2770
  169 DO 146 LI=1,KI1                                                     2780
      IF(LI.NE.1)    GOTO 147                                             2790
  148 LIM=1                                                               2800
      GO TO 149                                                           2810
  147 LIM=(LI-1)*11+1                                                     2820
      IF(LI.EQ.KI1)    GOTO 150                                           2830
  149 IF(KI1.LE.1)    GOTO 150                                            2840
  154 LI1=LI*11                                                           2850
      GO TO 151                                                           2860
  150 LI1=NZ                                                              2870
  151 IF(LIM.GT.LI1)  GOTO 146                                            2880
      WRITE(NA,125)    (LBA(LM),LM=LIM,LI1)                               2890
  125 FORMAT(10X,11(3X,I3,5X))                                            2900
      IF(LI.NE.1)    GOTO 153                                             2910
C     NEI-OUTSCATTERING GROUP ACCORDING TO THE COUNTING IN THE ABN-SET    2920
C     I.E. LOWEST GROUP NUMBER CORRESPONDS TO HIGHEST ENERGY BOUNDARIES   2930
C     WAHR-PROBABILITY FOR INELASTIC SCATTERING OUT OF GROUP I  INTO K     2940
  152 WRITE(NA,124) NEI,(WAHR(LM),LM=1,LI1)                               2950
  124 FORMAT (3X,I2,5X,11(E10.3,1X))                                      2960
      GO TO 146                                                           2970
  153 WRITE(NA,129)(WAHR(LM),LM=LIM,LI1)                                  2980
  129 FORMAT(10X,11(E10.3,1X))                                            2990
  146 CONTINUE                                                            3000
      NZ1=NZ+1                                                            3010
      DO 500 K=1,NZ                                                       3020
  500 WEIN(K)=WAHR(K)                                                     3030
      WRITE(LIZ) NZ1,NEI,(WEIN(K),K=1,NZ)                                 3040
    1 CONTINUE                                                            3050
    5 CONTINUE                                                            3060
  999 KL=KL+1                                                             3070
      RETURN                                                              3080
 1001 STOP                                                                3090
      END                                                                 3100
```

```
      SUBROUTINE AKED (E,    ET,SGIP,JMAT,KMAX,LMAX,SU,QUOT,WERT,AE,       10
     1EMAX,EMIN,IA,NAB,NFE,EF,FI,NE,NX,NET,NETF,NETP,SGIT,NAE,NAEF,        20
     2NAEP,ISG,ISGF,ISGP,IWE,IWF,IWP)                                      30
      REAL*8    NAM,      FELD,KFEL,NAM2,NAM3,ET,AE,EMAX,E,EMIN           40
      DIMENSION  FELD(6),KFEL(6),NFEL(6),SU(NX),QUOT(NX),E(NE),           50
     1AE(NAE),KMAX(NAE),WERT(IWE),ET(NET),SGIP(NAE,ISG),SGIT(NET),        60
     2EF(NFE),FI(NFE)                                                     70
      COMMON NAM,ISTRUK,ISPA,NA,LIZ                                       80
      EQUIVALENCE  (FELD(1),KFEL(1))                                      90
      CALL FSPIE                                                         100
      NETF=0                                                             110
      NAEF=0                                                             120
      IWF=0                                                              130
      ISGF=0                                                             140
      NETP=0                                                             150
      NAEP=0                                                             160
      IWP=0                                                              170
      ISGP=0                                                             180
      KEN=NFE                                                            190
      IF(NFE.EQ.1)  KEN=0                                                200
      CALL DOUB (8HBEST    ,NAM2)                                        210
```

```
      CALL DOUB(8HSGI     ,NAM3)                                        220
C     READING OF ENERGIES,SIGMA TOT,LEVEL EXCITATION SIGMA FROM KEDAK   230
      KFEL(1)=NAM                                                       240
      KFEL(2)=NAM2                                                      250
      KFEL(3)=NAM3                                                      260
C     INELASTIC SCATTERING CROSS SECTIONS WITH ENERGY SCALE FROM KNDF   270
C     ABOVE THRESHOLD FOR INELASTIC SCATTERING EMIN                     280
      NFEL(1)=3                                                         290
   10 CALL NDFLOC (N,NFEL,FELD,NDAT,NCO)                                300
      L=0                                                               310
   11 IF(FELD(5).NE.0.0)   GOTO 36                                      320
      L=1                                                               330
      SGIT(1)=FELD(5)                                                   340
      ET(1)=FELD(4)                                                     350
      CALL NDFNXT(N,NFEL,FELD,NDAT,NCO)                                 360
      IF(N.EQ.1)   GOTO 11                                              370
      GOTO 1000                                                         380
   36 L=L+1                                                             390
      IF(L.LE.NET)  GO TO 300                                           400
      L=1                                                               410
      NETF=NETF+1                                                       420
  300 ET(L)=FELD(4)                                                     430
      SGIT(L)=FELD(5)                                                   440
      IF(FELD(4).GE.E(NE))   GOTO 12                                    450
      CALL NDFNXT (N,NFEL,FELD,NDAT,NCO)                                460
      IF(N.EQ.1)   GOTO 36                                              470
   12 LMA=L                                                             480
      IF(NETF.EQ.0)  GO TO 301                                          490
      NETP=(NETF-1)*NET+L+1                                             500
      RETURN                                                            510
  301 EMIN    =ET(1)                                                    520
C     READING OF INELASTIC EXCITATION CROSS SECTIONS AND DETERMINATION  530
C     OF THE NUMBER OF EXCITATION LEVELS JMAT AND THE MAXIMUM ENERGY    540
C     EMAX, UP TO WHICH LEVEL EXCITAION CROSS SECTIONS ARE AVAILABLE ON 550
C     KEDAK (CORRESPONDS BOUNDARY BETWEEN CONTINUUM AND DISCRETE REGION) 560
C     A KEDAK CONVENTION IS PRESUPPOSED HERE: THE TOTAL INELASTIC       570
C     SCATTERING CROSS SECTION AND THE INELASTIC EXCITAION CROSS        580
C     SECTIONS FOR THE DIFFERENT LEVELS HAVE TO BE STORED AT THE SAME   590
C     ENERGY POINTS WHERE DATA FOR THE EXCITATION FUNCTIONS ARE GIVEN   600
C     STARTING AT THE HIGHEST ENERGY BELOW THE LEVEL ENERGY OF THE      610
C     EXCITATION LEVEL CONCERNED                                        620
      NFEL(1)=4                                                         630
      FELD(4)=0.0                                                       640
      CALL DOUB (8HSGIZ    ,NAM3)                                       650
      KFEL(3)=NAM3                                                      660
      CALL NDFLOC (N,NFEL,FELD,NDAT,NCO)                                670
      AE(1)=FELD(4)                                                     680
      J=0                                                               690
   21 CALL NDFLOC (N,NFEL,FELD,NDAT,NCO)                                700
      J=J+1                                                             710
      IF(J.LE.NAE)  GO TO 302                                           720
      J=1                                                               730
      NAEF=NAEF+1                                                       740
  302 AE(J)=FELD(4)                                                     750
      K=0                                                               760
   20 IF(FELD(5).LT.ET(1))   GOTO 121                                   770
    4 IF(FELD(5).LT.AE(J))   GOTO 121                                   780
  120 K=K+1                                                             790
      IF(K.LE.ISG)  GO TO 303                                           800
      K=1                                                               810
      ISGF=ISGF+1                                                       820
  303 SGIP(J,K)=FELD(6)                                                 830
  121 CALL NDFNXT(N,NFEL,FELD,NDAT,NCO)                                 840
      IF(N.EQ.1)   GOTO 20                                              850
      IF(ISGF.EQ.0)  GO TO 304                                          860
      ISGP=(ISGF-1)*ISG+K+1                                             870
      RETURN                                                            880
  304 IF(J.NE.1)    GOTO 22                                             890
      EMAX    =ET(K)                                                    900
C     KMAX(J) - CONSTANT WHICH HAS TO BE ADDED TO EMIN (AND ALL HIGHER  910
C     ENERGIES) TO OBTAIN THE FIRST ENERGY (AND HIGHER ENERGIES RESP.)  920
C     AT WHICH CROSS SECTION VALUES FOR THE LEVEL J ARE AVAILABLE ON    930
C     KEDAK                                                             940
   22 KMAX(J)=K                                                         950
      IF(FELD(4).NE.AE(J)) GO TO 21                                     960
      IF(NAEF.EQ.0)  GO TO 305                                          970
      NAEP=(NAEF-1)*NAE+J+1                                             980
      RETURN                                                            990
  305 JMAT=J                                                           1000
      DO 311 J=1,JMAT                                                  1010
      IF(KMAX(1).GE.KMAX(J))  GOTO 311                                 1020
      WRITE(NA,312)  J                                                 1030
  312 FORMAT (' ***ERROR 5.02 : THE NUMBER OF ENERGIES STORED FOR THE  1040
     1EXCITATION CROSS SECTIONS OF LEVEL J IS LARGER THAN THAT FOR THE 1050
     2FIRST (LOWEST) LEVEL.THIS IS AN ERROR ON KEDAK AND HAS TO BE     1060
     3CORRECTED. J =  ',I2)                                            1070
      GOTO 1000                                                        1080
  311 CONTINUE                                                         1090
      NE1=NE-1                                                         1100
  180 FORMAT (' ***ERROR 5.03 : ONE OF THE BOUNDARIES OF THE ENERGY    1110
     1RANGE IN WHICH INELASTIC SCATTERING IS POSSIBLE EMAX (- UPPER     1120
     2ENERGY LIMIT OF THE DISCRETE REGION) OR EMIN ( - LAST KEDAK-ENERGY 1130
     3AT WHICH THE TOTAL INELASTIC SCATTERING CROSS SECTION IS STILL    1140
     4EQUAL TO ZERO) IS NOT CONTAINED IN ANY OF THE ENERGY GROUPS OF    1150
     5THE GIVEN GROUP STRUCTURE. THAT MEANS THE GIVEN STRUCTURE OF      1160
     6ENERGY GROUPS DOES NOT COVER THE WHOLE ENERGY RANGE.')           1170
C     DETERMINATION OF THE ENERGY GROUP IA, IN WHICH EMIN IS LYING, AND 1180
C     OF THE ENERGY GROUP NAB, IN WHICH EMAX IS LYING.                 1190
      DO 84  L=1,NE1                                                   1200
      IF(EMIN     .GE.E(L).AND.EMIN     .LT.E(L+1))  GOTO 208          1210
      IF(EMIN     .GE.E(L+1))  GOTO 84                                 1220
      IF(EMIN     .GE.E(L))  GOTO 211                                  1230
      IF(L.NE.1)    GOTO 209                                           1240
  211 WRITE(NA,180)                                                    1250
      GOTO 1000                                                        1260
  208 IA=L                                                             1270
  209 IF(EMAX     .GT.E(L).AND.EMAX     .LE.E(L+1))  GOTO 210          1280
      IF(EMAX     .GT.E(L+1))  GOTO 84                                 1290
      WRITE(NA,180)                                                    1300
      GOTO 1000                                                        1310
   84 CONTINUE                                                         1320
  210 NAB=L                                                            1330
```

```
      IF(ET(LMA).LT.E(NAB+1))   GOTO 315                                1340
      DO 313 L=1,LMA                                                    1350
      IF(ET(L).GE.E(NAB+1))  GOTO 314                                   1360
  313 CONTINUE                                                          1370
C     LMAX - (NUMBER OF KEDAK ENERGIES + 1) BETWEEN EMIN AND THE UPPER  1380
C     ENERGY LIMIT E(NAB+1) OF GROUP NAB                                1390
  314 LMAX=L                                                            1400
      GOTO 316                                                          1410
  315 LMAX=LMA                                                          1420
C     INTERPOLATION OF THE WEIGHTING FUNCTION AT THE KEDAK ENERGY POINTS 1430
  316 KEN1=KEN-1                                                        1440
      IF(LMAX.LE.IWE)  GO TO 306                                        1450
      IWP=LMAX-IWE+1                                                    1460
      IWF=1                                                             1470
      RETURN                                                            1480
  306 IF(KEN.EQ.0)  GOTO 156                                            1490
   15 DO 32 LF=1,LMAX                                                   1500
      WERT(LF)=0.                                                       1510
      DO 16 IF=1,KEN1                                                   1520
      IF(ET(LF).LT.EF(IF))  GOTO 16                                     1530
      IF(ET(LF).GE.EF(IF+1))  GOTO 1116                                 1540
   38 WERT(LF)=FI(IF)+(ET(LF)-EF(IF))*(FI(IF+1)-FI(IF))/(EF(IF+1)-EF(IF) 1550
     1)                                                                 1560
      GO TO 32                                                          1570
 1116 IF(ET(LF).NE.EF(KEN))   GOTO 16                                   1580
      WERT(LF)=FI(KEN)                                                  1590
      GOTO 32                                                           1600
   16 CONTINUE                                                          1610
   32 CONTINUE                                                          1620
      GO TO 39                                                          1630
  156 DO18 KF=1,LMAX                                                    1640
      EK=ET(KF)                                                         1650
      WERT(KF)=PHI(EK)                                                  1660
   18 CONTINUE                                                          1670
C     INTERPOLATION OF SIGMA TOTAL AND THE WEIGHTING FUNCTION AT THE    1680
C     ENERGY GROUP BOUNDARIES                                           1690
   39 DO 50 II=IA,NAB                                                   1700
      NE1=NE-1                                                          1710
C     CRITICAL CASES                                                    1720
      IF(E(IA+1).GT.ET(1))  GOTO 7                                      1730
    8 IF(II.EQ.IA)   GOTO 50                                            1740
    9 IA1=IA+1                                                          1750
      IF(II-IA1)  90,108,90                                             1760
    7 IF(II-IA) 90,108,90                                               1770
  108 IF(E(II).GE.ET(1))   GOTO 112                                     1780
  109 LA=1                                                              1790
      SG1=0.                                                            1800
      EA=E(II)                                                          1810
      CALL TRA(EA,FHI1,NFE,EF,FI)                                       1820
      GO TO 91                                                          1830
  112 IF(E(II).EQ.ET(1))   GOTO 116                                     1840
      GO TO 1000                                                        1850
  116 LA=1                                                              1860
      SG1=SGIT(1)                                                       1870
      FHI1=WERT(1)                                                      1880
      EA=E(II)                                                          1890
      GO TO 91                                                          1900
   90 LA=0                                                              1910
   91 SUM(II)=0.                                                        1920
      SUMM=0.                                                           1930
      LMX1=LMAX-1                                                       1940
      DO 40 LL=1,LMX1                                                   1950
      IF(LA.NE.0)  GOTO 102                                             1960
  101 IF(E(II).LT.ET(LL))  GOTO 40                                      1970
  118 IF(E(II).GE.ET(LL+1))  GOTO 40                                    1980
  117 LA=LL                                                             1990
      SG1=SGIT(LL)+(SGIT(LL+1)-SGIT(LL))*(E(II)-ET(LL))/(ET(LL+1)-ET(LL) 2000
     1)                                                                 2010
      EA=E(II)                                                          2020
      CALL TRA(EA,FHI1,NFE,EF,FI)                                       2030
  102 IF(E(II+1).GT.ET(LL))  GOTO 122                                   2040
      GO TO 40                                                          2050
C     THE END GROUP IS THE CASE IN QUESTION                             2060
  122 IF(II.NE.NAB)   GOTO 107                                          2070
  123 NE1=NE-1                                                          2080
      IF(NAB.NE.NE1)   GOTO 107                                         2090
  124 IF(E(NAB+1).LT.ET(LMAX))  GOTO 107                                2100
  126 EE=ET(LMAX)                                                       2110
      LE=LMAX                                                           2120
      SG2=SGIT(LMAX)                                                    2130
      FHI2=WERT(LMAX)                                                   2140
      GO TO 100                                                         2150
  107 IF(E(II+1).GT.ET(LL+1))  GO TO 40                                 2160
  127 LE=LL+1                                                           2170
      SG2=SGIT(LL)+(SGIT(LL+1)-SGIT(LL))*(E(II+1)-ET(LL))/(ET(LL+1)-ET(L 2180
     1L))                                                               2190
      EE=E(II+1)                                                        2200
      CALL TRA(EE,FHI2,NFE,EF,FI)                                       2210
      GO TO 100                                                         2220
   40 CONTINUE                                                          2230
      GO TO 41                                                          2240
C     CALCULATION OF THE INTEGRAL OVER THE WEIGHTING FUNCTION AND THE   2250
C     INTEGRAL OVER SIGMA TOTAL*WEIGHTING FUNCTION BY TRAPEZOIDAL RULE  2260
  100 LE1=LE-1                                                          2270
      DO 30 IL=LA,LE1                                                   2280
      IF(LA.NE.LE1)  GOTO 104                                           2290
    3 IF(E(II).GE.ET(1))   GOTO 103                                     2300
   44 FU1=SGIT(LA)*WERT(LA)                                             2310
      FU2=SG2*FHI2                                                      2320
      DIF1=ET(LA)-EA                                                    2330
      DIFF=EE-ET(LA)                                                    2340
      SUP=DIF1*(WERT(LA)+FHI1)/2.+DIFF*(FHI2+WERT(LA))/2.               2350
      GOTO 28                                                           2360
  103 FU1=SG1*FHI1                                                      2370
      FU2=SG2*FHI2                                                      2380
      DIFF=EE-EA                                                        2390
      SUP=DIFF*(FHI2+FHI1)/2.                                           2400
      GO TO 28                                                          2410
  104 IF(IL.NE.LA)   GOTO 19                                            2420
    5 IF(E(II).GE.ET(1))    GOTO 34                                     2430
    6 FU1=SGIT(LA)*WERT(LA)                                             2440
      DIF1=ET(LA)-EA                                                    2450
```

```
      DIFF=ET(LA+1)-ET(LA)                                              2460
      SUP=DIF1*(WERT(LA)+FHI1)/2.+DIFF*(WERT(LA+1)+WERT(LA))/2.         2470
      GOTO 35                                                           2480
   34 FU1=SG1*FHI1                                                      2490
      DIFF=ET(LA+1)-EA                                                  2500
      SUP=DIFF*(WERT(LA+1)+FHI1)/2.                                     2510
      GO TO 35                                                          2520
   19 IF(IL.NE.LE1)  GOTO 26                                            2530
   27 FU1=FU2                                                           2540
      DIFF=EE-ET(LE1)                                                   2550
      SUP=DIFF*(FHI2+WERT(LE1))/2.                                      2560
      FU2=SG2*FHI2                                                      2570
      GO TO 28                                                          2580
   26 FU1=FU2                                                           2590
      DIFF=ET(IL+1)-ET(IL)                                              2600
      SUP=DIFF*(WERT(IL+1)+WERT(IL))/2.                                 2610
   35 FU2=SGIT(IL+1)*WERT(IL+1)                                         2620
   28 SUMM=SUMM+DIFF*(FU1+FU2)/2.                                       2630
      SU(II)=SU(II)+SUP                                                 2640
   30 CONTINUE                                                          2650
   41 IF(SU(II).EQ.0.)   GOTO 31                                        2660
   29 QUOT(II)=SUMM/SU(II)                                              2670
      GO TO 50                                                          2680
   31 QUOT(II)=0.                                                       2690
   50 CONTINUE                                                          2700
      RETURN                                                            2710
 1000 STOP                                                              2720
      END                                                               2730
```

```
      SUBROUTINE XKON(NZG,NUGR,DI,    EMAX,W,A,NE,ENG,NF,E,F,XNUE,NX)      10
C     XKON CALCULATES TRANSITION PROBABILITIES FOR INELASTIC SCATTERING    20
C     IN THE 'CONTINUUM REGION'.                                           30
      REAL*8 ELD,EUD,EXEM,EINS,SU1,SU2,EMD,WD,EXEL,EXD,                    40
     1    NAM,     EMAX,W,SW                                              50
      DIMENSION W(NX),          ENG(NE),F(NF),E(NF)                      60
      COMMON NAM,ISTRUK,ISPA,NA,LIZ                                      70
C     XNUE IS THE ADJUSTABLE PARAMETER FOR THE CALCULATION OF THE          80
C     NUCLEAR TEMPERATURE AND IS AN INPUT QUANTITY.                        90
      CALL FSPIE                                                        100
      XN=XNUE*A                                                         110
      KE=0                                                              120
      KEN=NF                                                            130
      IF(NF.EQ.1)  KEN=0                                                140
  401 IF(DI)2,2,1                                                       150
C     DI>0. MEANS:IN ENERGY GROUP NUGR BOTH RESOLVED AND UNRESOLVED     160
C     LEVELS HAVE TO BE CONSIDERED.EMAX(MM) IS THE HIGHEST ENERGY,      170
C     FOR WHICH THE W ARE CALCULATED FROM RESOLVED ENERGY LEVELS.       180
    1 D=DI                                                              190
      EANF=SNGL(EMAX)                                                   200
  202 EEND=ENG(NUGR+1)                                                  210
C     INDIRECT ASSUMPTION FOR DEFINITION OF EEND :                      220
C     HIGHEST ENERGY OF THE GROUP STRUCTURE IS LESS OR EQUAL THAN       230
C     THE UPPER ENERGY LIMIT ON KEDAK                                   240
      GOTO3                                                             250
    2 D=1.                                                              260
      EANF=ENG(NUGR)                                                    270
      GO TO 202                                                         280
    3 IF(KEN)4,4,5                                                      290
C     FOLLOWING IS THE CALCULATION OF THE AVERAGED NUCLEAR TEMPERATURE.  300
C     FOR KEN>0(STATEMENT NUMBER 5) THE AVERAGED NUCLEAR TEMPERATURE     310
C     IS CALCULATED USING AN ENERGY POINTWISE FLUX,SUBMITTED BY INPUT.   320
    5 DO 198 M=1,KEN                                                    330
      IF(E (M)-EANF)198,500,197                                         340
  500 MANF=M                                                            350
      GO TO 195                                                         360
  197 MANF=M                                                            370
      GO TO 194                                                         380
  198 CONTINUE                                                          390
  195 FANF=F(MANF)                                                      400
      GO TO 200                                                         410
  194 FANF=F(MANF-1)+((F(MANF)-F(MANF-1))*(EANF-E(MANF-1)))/(E(MANF)-    420
     1E(MANF-1))                                                        430
  200 MAN=MANF-1                                                        440
      DO 196 M=MAN ,KEN                                                 450
      IF(E (M)-EEND) 196,191,192                                        460
  191 MEND=M                                                            470
      GO TO 190                                                         480
  192  MEND=M                                                           490
      GO TO 189                                                         500
  196  CONTINUE                                                         510
  190 FEND=F(MEND)                                                      520
      GO TO 201                                                         530
  189 FEND=F(MEND-1)+ (F(MEND)-F(MEND-1))*(EEND-E(MEND-1))/(E(MEND)-    540
     1E(MEND-1))                                                        550
  201 JA=MANF                                                           560
      JE=MEND-2                                                         570
      IF(JE.LT.JA) GO TO 250                                            580
      S0=SQRT(E(MANF)/XN)*F(MANF)                                       590
      SINT=(SQRT(EANF/XN)*FANF+S0)/2.*(E(MANF)-EANF)+(SQRT(E(MEND-1)/XN)  600
     1*F(MEND-1)+SQRT(EEND/XN)*FEND)/2.*(EEND-E(MEND-1))                610
      XINT=(FANF+F(MANF))/2.*(E(MANF)-EANF)+(F(MEND-1)+FEND)/2.*        620
     1(EEND-E(MEND-1))                                                  630
      DO 186 J=JA,JE                                                    640
      DELT=E(J+1)-E(J)                                                  650
      S1=S0                                                             660
      S0=SQRT(E(J+1)/XN)*F(J+1)                                         670
      SINT=SINT+(S1+S0)/2.*DELT                                         680
  186 XINT=XINT+(F(J)+F(J+1))/2.*DELT                                   690
      THE  =SINT/XINT*0.001                                             700
  251 THE2=THE**2                                                       710
      GO TO 6                                                           720
  250 THE =SQRT((EEND+EANF)/(2.*XN))*0.001                              730
      GO TO 251                                                         740
C     IF KEN=0(STATEMENT NUMBER4),THE AVERAGE NUCLEAR TEMPERATURE       750
C     IS WEIGHTED BY A FLUX,WHICH IS CALCULATED FROM A FUNCTION PHI(E).  760
    4 DE=EEND-EANF                                                      770
      DED=DE/14.                                                        780
      E0=EANF+DED                                                       790
```

```
      X1=PHI(EANF)                                                          800
      X0=PHI(E0)                                                            810
      S1=SQRT(EANF/XN)*X1                                                   820
      S0=SQRT(E0/XN)*X0                                                     830
      SINT=(S1+S0)/2.*DED                                                   840
      XINT=(X1+X0)/2.*DED                                                   850
      DO 99 KF=1,13                                                         860
      E0=E0+DED                                                             870
      X1=X0                                                                 880
      S1=S0                                                                 890
      X0=PHI(E0)                                                            900
      S0=SQRT(E0/XN)*X0                                                     910
      SINT=SINT+(S1+S0)/2.*DED                                              920
   99 XINT=XINT+(X1+X0)/2.*DED                                              930
      THE  =SINT/XINT*0.001                                                 940
      THE2=THE**2                                                           950
C     FOLLOWING IS THE CALCULATION OF THE INELASTIC SCATTERING              960
C     TRANSITION PROBABILITIES.                                             970
    6 SW=0.                                                                 980
      EU=ENG(1)/THE*0.000001                                                990
      NU=NUGR-1                                                            1000
      DO 7 K=1,NU                                                          1010
      EL=EU                                                                1020
      EU=ENG(K+1)/THE*0.000001                                             1030
      EM=EU-EL                                                             1040
      ELD=DBLE(EL)                                                         1050
      EUD=DBLE(EU)                                                         1060
      EMD=DBLE(EM)                                                         1070
      EINS=DBLE(1.0)                                                       1080
      IF(EM-0.01)600,600,601                                               1090
C     IF (E(H)/THETA-E(H+1)/THETA) LESS OR EQUAL 0.01,(STATEMENT           1100
C     NUMBER 600),EXD IS USED TO CALCULATE THE TRANSITION PROBABILITIES,    1110
C     OTHERWISE(STATEMENT NUMBER 601) THE DOUBLE PRECISION EXPONENTIAL      1120
C     FUNCTION IS SUFFICIENT.                                              1130
  600 WD=-ELD*EXD(-EMD)-EMD*EXD(-EMD)-EXD(-EMD)-EMD                        1140
      EXEL=DEXP(-ELD)                                                      1150
      WD=EXEL*WD                                                           1160
      GO TO 602                                                            1170
  601 EXEM=DEXP(-EMD)                                                      1180
      SU1=EINS+ELD                                                         1190
      SU2=EINS+EUD                                                         1200
      SU2=SU2*EXEM                                                         1210
      WD=SU1-SU2                                                           1220
  602 EXEL=DEXP(-ELD)                                                      1230
      WD=EXEL*WD                                                           1240
      W(K)=WD*DBLE(THE2)                                                   1250
      IF(W(K).LT.0.0) KE=K                                                 1260
    7 CONTINUE                                                             1270
      IF(KE.GT.0) GOTO15                                                   1280
      GO TO 16                                                             1290
   15 DO 9 NG=1,KE                                                         1300
    9 W(NG)=0.0                                                            1310
   16 EL=EU                                                                1320
      EU=EEND/THE*0.000001                                                 1330
      EM=EU-EL                                                             1340
      ELD=DBLE(EL)                                                         1350
      EUD=DBLE(EU)                                                         1360
      EMD=DBLE(EM)                                                         1370
      EINS=DBLE(1.0)                                                       1380
      EXEM=DEXP(-EMD)                                                      1390
      EXEL=DEXP(-ELD)                                                      1400
      SU1=EINS+ELD                                                         1410
      SU2=EINS+EUD                                                         1420
      SU2=EXEM*SU2                                                         1430
      WD=SU1-SU2                                                           1440
      WD=EXEL*WD                                                           1450
      W(NUGR)=WD*DBLE(THE2)                                                1460
      DO 501 K=1,NUGR                                                      1470
  501 SW=SW+W(K)                                                           1480
      DO 8 K=1,NUGR                                                        1490
    8 W(K)=W(K)/SW*DBLE(D)                                                 1500
      RETURN                                                               1510
      END                                                                  1520
```

```
      DOUBLE PRECISION FUNCTION EXD(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 EXD=XN                                                               170
    5 RETURN                                                               180
      END                                                                  190
```

```
      DOUBLE PRECISION FUNCTION DNFAK(NN)                                   10
C     DNFAK CALCULATES N*(N-1)*(N-2)*.......*(N-(N-1)) FOR THE              20
C     SERIES DEVELOPED IN EXD.                                              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
```

```
      SUBROUTINE DOUB(IK,K)                                              10
      REAL*8 IK,K                                                        20
      K=IK                                                               30
      RETURN                                                             40
      END                                                                50
```

```
      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) GO TO 2                                               60
    1 FIS=PHI(EFI)                                                       70
      GO TO 3                                                            80
    2 DO 105 KI=1,KEN                                                    90
      IF(EF(KI).GE.EFI) GO TO 114                                       100
  113 KUA=KI                                                            110
      GO TO 105                                                         120
  114 KAB=KUA+1                                                         130
      GO TO 106                                                         140
  105 CONTINUE                                                          150
  106 FIS=FI(KUA)+(FI(KAB)-FI(KUA))*(EFI-EF(KUA))/(EF(KAB)-EF(KUA))     160
    3 RETURN                                                            170
      END                                                               180
```

```
      SUBROUTINE FLUMMI(A,B,EA,EB,E,EN,SGN,ECO,SCO,V,W,F,AR,FU,ABN,INT,  10
     1                  GR,FEKOE,FG,R,RSP,ESP,SPEK,SGNC,FEKO,ELSIG,      20
     2                  ELTOT,ET,ST,MAT,DAT,NLA,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,NR)                              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                                                                      170
C                                                                      180
      REAL*8 STOFF,MAT                                                 190
      DIMENSION A(ISM),B(ISM),EA(ISM),EB(ISM),E(ISM),                  200
     1          EN(ISD),SGN(ISD),ECO(ISD),SCO(ISD),V(ISD),W(ISD),F(ISD),210
     2          AR(ICOS),FU(ICOS),                                     220
     3          ABN(NE27),INT(NE27),GR(NE27),FEKOE(NE27),              230
     4          EG(NX),R(NX),RSP(NX),                                  240
     5          ESP(NSPEK),SPEK(LSPEK),                                250
     6          NST(6),LEG(6),MAZ(2),                                  260
     7          SGNC(ICOS,ISM),FEKO(ISM,NECU),ELSIG(6,NECU,NX),        270
     8          ELTOT(2,NX),                                           280
     9          MAT(KT),DAT(KT),                                       290
     A          ET(NTTT),ST(NTTT)                                      300
      COMMON STOFF,ISTRUK,ISPA,NOUT,KPR,IM,IL,KL                       310
C                                                                      320
      DATA NST/81,81,161,161,321,321/                                  330
C     NST(L)= ANZAHL DER AEQUIDISTANTEN STREUKOSINUSSTUETZPUNKTE DER   340
C             SGNC IM L-SYSTEM FUER DAS (L-1)-TE MOMENT                350
      DATA LEG/2,1,3,4,5,6/                                            360
C     LEG   = REIHENFOLGE BEI DER MOMENTENBERECHNUNG                   370
C                                                                      380
      WRITE (NOUT ,9000)                                               390
 9000 FORMAT(1HO/1HO/' PROGRAMM KENNZIFFER 6')                         400
      WRITE (NOUT ,9001)                                               410
 9001 FORMAT(' PROGRAMM ZUR BERECHNUNG ELASTISCHER STREUMATRIZEN'/)     420
      CALL FSPIE                                                       430
C                                                                      440
C*****SETZEN INTERNER KONSTANTEN*******************************************450
C     ISM   = ANZAHL DER ENERGIESTUETZPUNKTE PRO MAKROGRUPPE IM GROBNETZ 460
C     ISD   = MAXIMALE ANZAHL DER ENERGIESTUETZPUNKTE PRO MAKROGRUPPE    470
C             IM FEINNETZ                                              480
C     NK    = ANZAHL VON GRUNDPUNKTEN IM UEBERSTREUBEREICH             490
C     NR    = MAXIMALZAHL VON GRUNDPUNKTEN IM NICHT-UEBERSTREUBEREICH  500
C     NS    = MAXIMALE FEINGRUPPENZAHL PRO GROBGRUPPE                  510
      PM    = 1                                                        520
C     PM    = ANTEIL VON MUEL BEI DER KORREKTUR DES 1. MOMENTES        530
C     NECU  = MAXIMALE STREUBREITE                                     540
C     NMAX  = MAXIMALER LEGENDRE-APPROXIMATIONSGRAD                    550
C     NOUT  = UNIT-NUMMER DER AUSGABE-DATEI                            560
C     ICOS  = ANZAHL DER AEQUIDISTANTEN STREUKOSINUSSTUETZPUNKTE DER VON 570
C             KNOF GELESENEN DIFFERENTIELLEN STREUQUERSCHNITTE (SGNC)  580
      NF    = 10                                                       590
C     NF    = SPEICHEREINHEIT FUER ENERGIEDIFF. LEGENDRE-KOEFF.        600
C                                                                      610
C*****INITIALISIERUNG INTERNER GROESSEN*************************************620
      KIM = 0                                                          630
      NEN = 0                                                          640
      ITA = 0                                                          650
      ISO=1                                                            660
      NSYS = 1                                                         670
      NSTIS = NST(6)                                                   680
      NUEB = NECU                                                      690
      OD = 2./(ICOS-1)                                                 700
      NECUP=0                                                          710
      ISDP=0                                                           720
      ISMP=0                                                           730
      ICOSP=0                                                          740
      ISCOP=0                                                          750
      ISECP=0                                                          760
      NTTP=0                                                           770
      KSPE=1                                                           780
C                                                                      790
```

```
C*****LESEN DES ATOMGEWICHTES*********************************************
      CALL LOOK0(XMAT,MASSE,COM,&1001)
      ALFA = ((XMAT-1.)/(XMAT+1.))**2
C
C*****UMSORTIEREN DER GRUPPENGRENZEN**************************************
      KSPEK=NSPEK
      IF(NSPEK.GT.1)  GO TO 305
      KSPE=0
      KSPEK=0
  305 DO 302 I=1,NX
      II=NX-I+1
  302 ABN(I)=EG(II)
      IF(ABN(NX)-1.E-3)301,303,304
  301 WRITE(NOUT,350)
  350 FORMAT(//' ***ERROR 6.8 : THE SMALLEST GROUP BOUNDARY MUST BE GREA
     1TER THAN OR EQUAL TO 1.E-3')
      GO TO 8000
  304 NEGR=NE27
      ABN(NEGR)=AMAX1(1.E-3,ALFA*ABN(NX))
      GO TO 4
  303 NEGR=NX
C
C*****BESTIMMUNG DER GRUPPENLETHARGIEN************************************
    4 NGR = NEGR-1
      QA = ABN(1)/ABN(2)
      DO 5  I = 1,NGR
      RSP(I) = 0.
    5 R(I)=ALOG(ABN(I)/ABN(I+1))
C
C*****LESEN DER SGNC-ENERGIEN UND BESTIMMUNG DER STREUBREITE**************
      IF(MASSE.EQ.1)   GOTO 6
      CALL LOOK3(NEN,EB,ISO,NGR,ABN,ISM,ISMP,GR,NEGR,ISEL)
      IF(ISMP.GT.0) RETURN
      ES = EB(1)
      GOTO 7
    6 ALFA = 1.E-4
      ES = ABN(1)
    7 NUE=2
      DO 11 I=1,NGR
      DO 9 II=I,NEGR
      IF(ABN(II).LT.ABN(I)*ALFA)  GO TO 10
    9 CONTINUE
      II=NEGR
   10 NUE=MAX0(NUE,II-I)
   11 CONTINUE
      IF(NUE.LE.NUEB)   GOTO 8
      NECUP=NUE-NUEB
      RETURN
    8 NUEB = NUE
      ISCOP=NUEB*ISD-ISCO
      IF(ISCOP.LT.0)  ISCOP=0
      IF(ISCOP.GT.0)  RETURN
      ISECP=ISD-ISEC
      IF(ISECP.LT.0)  ISECP=0
      IF(ISECP.GT.0)  RETURN
C
C*****BESTIMMUNG DER MAKROGRUPPENEINTEILUNG********************************
   12 KIM = MINO(NGR-IM,NUEB-1)
      IM = IM+KIM
      CALL MAKRO(ALFA,ISO,IL,IM,NGR,ABN,ISD,ISM,ISDP,NS,NK,NECU,NUEB,V,
     1           W,ELTOT,INTT,INT,NEGR,ISEL)
      IF(ISDP.GT.0)  RETURN
C
   13 NEK = NEN
      IF(NEN.EQ.0)   GOTO 16
      IF(EB(NEN).GE.ABN(IL))   GOTO 16
      WRITE(NOUT,913)   STOFF,EB(NEN)
      STOP
   16 CONTINUE
C
C
C*****  M A K R O G R U P P E N R E C H N U N G  ************************
C
      IR = 1
   20 NANF = INT(IR)+1
      IF(IR.EQ.1)   NANF = NANF-1
      NEND = INT(IR+1)
      NEN = NEK
      ISOT = 1
C
C****  BESTIMMUNG DES EINSTREUINTERVALLES*********************************
      EANF = ABN(NEND+1)
   22 EEND=ABN(NANF)
      IF(MASSE.GT.1)   GOTO 28
      NEN = 1
      EA(1) = ABN(IL)
   28 IF(MASSE.EQ.1)   GOTO 62
      DO 60  NE = 1,NEN
   60 EA(NE) = EB(NE)
   62 CONTINUE
C
C*****MAKROSKOPISCHER TOTALER QUERSCHNITT FUER FEINSTRUKTURWICHTUNG*****
      NTT=1
      IF(NTK.EQ.1) CALL MIXSGT(KT,MAT,DAT,NTTT,NTTP,NTT,ET,ST,EANF,EEND)
      IF(NTTP.GT.0)  RETURN
C
C*****EINORDNEN DES AUSSTREUINTERVALLES UND LESEN DER SGNC**************
      IF(EA(1).GE.EEND)   GOTO 88
      DO 64  NE = 1,NEN
      NI = NE
      IF(EA(NE).GE.EANF)  GOTO 66
   64 CONTINUE
   66 DO 68  NE = 1,NEN
      NO = NEN-NE+1
      IF(EA(NO).LE.EEND)  GOTO 70
   68 CONTINUE
C
   70 IF(NI.EQ.1)   GOTO 78
      NO=MINO(NO+2,NEN)
      NI=MAX0(NI-2,1)
      NEN = NO-NI+1
      DO 74  NE = NI,NO
```

```
   74 A(NE) = EA(NE)                                                    1920
      DO 76  NE = 1,NEN                                                 1930
   76 EA(NE) = A(NE+NI-1)                                               1940
      CALL LOOK2(NEN,EA,ICOS,ICOSP,AR,ISM,SGNC)                         1950
      IF(ICOSP.GT.0)   RETURN                                           1960
      GOTO 100                                                          1970
C                                                                       1980
   78 NEN=MINO(NO+2,NEN)                                                1990
      CALL LOOK2(NEN,EA,ICOS,ICOSP,AR,ISM,SGNC)                         2000
      IF(ICOSP.GT.0)   RETURN                                           2010
      IF(ES.LE.EANF)  GO TO 100                                         2020
      DO 84  NE = 1,NEN                                                 2030
      NA = NEN-NE+1                                                     2040
      NU = NEN-NE+2                                                     2050
      EA(NU) = EA(NA)                                                   2060
      DO 84  IP = 1,ICOS                                                2070
   84 SGNC(IP,NU) = SGNC(IP,NA)                                         2080
      EA(1) = EANF                                                      2090
      NEN = NEN+1                                                       2100
      DO 86  IP = 1,ICOS                                                2110
   86 SGNC(IP,1) = 0.7957747E-01                                        2120
      GOTO 100                                                          2130
C                                                                       2140
C*****KOSINUS UND ENERGIEN BEI ISOTROPIE IM CM-SYSTEM******************* 2150
   88 DO 90  IP = 1,ICOS                                                2160
   90 AR(IP) = (IP-1)*DD-1.                                             2170
      NEN = 0                                                           2180
      CALL PUNK(NGR,NEGR,ABN,NANF,NEND,NEN,ALFA,NK,NR,ISM,ISMP,ISN,E)   2190
      IF(ISMP.GT.0)   RETURN                                            2200
      ISOT = 0                                                          2210
      GOTO 115                                                          2220
C                                                                       2230
C*****TRANSFORMATION DER SGNC************************************** 2240
  100 IF(NSYS.EQ.1)   CALL TRAFO(ICOS,NEN,ISM,SGNC,XMAT,ALFA,AR)        2250
C                                                                       2260
C*****ENERGIEINTERPOLATION DER SGNC************************************ 2270
      CALL PUNK(NGR,NEGR,ABN,NANF,NEND,NEN,ALFA,NK,NR,ISM,ISMP,ISN,E)   2280
      IF(ISMP.GT.0)   RETURN                                            2290
      CALL PUSUM(NEN,EA,ISN,E,V)                                        2300
      NU=0                                                              2310
      NO=0                                                              2320
  104 IF(E(NU+1).GE.EANF)  GO TO 106                                    2330
      NU=NU+1                                                           2340
      GO TO 104                                                         2350
  106 IF(E(ISN-NO).LE.EEND)  GO TO 108                                  2360
      NO=NO+1                                                           2370
      GO TO 106                                                         2380
  108 ISK=ISN-NU-NO                                                     2390
      DO 111  IP = 1,ICOS                                               2400
      DO 110  NE = 1,NEN                                                2410
  110 B(NE) = SGNC(IP,NE)                                               2420
      CALL IPOLA(NEN,EA,B,ISN,E,A,F)                                    2430
      DO 111 NE=1,ISK                                                   2440
      NO=NE+NU                                                          2450
      IF(E(NO).LE.ES)  A(NO)=A(1)                                       2460
  111 SGNC(IP,NE)=A(NO)                                                 2470
      DO 113 NE=1,ISK                                                   2480
  113 E(NE)=E(NE+NU)                                                    2490
      ISN = ISK                                                         2500
C                                                                       2510
C*****ENERGIEDIFFERENTIELLE LEGENDRE-KOEFFIZIENTEN ********************* 2520
  115 CALL LECAL (MASSE,XMAT,ALFA,ISOT,LEG,NLE,NANF,NEND,NUEB,IL,IM,    2530
     1            NEGR,ABN,ICOS,AR,ISN,E,SGNC,NST,NSTIS,ISM,ISD,NECU,   2540
     2            ITA,NF,GR,FEKOE,FU,A,ECO,SCO,V,W,F,FEKO)              2550
C                                                                       2560
C*****LESEN DER SGN UND MUEL************************************************ 2570
      CALL LOOK1(ISD,K,EN,SGN,EANF,EEND,0)                              2580
      IF(ISOT.EQ.0)   GOTO 120                                          2590
      CALL LOOK1(ISD,M,ECO,SCO,EANF,EEND,1)                             2600
      IF(M.LT.ISD)  GO TO 116                                           2610
      ISDP=100                                                          2620
      RETURN                                                            2630
  116 IF(ES.LT.EANF)  GO TO 120                                         2640
      DO 112  J = 1,M                                                   2650
      IF(ECO(J).LT.ES)   SCO(J) = COM                                   2660
  112 CONTINUE                                                          2670
  120 IF(IABS(ISEL).GT.1)  GO TO 122                                    2680
      DO 118  J = 1,K                                                   2690
  118 SGN(J) = 1.                                                       2700
C                                                                       2710
C*****MULTIGRUPPEN-ENERGIEINTEGRATION********************************** 2720
  122 CALL GRUPIN (MASSE,XMAT,ALFA,COM,ISOT,PM,LEG,NLE,NANF,NEND,NUEB,  2730
     1             IL,IM,NGR,NEGR,ABN,ISN,E,K,EN,SGN,M,ECO,SCO,NTT,ET,  2740
     2             ST,MAZ,KSPE,KSPEK,ESP,SPEK,NSPEK,LSPEK,ISM,ISD,      2750
     3             NECU,ISCO,ISEC,NF,F,A,GR,SGNC,FEKO,V,W,ISTT,RSP,     2760
     4             ELSIG)                                               2770
C                                                                       2780
C*****AUSGABE VON INFORMATIONEN*********************************************** 2790
      IF(ISEL.LT.0)   CALL INFORM(ALFA,NEGR,ABN,R,RSP,IL,IM,INTT,INT,   2800
     1                            NST,NSTIS,IR,ISTT,K,NTK,NTT,NOUT)     2810
C                                                                       2820
      IF(IR+1.GE.INTT)   GOTO 290                                       2830
      IR = IR+1                                                         2840
      GOTO 20                                                           2850
C                                                                       2860
C*****MULTIGRUPPENKONSTANTEN************************************************ 2870
  290 CALL MUKON(ELSIG,ELTOT,NLE,NECU,NUEB,IL,IM,NGR)                   2880
C                                                                       2890
C*****AUSDRUCKEN DER ERGEBNISSE********************************************** 2900
      IM = IM-KIM                                                       2910
  300 CALL PRINT(ELSIG,ELTOT,NLA,NLE,NECU,NUEB,ISEL,NGR,KSPE,MAZ,NTK,   2920
     1           KIM)                                                   2930
      GO TO 8000                                                        2940
C                                                                       2950
 1001 WRITE (NOUT,1002) STOFF                                           2960
 8000 KL = KL+1                                                         2970
      RETURN                                                            2980
C                                                                       2990
C                                                                       3000
  909 FORMAT(1HO)                                                       3010
  913 FORMAT(//' ***ERROR 6.1 : FOR  ',A8,' SCATTERING MATRICES CANNOT B 3020
     1E CALCULATED'/16X'FOR ENERGIES ABOVE',1PE10.3,' EV FOR LACK OF SGN 3030
```

```
     2C ON KEDAK')                                                          3040
 1002 FORMAT(//' ***ERROR 6.7 : FOR  ',A8,' SCATTERING MATRICES CANNOT B 3050
     1E CALCULATED FOR'/16X,'LACK OF ISOTI (ATOMIC WEIGHT) ON KEDAK')       3060
      END                                                                   3070
```

```
      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
      IF(A(I-1).LE.A(I))   GOTO 2                                         150
      B = A(I)                                                            160
      A(I) = A(I-1)                                                       170
      A(I-1) = B                                                          180
      K = 1                                                               190
    2 CONTINUE                                                            200
      N = -N                                                              210
      IA = IA-N                                                           220
      IF(K.EQ.1)   GOTO 1                                                 230
      IF(KK.EQ.1)   GOTO 3                                                240
      KK = 1                                                              250
      GOTO 1                                                              260
C                                                                         270
C*****SUMMIEREN*****************************************************     280
    3 SP = 0.                                                             290
      SN = 0.                                                             300
      IF(A(1).GE.0.)   GOTO 8                                             310
      IF(A(M).LE.0.)   GOTO 10                                            320
      DO 4  I = 2,M                                                       330
      IF((A(I-1).LE.0.).AND.(A(I).GE.0.))   GOTO 5                        340
    4 CONTINUE                                                            350
    5 IA = I                                                              360
      IB = I-1                                                            370
      DO 6  I = IA,M                                                      380
    6 SP = SP+DBLE(A(I))                                                  390
      DO 7  I = 1,IB                                                      400
    7 SN = SN+DBLE(A(IB+1-I))                                             410
      GOTO 12                                                             420
    8 DO 9  I = 1,M                                                       430
    9 SP = SP+DBLE(A(I))                                                  440
      GOTO 12                                                             450
   10 DO 11  I = 1,M                                                      460
   11 SN = SN+DBLE(A(M+1-I))                                              470
```

```
   12 S = SNGL(SN+SP)                                                     480
      RETURN                                                              490
   13 S = A(1)                                                            500
      IF(M.EQ.2)   S = S+A(2)                                             510
      RETURN                                                              520
      END                                                                 530
```

```
      SUBROUTINE IPOLA(M,A,B,N,X,Y,T)                                      10
C                                                                          20
C*****STETIG DIFFB. INTERPOLATION DURCH POLYNOME 4. GRADES**********      30
C                                                                          40
      DIMENSION  A(M),B(M),T(M),X(N),Y(N)                                  50
C                                                                          60
C*****TANGENTEN*****************************************************     70
      T(1)=(B(2)-B(1))/(A(2)-A(1))                                         80
      T(M)=(B(M)-B(M-1))/(A(M)-A(M-1))                                     90
      MN = M-1                                                            100
      DO 2  J = 2,MN                                                      110
      T(J) = 0.                                                           120
      IF((B(J+1).GT.B(J)).AND.(B(J).GT.B(J-1)))                           130
     1T(J) = (B(J+1)-B(J-1))/(A(J+1)-A(J-1))                              140
      IF((B(J+1).LT.B(J)).AND.(B(J).LT.B(J-1)))                           150
     1T(J) = (B(J+1)-B(J-1))/(A(J+1)-A(J-1))                              160
    2 CONTINUE                                                            170
C                                                                         180
C*****INTERPOLATION*************************************************     190
      Y(1) = B(1)                                                         200
      Y(N) = B(M)                                                         210
      NM = N-1                                                            220
      J = 1                                                               230
      DO 26  I = 2,NM                                                     240
   18 IF(X(I)-A(J))   20,22,24                                            250
   20 S = X(I)-UM                                                         260
      Y(I) = (((A4*S+A3)*S+A2)*S+A1)*S+VM                                 270
      GOTO 26                                                             280
   22 Y(I) = B(J)                                                         290
      GOTO 26                                                             300
   24 J = J+1                                                             310
      U = 0.5*(A(J)-A(J-1))                                               320
      V = 0.5*(B(J)-B(J-1))                                               330
      TP = 0.5*(T(J)+T(J-1))                                              340
      TM = 0.5*(T(J)-T(J-1))                                              350
      A1 = 0.5*(3*V/U-TP)                                                 360
      A2 = -0.5*TM/U                                                      370
      A3 = 0.5*(TP-V/U)/(U*U)                                             380
      A4 = 0.5*TM/(U*U*U)                                                 390
      UM = 0.5*(A(J-1)+A(J))                                              400
      VM = 0.5*(B(J-1)+B(J))                                              410
      GOTO 18                                                             420
   26 CONTINUE                                                            430
      RETURN                                                              440
      END                                                                 450
```

```
      SUBROUTINE PUSUM(KA,A,KE,E,B)                                     10
C                                                                       20
C*****STUETZPUNKTMENGEN VEREINIGEN*************************************  30
C                                                                       40
      DIMENSION  A(KA),E(KE),B(KE)                                      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(K.GT.KA)  GO TO 10                                            130
      IF(I.GT.KE)   GOTO 14                                            140
      IF(A(K)-B(I))   4,5,6                                            150
    4 E(J) = A(K)                                                      160
      J = J+1                                                          170
      K = K+1                                                          180
      GOTO 3                                                           190
    5 E(J) = A(K)                                                      200
      J = J+1                                                          210
      I = I+1                                                          220
      K = K+1                                                          230
      GOTO 3                                                           240
    6 E(J) = B(I)                                                      250
      J = J+1                                                          260
      I = I+1                                                          270
      GOTO 3                                                           280
   10 IF(I.GT.KE)  GO TO 18                                            290
      DO 12 K=I,KE                                                     300
      E(J)=B(K)                                                        310
   12 J=J+1                                                            320
      GO TO 18                                                         330
   14 DO 16 I=K,KA                                                     340
      E(J)=A(I)                                                        350
   16 J=J+1                                                            360
   18 KE=J-1                                                           370
      RETURN                                                           380
C                                                                      390
      END                                                              400
```

```
      SUBROUTINE MAKRO(ALFA,ISO,IL,IM,NGR,ABN,ISD,ISM,ISDP,NS,NK,NECU,  10
     1                 NUEB,V,W,LST,INTT,INT,NEGR,ISEL)                 20
C                                                                       30
C*****BESTIMMUNG EINER DEN SGN-STELLEN UND DER GRUPPENSTUETZPUNKTZAHL AN  40
C*****GEPASSTEN MAKROGRUPPENEINTEILUNG*********************************  50
C                                                                       60
      REAL*8  STOFF                                                     70
      DIMENSION  ABN(NEGR),INT(NEGR),LST(NGR),V(ISD),W(ISD)             80
      COMMON  STOFF,ISTRUK,ISPA,NOUT                                    90
C                                                                      100
C*****ANZAHL DER SGN IN DER N-TEN GRUPPE*******************************  110
      DO 10  N = IL,IM                                                 120
   10 LST(N) = 0                                                       130
      EA = ABN(IM+1)                                                   140
      EE = ABN(IL)                                                     150
   11 CALL LOOK1(ISD,K,V,W,EA,EE,0)                                    160
      DO 12  N = IL,IM                                                 170
      A = ABN(N+1)                                                     180
      B = ABN(N)                                                       190
      DO 12  MM = 1,K                                                  200
      E = V(K-MM+1)                                                    210
      IF(A.LT.E.AND.E.LE.B)    LST(N) = LST(N)+1                       220
   12 CONTINUE                                                         230
      IF(K.LT.ISD)   GOTO 13                                           240
      EA = V(K)                                                        250
      GOTO 11                                                          260
   13 IF(ISEL.LT.0)   WRITE(NOUT,100)                                  270
      ISDP = 0                                                         280
      NTO = 0                                                          290
      DO 14  N = IL,IM                                                 300
      NTO = NTO+LST(N)                                                 310
      IF(ISEL.LT.0)   WRITE(NOUT,102)   N,LST(N)                       320
      LSS = LST(N)                                                     330
C         = SGN-STELLEN IN DER N-TEN GRUPPE                            340
      LSG = NK+5                                                       350
C         = GRUNDPUNKTE PRO GRUPPE                                     360
      LSM = (ISM-NS*(NK+5))/NS                                         370
C         = SGNC-ENERGIESTUETZSTELLEN PRO GRUPPE                       380
   14 ISDP = MAX0(ISDP,LSG+LSM+LSS-ISD)                                390
      IF(ISEL.LT.0)   WRITE(NOUT,103)   NTO                            400
      IF(ISDP.GT.0)   RETURN                                           410
C                                                                      420
C*****MAKROGRUPPENEINTEILUNG*******************************************  430
      IT = ISO                                                         440
      ID = ISD-ISM                                                     450
      INT(1) = IL-1                                                    460
      IR = 2                                                           470
    3 II = INT(IR-1)+1                                                 480
      IS = 0                                                           490
      DO 4  I = II,IM                                                  500
      IS = IS+LST(I)                                                   510
      IF((IS.GE.ID).OR.(1+I-II.GT.NS))   GOTO 5                        520
      IF(I.NE.IT)   GOTO 4                                             530
      IF(I.EQ.IM.OR.I.EQ.II)   GOTO 4                                  540
      IT = 0                                                           550
      GOTO 5                                                           560
    4 CONTINUE                                                         570
      INT(IR) = IM                                                     580
      INT(1) = IL                                                      590
      INTT = IR                                                        600
      IE = IR-1                                                        610
      GOTO 7                                                           620
```

```
    5 INT(IR) = MAXO(II,I-1)
      IR = IR+1
      GOTO 3
C
C*****SCHREIBEN DER MAKROGRUPPENEINTEILUNG*******************************
    7 IF(ISEL.GT.0)   RETURN
      WRITE(NOUT,94)
      DO 8  I = 1,IE
      IP = INT(I)+1
      IF(I.EQ.1)   IP = IP-1
    8 WRITE(NOUT,96)   I,IP,INT(I+1)
C
      RETURN
C
   94 FORMAT(///11X,'M A K R O G R U P P E N'//)
   96 FORMAT(1HO,2X,I2,'. MAKROGRUPPE',5X,I3,'. BIS ',I3,'. FEINGRUPPE')
  100 FORMAT(//14X,'VERTEILUNG DER SGN'//)
  102 FORMAT(1X,I3,'. FEINGRUPPE',12X,I4,' SGN')
  103 FORMAT(1HO,6X,'INSGESAMT',12X,I4,' SGN')
C
      END
```

```
      SUBROUTINE MIXSGT(KT,MAT,DAT,NTT,NTP,NT,ET,ST,EA,EE)
C
C*****TOTALER QUERSCHNITT EINER MISCHUNG*********************************
C
      REAL*8  MAT(KT),A(5),STOFF
      DIMENSION  DAT(KT),ET(NTT),ST(NTT),NW(4),NAD(2)
      COMMON STOFF,ISTRUK,ISPA,NOUT
      DATA NW(1),A(2),A(3) /3,'BEST ','SGT  '/
C
      DO 10  K = 1,KT
      D = DAT(K)
      A(1) = MAT(K)
      NU = 0
      CALL NDFLOC(KP,NW,A,NAD,KC)
      IF(KP.NE.1)   GOTO 12
      E = A(4)
      S = A(5)
      IF(E-EA)   6,4,14
    4 CALL ADD(K,NTT,NTP,NT,ET,ST,NU,D,E,S,EV,SV,EW,SW,EA,EE)
      IF(NTP.GT.0)   RETURN
    6 EV = E
      SV = S
      CALL NDFNXT(KP,NW,A,NAD,KC)
      IF(KP.EQ.1)   GOTO 7
      E = EE
      S = SV
      GOTO 8
    7 E = A(4)
      S = A(5)
      IF(E-EA)   6,4,8
    8 CALL ADD(K,NTT,NTP,NT,ET,ST,NU,D,E,S,EV,SV,EW,SW,EA,EE)
      IF(NTP.GT.0)   RETURN
      IF(E.LT.EE)   GOTO 6
   10 CONTINUE
      RETURN
C
   12 WRITE(NOUT,20)   MAT(K)
      STOP
   14 WRITE(NOUT,22)   MAT(K),EA
      STOP
C
   20 FORMAT(//' ***ERROR 6.5 : FOR  ',A8,' IN THE FINE-STRUCTURE MIXTUR
     1E NO SGT'/16X,'ARE ON KEDAK')
   22 FORMAT(//' ***ERROR 6.6 : FOR  ',A8,' IN THE FINE-STRUCTURE MIXTUR
     1E NO SGT'/16X,'ARE ON KEDAK FOR ENERGIES BELOW',1PE10.3,' EV')
C
      END
```

```
      SUBROUTINE ADD(K,NTT,NTP,NT,ET,ST,NU,D,E,S,EV,SV,EW,SW,EA,EE)
C
      DIMENSION  ET(NTT),ST(NTT)
C
C*****ERSTES MATERIAL****************************************************
      IF(K.GT.1)   GOTO 10
      IF(NU.GT.0)   GOTO 6
      IF(E.GT.EA)   GOTO 2
      ET(1) = E
      ST(1) = S*D
      GOTO 4
    2 T = (S-SV)/(E-EV)
      ET(1) = EA
      ST(1) = D*(S+T*(EA-E))
    4 NU = 1
      NT = 1
      IF(E.LT.EE)   RETURN
      ET(2) = EE
      ST(2) = D*(S+T*(EE-E))
      NU = 2
      NT = 2
      RETURN
    6 NU = NU+1
      NT = NT+1
      IF(NT.GT.NTT)   GOTO 22
      IF(E.LE.EE)   GOTO 8
      ET(NU) = EE
      ST(NU) = ST(NU-1)
      RETURN
    8 ET(NU) = E
      ST(NU) = S*D
      RETURN
C
C*****WEITERE MATERIALIEN************************************************
```

```
   10 IF(NU.GT.0)   GOTO 12
      EW = ET(1)
      SW = ST(1)
      IF(E.GT.EA)   GOTO 12
      ST(1) = ST(1)+D*S
      EV = E
      SV = S
      NU = 1
      RETURN
   12 T = (S-SV)/(E-EV)
      NP = NU+1
      DO 14  I = NP,NT
      IF(ET(I).GT.E)   GOTO 16
      Z = SV+T*(ET(I)-EV)
      EW = ET(I)
      SW = ST(I)
   14 ST(I) = ST(I)+D*Z
      RETURN
   16 IF(E.EQ.ET(I-1))   GOTO 20
      Z = SW+(ST(I)-SW)/(ET(I)-EW)*(E-EW)
      IF(NT+1.EQ.NTT)   GOTO 22
      DO 18  J = I,NT
      JJ = NT+I-J
      ET(JJ+1) = ET(JJ)
   18 ST(JJ+1) = ST(JJ)
      NT = NT+1
      ET(I) = E
      ST(I) = Z+D*S
      NU = I
      EV = E
      SV = S
      RETURN
   20 NU = I-1
      EV = E
      SV = S
      RETURN
C
   22 NTP = 1000
      RETURN
      END
```

```
      SUBROUTINE TRAFO(IC,NE,ISM,S,XM,AL,A)
C
C*****TRANSFORMATION DER SGNC INS L-SYSTEM*********************************
C
      DIMENSION A(IC),S(IC,ISM)
C
      XMM = XM-1
      XMP = XM+1
      QM = XM*XM
      DO 2  I = 1,IC
      V = SQRT(0.5*(1.+AL+(1.-AL)*A(I)))
      A(I) = 0.5*(XMP*V-XMM/V)
      B = SQRT(A(I)*A(I)+QM-1.)
      F = (A(I)+B)*(A(I)+B)/(XM*B)
      DO 2  N = 1,NE
    2 S(I,N) = S(I,N)*F
C
      RETURN
      END
```

```
      SUBROUTINE INFORM(ALFA,NEGR,ABN,R,RSP,IL,IM,INTT,INT,NST,NSTIS,
     1                  IR,ISTT,K,NTK,NTT,NOUT)
C
C*****INFORMATIONEN************************************************************
C
      DIMENSION  ABN(NEGR),R(NEGR),RSP(NEGR),INT(NEGR),NST(6),NA(6),
     1           NB(6)
C
      IF(IR.GT.1)   GOTO 6
      WRITE(NOUT,919)
      WRITE(NOUT,935)   ALFA
    3 DO 5  I = 1,6
      NA(I) = I-1
    5 NB(I) = NSTIS
      WRITE(NOUT,936)   (NA(I),I = 1,6),(NB(I),I = 1,6),
     1                  (NST(I),I = 1,6)
    6 IF(IR+1.LT.INTT)   GOTO 7
      WRITE(NOUT,932)
      DO 4  I = IL,IM
    4 WRITE(NOUT,933)   I,ABN(I),ABN(I+1),R(I),RSP(I)
      WRITE(NOUT,934)
    7 I1 = INT(IR+1)+1
      I2 = INT(IR)+1
      IF(IR.EQ.1)   I2 = I2-1
      WRITE(NOUT,909)
      EFIN = AMAX1(ALFA*ABN(I1),ABN(IM+1))
      WRITE(NOUT,920)   IR,IR,ABN(I1),ABN(I2)
      WRITE(NOUT,921)   IR,EFIN,ABN(I2)
      WRITE(NOUT,922)   IR,ISTT
      WRITE(NOUT,925)   K
      IF(NTK.EQ.1)  WRITE(NOUT,126) NTT
      RETURN
C
  909 FORMAT(1HO)
  919 FORMAT(1HO//24X,'I N F O R M A T I O N E N'//)
  920 FORMAT(1HO,I2,'. AUSSTREUINTERVALL = ',I2,'. MAKROGRUPPE', 5X,E10.
     14,' EV',' -  ',E10.4,' EV')
  921 FORMAT(1HO,I2,'. EINSTREUINTERVALL',23X,E10.4,' EV',' -  ',E10.4,
     1' EV')
  922 FORMAT(1HO,'ZAHL DER ENERGIESTUETZPUNKTE IM ',I2,'. AUSSTREUINTERV
     1ALL',18X,I4)
  925 FORMAT(1HO,'ZAHL DER GELESENEN SGN IM AUSSTREUINTERVALL',28X,I4)
  932 FORMAT(////16X,'F E I N G R U P P E N E I N T E I L U N G'///)
```

```
  933 FORMAT(1X,I3,'.GRUPPE',1X,1PE10.3,' EV  -',1PE10.3,' EV',1X,'DU =   440
     1',E9.2,1X,'RSP = ',1PE11.4)                                         450
  934 FORMAT(////18X,'DU = LETHARGIEDIFFERENZ'//18X,'RSP = GRUPPENINTEGR  460
     1AL UEBERS SPEKTRUM')                                                470
  935 FORMAT(1HO,'ALFA = ',F8.5)                                          480
  936 FORMAT(1HO,'WINKELSTUETZSTELLEN'//12X,'MOMENT',5X,6(3X,I3)/12X,'IS  490
     1OTROPIE',3X,6(3X,I3)/12X,'ANISOTROPIE',1X,6(3X,I3))                 500
  126 FORMAT(1HO,'ZAHL DER SGT FUER FEINSTRUKTURWICHTUNG IM AUSSTREUINTE  510
     1RVALL',11X,I5)                                                      520
      END                                                                 530




      SUBROUTINE PUNK(NGR,NEGR,ABN,NA,NE,NEN,ALFA,NK,NR,ISM,ISMP,ISN,E)    10
C                                                                           20
C*****GRUNDPUNKTE INTERVALLWEISE LOGARITHMISCH AEQUIDISTANT*************   30
C                                                                           40
      REAL*8  D,ED,EX,EP                                                    50
      DIMENSION  ABN(NEGR),E(ISM)                                           60
C                                                                           70
      ISMP = MAXO(0,(NE-NA+1)*(NK+NR)+NEN-ISM)                              80
      IF(ISMP.GT.0)   RETURN                                                90
      EX = DBLE(1./(NK-1))                                                 100
      E(1) = ABN(NE+1)                                                     110
      J = 2                                                                120
      DO 10  NN = NA,NE                                                    130
      N = NA+NE-NN                                                         140
      ED = DBLE(E(J-1))                                                    150
      AB = ABN(N)                                                          160
      A = AMIN1(AB,ABN(N+1)/ALFA)                                          170
    4 D = DBLE(A/ABN(N+1))                                                 180
      D = D**EX                                                            190
    6 EP = ED*D                                                            200
      E(J) = SNGL(EP)                                                      210
      IF(E(J).GT.A)   GOTO 8                                               220
      ED = EP                                                              230
      J = J+1                                                              240
      GOTO 6                                                               250
    8 E(J-1) = A                                                           260
      IF(A.GE.AB)   GOTO 10                                                270
      ED = DBLE((AB/A)**(1./NR))                                           280
      IF(ED.GE.D)   D = ED                                                 290
      ED = DBLE(A)                                                         300
   11 EP = ED*D                                                            310
      E(J) = SNGL(EP)                                                      320
      IF(E(J).GT.AB)   GOTO 9                                              330
      ED = EP                                                              340
      J = J+1                                                              350
      GOTO 11                                                              360
    9 E(J-1) = AB                                                          370
   10 CONTINUE                                                             380
      ISN = J-1                                                            390
      RETURN                                                               400
      END                                                                  410
```

```
      SUBROUTINE LOOKO(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
      XMAT=1.                                                              250
      MASSE=1                                                              260
      COM=0.6666667                                                        270
      RETURN                                                               280
      END                                                                  290
```

```
      SUBROUTINE LOOK1(ISD,K,E,SGN,EO,EE,NT)                                10
C                                                                           20
C*****LESEN DER SGN UND MUEL VON KEDAK**************************************  30
C                                                                           40
      REAL*8  STOFF,A(5),B(2)                                               50
      DIMENSION E(ISD),SGN(ISD),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 '/                                 90
C                                                                          100
      A(3) = B(NT+1)                                                       110
    1 NWORT(1) = 3                                                         120
      A(1) = STOFF                                                         130
      CALL NDFLOC(KP,NWORT,A,NADAT,KC)                                     140
      IF(KP.NE.1)   STOP                                                   150
      K = 1                                                                160
      E(1) = A(4)                                                          170
```

```
      SGN(1) = A(5)                                                     180
      IF(E(1)-EO)   5,4,3                                               190
    3 WRITE(NOUT,40)   STOFF,EO,A(3)                                    200
      STOP                                                              210
    4 K = K+1                                                           220
    5 CALL NDFNXT(KP,NWORT,A,NADAT,KC)                                  230
      IF(KP.NE.1)   GOTO 14                                             240
      IF(K.GT.1)   GOTO 11                                              250
      IF(A(4)-EO)   8,9,10                                              260
    8 E(1) = A(4)                                                       270
      SGN(1) = A(5)                                                     280
      GOTO 5                                                            290
    9 E(1) = A(4)                                                       300
      SGN(1) = A(5)                                                     310
      GOTO 4                                                            320
   10 K = 2                                                             330
   11 E(K) = A(4)                                                       340
      IF(K.EQ.ISD)   RETURN                                             350
      SGN(K) = A(5)                                                     360
      IF(E(K)-EE)   4,16,12                                             370
   12 Y = FG(E(K-1),EE,E(K),SGN(K-1),SGN(K))                            380
      E(K) = EE                                                         390
      SGN(K) = Y                                                        400
      GOTO 16                                                           410
   14 E(K) = EE                                                         420
      SGN(K) = SGN(K-1)                                                 430
      WRITE(NOUT,42)   A(3),STOFF,E(K-1),A(3),E(K-1)                    440
   16 IF(E(1).EQ.EO)   RETURN                                           450
      Y = FG(E(1),EO,E(2),SGN(1),SGN(2))                                460
      E(1) = EO                                                         470
      SGN(1) = Y                                                        480
      RETURN                                                            490
C                                                                       500
   40 FORMAT(//' ***ERROR 6.2 : FOR  ',A8,' SCATTERING MATRICES CANNOT B 510
     1E CALCULATED'/16X'FOR ENERGIES BELOW',1PE10.3,' EV FOR LACK OF  ', 520
     2A8,' ON KEDAK')                                                   530
   42 FORMAT(//' ***WARNING 6.1 : THE  ',A8,' FOR  ',A8,' AT ENERGIES AB 540
     1OVE',1PE10.3,' EV'/18X,'ARE SET EQUAL TO THE  ',A8,' AT',E10.3,' E 550
     2V'//)                                                             560
C                                                                       570
      END                                                               580
```

```
      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(ICOS,ISM),AR(ICOS)        60
      COMMON STOFF,ISTRUK,ISPA,NOUT                                      70
      DATA F(2),F(3) /'BEST ','SGNC '/                                   80
C                                                                        90
      ICOSP = 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 AR(IP) = F(5)                                                     180
      SGNC(IP,NE) = F(6)                                                190
      IP = IP+1                                                         200
      CALL NDFNXT(KP,NWORT,F,NADAT,KC)                                  210
      IF(KP.EQ.1)   GOTO 3                                              220
      IF(IP-1-ICOS)   8,4,10                                            230
    4 CONTINUE                                                          240
      RETURN                                                            250
    8 WRITE(NOUT,44)   STOFF,ICOS,EA(NE)                                260
      STOP                                                              270
   10 ICOSP = IP-1-ICOS                                                 280
      RETURN                                                            290
C                                                                       300
   44 FORMAT(//' ***ERROR 6.3 : FOR  ',A8,' THE SGNC COSINE MESH HAS LES 310
     1S'/16X,'THAN ',I3,' MESHPOINTS AT',1PE10.3,' EV')                 320
C                                                                       330
      END                                                               340
```



```
      SUBROUTINE LOOK3(NE,EA,ISO,NGR,ABN,ISM,ISMP,LST,NEGR,ISEL)         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
    2 NWORT(1) = 4                                                      100
      F(1) = STOFF                                                      110
      F(4) = 0.                                                         120
      NE = 1                                                            130
    4 CALL NDFLOC(KP,NWORT,F,NADAT,KC)                                  140
      IF(KP.EQ.1)  GO TO 5                                              150
      CALL NDFLOC(KP,NWORT,F,NADAT,KC)                                  160
      IF(KP.EQ.1)  GO TO 5                                              170
      IF(NE-1)13,13,6                                                   180
    5 EA(NE)=F(4)                                                       190
      F(4) = F(4)+F(4)*(1.E-06)                                         200
      NE = NE+1                                                         210
      IF(NE.LE.ISM)   GOTO 4                                            220
      ISMP=50                                                           230
      RETURN                                                            240
    6 WRITE(NOUT,62)                                                    250
      IF(EA(1).GE.ABN(1))  GO TO 12                                     260
C                                                                       270
```

```
C*****ANZAHL DER SGNC IN DER N-TEN GRUPPE*********************************
      NE=NE-1
      NTO = 0
      DO 10  N = 1,NGR
      LST(N) = 0
      DO 8  M = 1,NE
      IF((ABN(N+1).LE.EA(M)).AND.(EA(M).LT.ABN(N)))   LST(N) = LST(N)+1
    8 CONTINUE
   10 NTO = NTO+LST(N)
      IF(ISEL.GT.0)  GO TO 11
      WRITE(NOUT,52)
      DO 7 N=1,NGR
    7 WRITE(NOUT,54) N,LST(N)
      WRITE(NOUT,56)   NTO
C
C*****ANISOTROPIE-SCHWELLE***************************************************
   11 DO 14 N = 1,NGR
      NN = NGR-N+1
      IF(LST(NN).NE.0)   GOTO 16
   14 CONTINUE
   16 ISO = NN+1
      RETURN
C
   12 IF(ISEL.GT.0)  GO TO 15
      WRITE (NOUT,52)
      WRITE(NOUT,58)
   15 EA(1) = ABN(1)
      ISO=1
      RETURN
C
   13 WRITE(NOUT,60)   STOFF
      STOP
C
   52 FORMAT(1HO//14X,'VERTEILUNG DER SGNC'//)
   54 FORMAT(1X,I3,'. FEINGRUPPE',12X,I4,' SGNC')
   56 FORMAT(1HO,6X,'INSGESAMT',12X,I4,' SGNC')
   58 FORMAT(5X,'ENERGIEBEREICH LIEGT IM BEREICH ISOTROPER STREUUNG')
   60 FORMAT(//' ***ERROR 6.4 : FOR  ',A8,' SCATTERING MATRICES CANNOT B
     1E CALCULATED'/16X'FOR LACK OF SGNC ON KEDAK')
   62 FORMAT(//' ***MESSAGE 6.1 : WARNING NDF. 2 MAY BE IGNORED')
C
      END
```

```
      SUBROUTINE LECAL(MASSE,XMAT,ALFA,ISOT,LEG,NLE,NANF,NEND,NUEB,IL,
     1                 IM,NEGR,ABN,ICOS,AR,ISN,E,SGNC,NST,NSTIS,ISM,ISD,
     2                 NECU,ITA,NF,GR,FEKOE,FU,EW,A,H,V,W,F,FEKO)
C
C*****BERECHNUNG DER ENERGIEDIFFERENTIELLEN LEGENDRE-KOEFFIZIENTEN******
C
      DIMENSION  NST(6),LEG(6),AR(ICOS),FU(ICOS),ABN(NEGR),GR(NEGR),
     1           FEKOE(NEGR),A(ISD),H(ISD),E(ISM),EW(ISM),V(ISD),W(ISD),
     2           F(ISD),SGNC(ICOS,ISM),FEKO(ISM,NECU)
C
      EP = 0.8
      XP = XMAT+1
      XM = XMAT-1
      IF(MASSE.EQ.1)   XM = 0.
      NM = NUEB-1
      IA = NANF
      IC = MINO(NEGR,NEND+NUEB)
      IB = IC-1
      IF(ITA.EQ.0.AND.ISOT.EQ.0)
     1CALL LEGINT(NLE,NSTIS,XMAT,ITA)
      REWIND NF
C
C*****ENERGIEDIFF. LEGENDRE-KOEFF. (L-1)-TER ORDNUNG*********************
      N = 0
      L = 1
      GOTO 2
    1 N=N+1
      L=LEG(N)
    2 IF(ISOT.EQ.0)   GOTO 3
      NSB = NSTIS
      NSA = NST(L)
      CALL LEGPOL(NSA,H,NLE)
C
    3 DO 28  J = 1,ISN
C
C*****GRENZEN FUER WINKELINTEGRATION*************************************
      GRM = 0.
      EL = AMAX1(ABN(IM+1),ALFA*E(J))
      DO 8  I = IA,IC
      IF(EL.LT.ABN(I))   GOTO 6
      GR(I) = -1.
      GOTO 8
    6 IF(E(J).GT.ABN(I))   GOTO 7
      GR(I) = 1.
      GOTO 8
    7 G = SQRT(ABN(I)/E(J))
      GR(I) = 0.5*(XP*G-XM/G)
      GRA = ABS(GR(I))
      IF((GRA.LT.1.).AND.(GRM.LT.GRA))   GRM = GRA
    8 CONTINUE
      IF(ISOT.EQ.0)   GOTO 11
C
C*****MOMENTE BEI ANISOTROPIE IM SP-SYSTEM*******************************
      IF(GRM.LT.EP)   NSB = NST(L)
      IF(NSA.EQ.NSB)   GOTO 9
      NSA = NSB
      CALL LEGPOL(NSA,H,NLE)
    9 DO 10  IP = 1,ICOS
   10 FU(IP) = SGNC(IP,J)
      CALL IPOLA(ICOS,AR,FU,NSA,H,A,F)
      CALL LEGANS(L,NSA,A,IA,IB,NEGR,GR,FEKOE,V,W)
      NSB = NSTIS
      GOTO 12
C
C*****MOMENTE BEI ISOTROPIE IM SP-SYSTEM*********************************
```

```
   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*FEKOE(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
      END                                                               990
```

```
      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
      D = 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
      END                                                               370
```

```
      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
      F0 = 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)*DF                         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
      END                                                              1030
```

```
      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
      GU = -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),POL(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
      DU = 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*DU*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
      NO = 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,ISOT,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,ISCO,ISEC,NF,E,EW,GR,WA,U,V,W,ISTT,   40
     4                  RSP,ELSIG)                                         50
C                                                                         60
C*****GEWICHTETE MULTIGRUPPEN-ENERGIEINTEGRATION************************** 70
C                                                                         80
      DIMENSION  LEG(6),ABN(NEGR),RSP(NEGR),ESP(NSPEK),SPEK(LSPEK),       90
     1           EH(ISM),EW(ISM),H(ISD),F(ISD),G(ISD),EN(ISD),V(ISD),     100
     2           W(ISD),E(ISD),WA(ISCO),U(ISEC),ET(NTT),ST(NTT),GR(NGR),  110
     3           MAZ(2),ELSIG(6,NECU,NGR)                                 120
C                                                                         130
      NP = NLE+1                                                          140
      XP = XMAT+1                                                         150
      XM = XMAT-1                                                         160
      IF(MASSE.EQ.1)   XM = 0.                                            170
      NM = NUEB-1                                                         180
C                                                                         190
C*****VEREINIGUNG DER ENERGIESTUETZPUNKTMENGEN*************************** 200
      DO 2  J = 1,ISN                                                     210
    2 E(J) = EH(J)                                                        220
      ISTT = ISN                                                          230
      CALL PUSUM(K,H,ISTT,E,V)                                            240
C                                                                         250
C*****INTERPOLATION DER TOTALEN ELASTISCHEN QUERSCHNITTE***************** 260
      CALL IPOLIN(K,H,F,ISTT,E,W,U)                                       270
C                                                                         280
C*****INTERPOLATION DER MITTLEREN STREUKOSINUS*************************** 290
      IF(ISOT.EQ.0)   GOTO 4                                              300
      CALL IPOLIN(M,G,EN,ISTT,E,V,U)                                      310
      GOTO 8                                                              320
    4 DO 6  J = 1,ISTT                                                    330
    6 V(J) = COM                                                          340
C                                                                         350
    8 DO 66  N = 1,NP                                                     360
      L = LEG(N)                                                          370
      LISOT = L*ISOT                                                      380
C*****LESEN UND INTERPOLATION DER NORMIERTEN ENERGIEDIFF. LEGENDRE-KOEFF 390
      DO 11  I = 1,NUEB                                                   400
      JI = (I-1)*ISTT                                                     410
      READ(NF)   (EW(J),J = 1,ISN)                                        420
      IF(ISOT.EQ.0.AND.I.EQ.NUEB)   GOTO 9                                430
      CALL IPOLIN(ISN,EH,EW,ISTT,E,WA(1+JI),U)                            440
      GOTO 11                                                             450
    9 XY = EW(ISN)                                                        460
      DO 10  J = 1,ISTT                                                   470
   10 WA(J+JI) = XY                                                       480
   11 CONTINUE                                                            490
C                                                                         500
C*****MUEL-ANGEPASSTE ENERGIEDIFF. LEGENDRE-KOEFF. ********************** 510
      DO 44  J = 1,ISTT                                                   520
      XY = 0.                                                             530
      JP = J+NM*ISTT                                                      540
      IF(LISOT.EQ.2)   V(J) = PM*(V(J)-WA(JP))                            550
      DO 12  NN = NANF,NEND                                               560
      IF((ABN(NN+1).LE.E(J)).AND.(E(J).LE.ABN(NN)))   GOTO 14             570
   12 CONTINUE                                                            580
      NN = NEND                                                           590
   14 EL = AMAX1(ABN(IM+1),ALFA*E(J))                                     600
      DO 42  I = 1,NUEB                                                   610
      JI = J+(I-1)*ISTT                                                   620
      NI = MINO(IM,NN+I-1)                                                630
      P = 0.                                                              640
      IF(ISOT.EQ.0)   GOTO 36                                             650
      GU = -1.                                                            660
      IF(EL.GE.ABN(NI+1))   GOTO 16                                       670
      GU = SQRT(ABN(NI+1)/E(J))                                           680
      GU = 0.5*(XP*GU-XM/GU)                                              690
   16 GO = 1.                                                             700
      IF(I.EQ.1)   GOTO 18                                                710
      LI = MINO(IM+1,NN+I-1)                                              720
      GO = -1.                                                            730
      IF(EL.GE.ABN(LI))   GOTO 18                                         740
      GO = SQRT(ABN(LI)/E(J))                                             750
      GO = 0.5*(XP*GO-XM/GO)                                              760
   18 IF(GU.LT.GO)   GOTO 20                                              770
      P = 0.                                                              780
      GOTO 36                                                             790
   20 IF(GO-GU.LT.2.)   GOTO 22                                           800
      P = 0.                                                              810
      IF(L.EQ.2)   P = 1.                                                 820
      GOTO 36                                                             830
   22 O2 = GO*GO                                                          840
      U2 = GU*GU                                                          850
      O3 = O2*GO                                                          860
      U3 = U2*GU                                                          870
      GOTO(24,26,28,30,32,34),L                                           880
   24 P = 0.75*(O2-U2)                                                    890
      GOTO 36                                                             900
   26 P = 0.5*(O3-U3)                                                     910
      GOTO 36                                                             920
   28 P = 0.1875*(O2*(3*O2-2)-U2*(3*U2-2))                                930
      GOTO 36                                                             940
   30 P = 0.75*(O3*(O2-1)-U3*(U2-1))                                      950
      GOTO 36                                                             960
```

```
   32 P = 0.03125*(O2*((O2-1)*(35*O2-10)-1)-U2*((U2-1)*(35*U2-10)-1))     970
      GOTO 36                                                            980
   34 P = 0.1875*(O3*(O2-1)*(9*O2-5)-U3*(U2-1)*(9*U2-5))                 990
   36 CONTINUE                                                          1000
      IF(EL.LT.ABN(NI+1).AND.I.LT.NUEB)   GOTO 40                       1010
      WA(JI) = WA(JP)-XY                                                1020
      IF(I.EQ.NUEB)   GOTO 42                                           1030
      IA = I+1                                                          1040
      DO 38  II = IA,NUEB                                               1050
   38 WA(J+(II-1)*ISTT) = 0.                                            1060
      WA(JI) = (WA(JI)+P*V(J))*W(J)                                     1070
      GOTO 44                                                           1080
   40 XY = XY+WA(JI)                                                    1090
   42 WA(JI) = (WA(JI)+P*V(J))*W(J)                                     1100
   44 CONTINUE                                                          1110
C                                                                       1120
C*****AUSSORTIEREN ZUR GEWICHTETEN INTEGRATION************************* 1130
      DO 64  NR = 1,NUEB                                                1140
      NI = (NR-1)*ISTT                                                  1150
      JA = 1                                                            1160
      DO 58  NT = NANF,NEND                                             1170
      NN = NANF+NEND-NT                                                 1180
C     NN-TE GRUPPE = AUSSTREUGRUPPE                                     1190
C     (NN+NR-1)-TE GRUPPE = EINSTREUGRUPPE                              1200
      AM = ABN(NN)                                                      1210
      DO 46  J = JA,ISTT                                                1220
      IF(E(J).GT.AM)   GOTO 48                                          1230
      JI = J-JA+1                                                       1240
      EN(JI) = E(J)                                                     1250
   46 F(JI) = WA(J+NI)                                                  1260
      J = ISTT+1                                                        1270
   48 IKK = J-JA                                                        1280
      JA = J-1                                                          1290
      IF(NN+NR-1.GT.IM)   GOTO 58                                       1300
      IF(IKK.GE.3)   GOTO 52                                            1310
      VAL = 0.                                                          1320
      GOTO 56                                                           1330
   52 EN(IKK) = AM                                                      1340
      T = (F(IKK-2)-F(IKK-1))/(EN(IKK-2)-EN(IKK-1))                     1350
      F(IKK) = F(IKK-1)+T*(AM-EN(IKK-1))                                1360
C                                                                       1370
C*****AUSWAHL DES BENOETIGTEN TEILSPEKTRUMS UND INTERPOLATION********** 1380
      CALL SPRAL(KSPE,KSPEK,MAZ,ESP,SPEK,NTT,ET,ST,L,IKK,EN,G,NSPEK,    1390
     1           LSPEK)                                                 1400
C                                                                       1410
C*****ERZEUGUNG DER NORMIERUNGSINTEGRALE******************************* 1420
      IF(NR.GT.1)   GOTO 54                                             1430
      CALL TRAPEZ(IKK,EN,G,F,GR(NN),U,0)                                1440
      IF(L.EQ.1)   RSP(NN) = GR(NN)                                     1450
C                                                                       1460
C*****SPEKTRUMSGEWICHTETE ENERGIEINTEGRATION*************************** 1470
   54 CALL TRAPEZ(IKK,EN,F,G,VAL,U,1)                                   1480
      VAL = VAL/GR(NN)                                                  1490
   56 ELSIG(L,NR,NN) = VAL                                              1500
   58 CONTINUE                                                          1510
   64 CONTINUE                                                          1520
   66 CONTINUE                                                          1530
C                                                                       1540
      RETURN                                                            1550
      END                                                               1560
```

```
      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
      END                                                               280
```

```
      SUBROUTINE SPRAL(KS,NS,MZ,E,S,NTT,ET,ST,L,IKK,EN,G,NP,NL)          10
C                                                                        20
C*****BEREITSTELLUNG DES WICHTUNGSSPEKTRUMS*************************** 30
C                                                                        40
      DIMENSION  E(NP),S(NL),EN(IKK),G(IKK),ET(NTT),ST(NTT),MZ(2)        50
C                                                                        60
      F0(A,B,X,Y) = (1/X+1/Y)*(B-A)                                      70
      F1(A,B,X,Y) = (1/(X*X)+1/(Y*Y))*(B-A)                              80
      F2(A,B,X,Y) = (1/(X*X*X)+1/(Y*Y*Y))*(B-A)                          90
      F3(A,B,X,Y) = (1/X**4+1/Y**4)*(B-A)                               100
      F4(A,B,X,Y) = (1/X**5+1/Y**5)*(B-A)                               110
      F5(A,B,X,Y) = (1/X**6+1/Y**6)*(B-A)                               120
C                                                                       130
      IF(KS.NE.0)  GO TO 2                                              140
```

```
C*****SPEKTRUM AUS DER FUNKTION PHI(E) BZW. PHIL(L,E) ******************
   40 IF(L.GT.1.AND.MZ(1).EQ.1)   GOTO 42
      DO 41  I = 1,IKK
   41 G(I) = PHI(EN(I))
      GOTO 7
   42 DO 43  I = 1,IKK
   43 G(I) = PHIL(L,EN(I))
      GOTO 7
C
C*****SPEKTRUM AUS PUNKTWEISER EINGABE***********************************
    2 NN = 2
      DO 6  I = 1,IKK
      DO 3  N = NN,NS
      M = N
      IF(MZ(1).NE.0)   M = M+(L-1)*NS
      IF(E(N)-EN(I))   3,4,5
    3 CONTINUE
    4 G(I) = S(M)
      NN = N
      GOTO 6
    5 G(I) = S(M-1)+(S(M)-S(M-1))/(E(N)-E(N-1))*(EN(I)-E(N-1))
      IF(N.GT.2)   NN = N-1
    6 CONTINUE
C
C*****UNGEWICHTETE INTERVALLBREITEN**************************************
    7 IF(NTT.GT.1)   GOTO 9
      IK = IKK-1
      DO 8  I = 1,IK
    8 EN(I) = EN(I+1)-EN(I)
      RETURN
C
C*****FEINSTRUKTURGEWICHTETE INTERVALLBREITEN****************************
    9 N = 1
      STE = -1
      IF(EN(IKK).LE.ET(2))   STE = ST(2)
      IF(EN(1).GE.ET(NTT-1))   STE = ST(NTT-1)
      STA = STE
      IF(STE.LT.0)   GOTO 10
      N = 0
      M = 0
   10 NN = 1
      IK = IKK-1
      DO 38  I = 1,IK
      IF(N.EQ.0)   GOTO 17
      DO 11 N = NN,NTT
      IF(ET(N)-EN(I))   11,11,12
   11 CONTINUE
      N = NTT
   12 DO 14  M = N,NTT
      IF(ET(M)-EN(I+1))   14,16,16
   14 CONTINUE
      M = NTT
   16 STA = ST(N)+(EN(I)-ET(N))*(ST(N-1)-ST(N))/(ET(N-1)-ET(N))
      STE = ST(M)+(EN(I+1)-ET(M))*(ST(M-1)-ST(M))/(ET(M-1)-ET(M))
   17 IF(MZ(2).EQ.0)   GOTO 18
      GOTO (18,21,24,27,30,33),L

C***** 0. MOMENT
   18 IF(M.GT.N)   GOTO 19
      W = F0(EN(I),EN(I+1),STA,STE)
      GOTO 36
   19 W = F0(EN(I),ET(N),STA,ST(N))+F0(ET(M-1),EN(I+1),STE,ST(M-1))
      IF(N.EQ.M-1)   GOTO 36
      MM = M-2
      DO 20  J = N,MM
   20 W = W+F0(ET(J),ET(J+1),ST(J+1),ST(J))
      GOTO 36
C***** 1. MOMENT
   21 IF(M.GT.N)   GOTO 22
      W = F1(EN(I),EN(I+1),STA,STE)
      GOTO 36
   22 W = F1(EN(I),ET(N),STA,ST(N))+F1(ET(M-1),EN(I+1),STE,ST(M-1))
      IF(N.EQ.M-1)   GOTO 36
      MM = M-2
      DO 23  J = N,MM
   23 W = W+F1(ET(J),ET(J+1),ST(J+1),ST(J))
      GOTO 36
C***** 2. MOMENT
   24 IF(M.GT.N)   GOTO 25
      W = F2(EN(I),EN(I+1),STA,STE)
      GOTO 36
   25 W = F2(EN(I),ET(N),STA,ST(N))+F2(ET(M-1),EN(I+1),STE,ST(M-1))
      IF(N.EQ.M-1)   GOTO 36
      MM = M-2
      DO 26  J = N,MM
   26 W = W+F2(ET(J),ET(J+1),ST(J+1),ST(J))
      GOTO 36
C***** 3. MOMENT
   27 IF(M.GT.N)   GOTO 28
      W = F3(EN(I),EN(I+1),STA,STE)
      GOTO 36
   28 W = F3(EN(I),ET(N),STA,ST(N))+F3(ET(M-1),EN(I+1),STE,ST(M-1))
      IF(N.EQ.M-1)   GOTO 36
      MM = M-2
      DO 29  J = N,MM
   29 W = W+F3(ET(J),ET(J+1),ST(J+1),ST(J))
      GOTO 36
C***** 4. MOMENT
   30 IF(M.GT.N)   GOTO 31
      W = F4(EN(I),EN(I+1),STA,STE)
      GOTO 36
   31 W = F4(EN(I),ET(N),STA,ST(N))+F4(ET(M-1),EN(I+1),STE,ST(M-1))
      IF(N.EQ.M-1)   GOTO 36
      MM = M-2
      DO 32  J = N,MM
   32 W = W+F4(ET(J),ET(J+1),ST(J+1),ST(J))
      GOTO 36
C***** 5. MOMENT
   33 IF(M.GT.N)   GOTO 34
      W = F5(EN(I),EN(I+1),STA,STE)
      GOTO 36
   34 W = F5(EN(I),ET(N),STA,ST(N))+F5(ET(M-1),EN(I+1),STE,ST(M-1))
      IF(N.EQ.M-1)   GOTO 36
```

```
      MM = M-2                                                          1270
      DO 35  J = N,MM                                                   1280
   35 W = W+F5(ET(J),ET(J+1),ST(J+1),ST(J))                             1290
   36 EN(I) = 0.5*W                                                     1300
   38 NN = M-1                                                          1310
C                                                                       1320
      RETURN                                                            1330
      END                                                               1340
```

```
      SUBROUTINE TRAPEZ(M,E,F,G,W,H,L)                                    10
C                                                                         20
C*****INTEGRATION NACH DER TRAPEZREGEL*************************************  30
C                                                                         40
      DIMENSION  E(M),F(M),G(M),H(M)                                      50
C                                                                         60
C     L = 0 : GEWICHTSFUNKTION KONSTANT = 1                               70
C     L = 1 : GEWICHTSFUNKTION NICHT KONSTANT                             80
C                                                                         90
      IF(L.EQ.0)   GOTO 8                                                100
      DO 2  J = 2,M                                                      110
    2 H(J-1) = (F(J-1)*G(J-1)+F(J)*G(J))*E(J-1)                          120
      GOTO 12                                                           130
    8 DO 10  J = 2,M                                                    140
   10 H(J-1) = (F(J)+F(J-1))*E(J-1)                                     150
   12 MM = M-1                                                          160
      CALL SUM(MM,H,W)                                                  170
      W = 0.5*W                                                         180
C                                                                       190
      RETURN                                                            200
      END                                                               210
```

```
      FUNCTION PHIL(L,E)                                                  10
      PHIL=1./E**L                                                        20
      RETURN                                                              30
      END                                                                 40
```

```
      SUBROUTINE MUKON(ELSIG,ELTOT,NLE,NECU,NUEB,IL,IM,NGR)               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
      DO 40  L = 1,NP                                                    390
      DO 40 NN=IL,IM                                                     400
      DO 38  I = 1,NUEB                                                  410
      NT=I+NN-1                                                          420
      ELSIG(L,I,NN) = AINT(ELSIG(L,I,NN)*1.E+5)*1.E-5                    430
      IF(NT.EQ.IM)  GO TO 40                                             440
   38 CONTINUE                                                           450
   40 CONTINUE                                                           460
C                                                                        470
      RETURN                                                             480
      END                                                                490
```

```
      SUBROUTINE PRINT(ELSIG,ELTOT,NLA,NLE,NECU,NUEB,ISEL,NGR,KSPEK,      10
     1                 MAZ,NTK,KIM)                                       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)                     70
      COMMON STOFF,ISTRUK,ISPA,NOUT,KPR,NEND,NANF                         80
C                                                                         90
      NP = NLE+1                                                         100
```

```
C                                                                       110
C*****AUSDRUCKEN DER STREUMATRIZEN*****************************************  120
      DO 3  L = 1,NP                                                    130
      LM = L-1                                                          140
      WRITE(NOUT,21) LM,LM,STOFF                                        150
      IF(IABS(ISEL).EQ.1)   WRITE(NOUT,28)                              160
      I1 = NANF                                                         170
    1 I2=I1+MINO(5,NEND-I1)                                             180
      WRITE(NOUT,24)   (I,I = I1,I2)                                    190
      DO 2  I = 1,NUEB                                                  200
      I3=MINO(I2,NEND+KIM-I+1)                                          210
      IF(I3.LT.I1)  GO TO 2                                             220
      WRITE(NOUT,22) (ELSIG(L,I,NN     ),NN=I1,I3)                      230
    2 CONTINUE                                                          240
      WRITE(NOUT,20)                                                    250
      IF(I2.GE.NEND)  GOTO 3                                            260
      I1 = I2+1                                                         270
      GOTO 1                                                            280
    3 CONTINUE                                                          290
      WRITE(NOUT,52)                                                    300
C                                                                       310
C*****INFORMATIONEN UEBER DIE WICHTUNG*************************************  320
      WRITE(NOUT,30)                                                    330
      IF(KSPEK.GT.0.AND.MAZ(1).EQ.0)WRITE(NOUT,32)                      340
      IF(KSPEK.GT.0.AND.MAZ(1).EQ.1)WRITE(NOUT,34)    NLE               350
      IF(KSPEK.EQ.0.AND.MAZ(1).EQ.0)WRITE(NOUT,36)                      360
      IF(KSPEK.EQ.0.AND.MAZ(1).EQ.1)WRITE(NOUT,38)    NLE               370
      WRITE(NOUT,40)                                                    380
      IF(NTK.EQ.1.AND.MAZ(2).EQ.0)WRITE(NOUT,42)                        390
      IF(NTK.EQ.1.AND.MAZ(2).EQ.1)WRITE(NOUT,44)    NLE                 400
      IF(NTK.EQ.0)  WRITE(NOUT,46)                                      410
C                                                                       420
C*****AUSDRUCKEN DER TOTALEN QUERSCHNITTE UND STREUKOSINUS**************  430
      WRITE(NOUT,27)   STOFF                                            440
      IF(IABS(ISEL).EQ.1)   WRITE(NOUT,28)                              450
      I1 = NANF                                                         460
    9 I2=I1+MINO(5,NEND-I1)                                             470
      WRITE(NOUT,24)   (I,I = I1,I2)                                    480
      DO 10  I = 1,2                                                    490
   10 WRITE(NOUT,25)   (ELTOT(I,NN),NN = I1,I2)                         500
      WRITE(NOUT,20)                                                    510
      IF(I2.GE.NEND)   GOTO 11                                          520
      I1 = I2+1                                                         530
      GOTO 9                                                            540
   11 WRITE(NOUT,54)                                                    550
C                                                                       560
C*****RESERVIEREN DER RESULTATE********************************************  570
      CALL DOPW(8HFLUM    ,MMM)                                         580
      I=0                                                               590
      WRITE (KPR) I,MMM                                                 600
      I1=NANF                                                           610
      I2=NEND                                                           620
      I=4                                                               630
      L=NLE-NLA+1                                                       640
      NN=I2-I1+1                                                        650
      WRITE (KPR)I,STOFF,NN,L                                           660
      I=3                                                               670
      DO 31 NN=I1,I2                                                    680
      WRITE (KPR) I,NN,ELTOT(1,NN),ELTOT(2,NN)                          690
   31 CONTINUE                                                          700
      DO 33  L = 1,NP                                                   710
      LM=L-1                                                            720
      DO 33 NN=I1,I2                                                    730
      LL=MINO(NUEB,I2+KIM-NN+1)                                         740
      I=LL+2                                                            750
      WRITE (KPR)    I,LM,NN,(ELSIG(L,K,NN ),K=1,LL)                    760
   33 CONTINUE                                                          770
C                                                                       780
      RETURN                                                            790
C                                                                       800
   20 FORMAT(1HO)                                                       810
   21 FORMAT(1HO//29X,'SGNC',I1,8X,'ELASTISCHE STREUMATRIX  ',I1,'. ORDN  820
     1UNG FUER  ',A8//)                                                 830
   22 FORMAT(23X,6F12.5)                                                840
   24 FORMAT(23X,6(2X,I3,'.GRUPPE'))                                    850
   25 FORMAT(23X,1P6E12.3)                                              860
   28 FORMAT(56X,'FUER SGN(E) = 1'/)                                    870
   27 FORMAT(1HO//31X,'TOTALE ELASTISCHE STREUQUERSCHNITTE SGN UND STREU  880
     1KOSINUS MUEL FUER ',A8//)                                         890
   30 FORMAT(////42X,'M A K R O W I C H T U N G '/)                     900
   32 FORMAT(42X,'ALLE MOMENTE WIE DAS 0. MOMENT MIT DEM'/              910
     1       42X,'EINGELESENEN PUNKTSPEKTRUM F(0,E)')                   920
   34 FORMAT(42X,'DAS L-TE MOMENT MIT DEM (L+1)-TEN EINGE-'/            930
     1       42X,'LESENEN PUNKTSPEKTRUM F(L,E), L = 0,1,..,',I2)        940
   36 FORMAT(42X,'ALLE MOMENTE WIE DAS 0. MOMENT MIT'/                  950
     1       42X,'F(0,E)   (STANDARD F(0,E) = 1/E)')                    960
   38 FORMAT(42X,'DAS L-TE MOMENT MIT F(L,E), L = 0,1,..,',I2/          970
     1       42X,'(STANDARD F(L,E) = 1/E**(L+1))')                      980
   40 FORMAT(///42X,'M I K R O W I C H T U N G  (FEINSTRUKTUR)'/)       990
   42 FORMAT(42X,'ALLE MOMENTE WIE DAS 0. MOMENT MIT FS(0,E)=1/SGT(E)'/ 1000
     1       42X,'SGT(E)=TOTALER QUERSCHNITT DER EINGELESENEN MISCHUNG') 1010
   44 FORMAT(42X,'DAS L-TE MOMENT MIT FS(L,E), L = 0,1,..,',I2/         1020
     1       42X,'(STANDARD FS(L,E)=(1/SGT(E))**(L+1) )'/               1030
     2       42X,'SGT(E)=TOTALER QUERSCHNITT DER EINGELESENEN MISCHUNG') 1040
   46 FORMAT(42X,'ALLE MOMENTE MIT FS(0,E) = 1'/                        1050
     1       42X,'(KEINE FEINSTRUKTURWICHTUNG)')                        1060
   52 FORMAT(//29X,'ERLAEUTERUNG'/29X,'L-TE ORDNUNG, G-TE GRUPPE, I-TE Z 1070
     1EILE: MATRIXELEMENT L-TER ORDNUNG'/29X,'FUER STREUUNG AUS DER G-TE 1080
     2N GRUPPE IN DIE (G+I-1)-TE GRUPPE, BEZOGEN'/29X,'AUF DEN TOTALEN E 1090
     3LASTISCHEN QUERSCHNITT (TOTALES 0.MOMENT) DER'/29X,'G-TEN GRUPPE') 1100
   54 FORMAT(//29X,'ERLAEUTERUNG'/29X,'G-TE GRUPPE, 1. ZEILE: TOTALER EL 1110
     1ASTISCHER QUERSCHNITT DER G-TEN'/29X,'GRUPPE'/29X,'G-TE GRUPPE, 2. 1120
     2 ZEILE: MITTLERER STREUKOSINUS DER G-TEN GRUPPE')                 1130
      END                                                               1140
```

```
      SUBROUTINE SPALT(NE,ENG,X)                                        10
C                                                                       20
C     BERECHNUNG DES SPALTSPEKTRUMS                                     30
      REAL*8 MAT,FEST(10),NFEST(10),MMM                                 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
      WRITE (NOUTP,9000)                                                90
 9000 FORMAT(1HO/1HO/' PROGRAMM KENNZIFFER 7')                          100
      WRITE (NOUTP,9001)                                                110
 9001 FORMAT(' PROGRAMM ZUR BERECHNUNG DES SPALTSPEKTRUMS'/)            120
      N=1                                                               130
      I=0                                                               140
      L=NE-NANF                                                         150
      IGRUP=NE-NEND                                                     160
      CALL DOPW (8HBEST    ,NFEST(2))                                   170
      CALL DOPW (8HCHICR   ,NFEST(3))                                   180
      CALL DOPW (8HSPALT   ,MMM)                                        190
      NSATZ(1)=3                                                        200
      NFEST(1)=MAT                                                      210
      CALL NDFLOC (NSUCH,NSATZ,FEST,NUDAT,NC)                           220
      IF(NSUCH)6,6,7                                                    230
    6 WRITE (NOUTP,8) FEST(1)                                           240
    8 FORMAT(' FUER DAS MATERIAL',A9,' GIBT ES KEIN SPALTSPEKTRUM')     250
      GO TO 5                                                           260
    7 E=FEST(4)                                                         270
      B=FEST(6)                                                         280
      C=FEST(7)                                                         290
      T=1./B                                                            300
      EF=  C/(4.*B*B)                                                   310
      EW=DSQRT(EF/T)                                                    320
      DO 9 K=L,IGRUP                                                    330
      EG=DSQRT(ENG(K)/T)                                                340
      EG1=DSQRT(ENG(K+1)/T)                                             350
      XG=EG1-EW                                                         360
      XG1=EG-EW                                                         370
      YG=EG1+EW                                                         380
      YG1=EG+EW                                                         390
      XG2=XG*XG                                                         400
      YG2=YG*YG                                                         410
      XG12=XG1*XG1                                                      420
      YG12=YG1*YG1                                                      430
      X(K)=0.2820947917738/EW*(DEXP(-XG12)-DEXP(-XG2)-DEXP(-YG12)       440
     1+DEXP(-YG2))-0.5*(DERF(XG1)-DERF(XG)+DERF(YG1)-DERF(YG))          450
    9 CONTINUE                                                          460
      IF(N.EQ.2) GO TO 10                                               470
      N=2                                                               480
      IJ=0                                                              490
      WRITE (JA) IJ,MMM                                                 500
   10 IJ=6                                                              510
      K=NE-L                                                            520
      J=NE-IGRUP                                                        530
      WRITE (JA) IJ,MAT,E,K,J                                           540
      NNN=IGRUP+1-L                                                     550
      WRITE(JA) NNN,(X(IJ),IJ=L,IGRUP)                                  560
      WRITE (NOUTP,12) MAT,E,K,J                                        570
   12 FORMAT(1HO,A9,'  EINFALLSENERGIE =',E16.8,'  VON GRUPPE',I3,' BIS' 580
     1,I3)                                                              590
      WRITE(NOUTP,14) I                                                 600
   14 FORMAT(' CHI ',I1)                                                610
      I=I+1                                                             620
      WRITE (NOUTP,13) (X(IJ),IJ=L,IGRUP)                               630
   13 FORMAT(1H ,7E16.8/(1X,7E16.8))                                    640
      CALL NDFNXT(NSUCH,NSATZ,FEST,NUDAT,NC)                            650
      IF(NSUCH) 5,5,7                                                   660
    5 KL=KL+1                                                           670
      RETURN                                                            680
      END                                                               690
```

```
C     BESTIMMUNG DER 1/V-WERTE IM KFK-SATZ                              10
      SUBROUTINE EDV (MM,A,NEF,XS,G,E,V,Y,NES,ES,F)                     20
      REAL*8 MAT,KZE                                                    30
      DIMENSION A(MM),XS(NEF),G(NEF),E(MM),V(MM),Y(MM)                  40
     1,ES(NES),F(NES)                                                   50
      COMMON MAT,ISTRUK,ISPA,NOUTP,JA,NANF,NEND,KL                      60
      WRITE (NOUTP,9000)                                                70
 9000 FORMAT(1HO/1HO/' PROGRAMM KENNZIFFER 8')                          80
      WRITE (NOUTP,9001)                                                90
 9001 FORMAT(' PROGRAMM ZUR BERECHNUNG DES 1/V- GRUPPENMITTELWERTES'/)   100
      DO 5 I=1,NEF                                                      110
      ES(I)=XS(I)                                                       120
    5 F(I)=G(I)                                                         130
      C=7.22929E-7                                                      140
      NF=NEF                                                            150
      IF(NEF.EQ.1)  NF=0                                                160
      CALL DOPW (8HS1/V    ,KZE)                                        170
      DO 914 I=1,MM                                                     180
      L=MM+1-I                                                          190
  914 E(L)=A(I)                                                         200
      IS=0                                                              210
      J=MM                                                              220
      IF(NF)25,3,25                                                     230
    3 ES(1)=E(J)                                                        240
      M=1                                                               250
      L=MM-1                                                            260
      DO 14 I=1,L                                                       270
      K=MM-I                                                            280
      ER1=E(K)                                                          290
      ER2=E(K+1)                                                        300
      DO 12 K=1,9                                                       310
      M=M+1                                                             320
      AK=K                                                              330
      AK=AK*0.1                                                         340
   12 ES(M)=ER2+AK*(ER1-ER2)                                            350
      IF(I-L)16,14,16                                                   360
   16 M=M+1                                                             370
   14 ES(M)=ER1                                                         380
```

```
      DO 13 I=1,M
   13 F(I)=PHI(ES(I))
   25 IS=IS+1
      IF(E(J)-ES(IS))10,22,25
   10 IF(IS-1)11,11,30
   11 NFEHL=1
  101 WRITE (NOUTP,100) NFEHL
  100 FORMAT(1H0,6HFEHLER I3)
      GO TO 999
   22 Y(J)=F(IS)
      GO TO 40
   30 XM=(F(IS)-F(IS-1))/(ES(IS)-ES(IS-1))
      Y(J)=XM*(E(J)-ES(IS-1))+F(IS-1)
      IS=IS-1
   40 KS=MM-1
      DO 1 I=1,KS
      J=MM-I
    4 KZ=0
      IJ1=IS
   77 IF(E(J)-ES(IS))68,71,70
   70 KZ=KZ+1
   80 IS=IS+1
      GO TO 77
   68 XM=(F(IS)-F(IS-1))/(ES(IS)-ES(IS-1))
      Y(J)=XM*(E(J)-ES(IS-1))+F(IS-1)
      LAR=0
      GO TO 550
   71 Y(J)=F(IS)
      LAR=1
  550 SUMZ=0.
      SUMN=0.
      S1=Y(J+1)/SQRT(E(J+1))
      S2=F(IJ1+1)/SQRT(ES(IJ1+1))
      SZ1=S1+S2
      SZ2=E(J+1)-ES(IJ1+1)
      SZ=SZ1*SZ2
      SUMZ=SUMZ+SZ
      SN1=F(IJ1+1)+Y(J+1)
      SN=SN1*SZ2
      SUMN=SUMN+SN
      IF(KZ-2)501,500,600
  600 KZ=IJ1+KZ-2
      IJ1=IJ1+1
      DO 2 N=IJ1,KZ
      S1=F(N)/SQRT(ES(N))
      S2=F(N+1)/SQRT(ES(N+1))
      SZ1=S1+S2
      SZ2=ES(N)-ES(N+1)
      SZ=SZ1*SZ2
      SUMZ=SUMZ+SZ
      SN1=F(N)+F(N+1)
      SN=SN1*SZ2
    2 SUMN=SUMN+SN
  500 S1=F(IS-1)/SQRT(ES(IS-1))
      S2=Y(J)/SQRT(E(J))
      SZ1=S1+S2
      SZ2=ES(IS-1)-E(J)
      SZ=SZ1*SZ2
      SUMZ=SUMZ+SZ
      SN1=Y(J)+F(IS-1)
      SN=SN1*SZ2
      SUMN=SUMN+SN
  501 IF(LAR)1,55,1
   55 IS=IS-1
    1 V(J)=C*SUMZ/SUMN
      V(MM)=0.8862269*C/SQRT(0.0253)
      WRITE (NOUTP,300) (I,V(I),I=1,MM)
  300 FORMAT(1H0,6HGRUPPE,7X,3H1/V/(I5,E17.8))
  916 L=0
      WRITE (JA)L,KZE
      DO 502 I=1,MM
      KP=MM-I+1
  502 Y(I)=V(KP)
      WRITE (JA) MM,(Y(I),I=1,MM)
      KL=KL+1
      RETURN
  999 STOP
      END
```

```
      SUBROUTINE REMO(NG,ABN,NSP,F,E,ERR,NLA,NLE,NGRE,NFG,NFI,NJM,NUJM,
     1ISEL,IWORK,WORK,L)
      DIMENSION IWORK(1),WORK(1),KDAT(2)
      REAL*8 FNEV(3)
      REAL*8 NHID
      REAL*8 MATN
      REAL*8 REM
      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 NHID/'H  H1'/
      DATA FNEV/'SGNC ' ,'SGT  ','SGN  '/
      DATA REM/'REMO '/
      KLL=KLL+1
      WRITE (NOUT ,9000)
 9000 FORMAT(1H0/1H0/' PROGRAMM KENNZIFFER 9')
      WRITE (NOUT ,9001)
 9001 FORMAT(' PROGRAMM ZUR BERECHNUNG DER ELASTISCHEN STREUMATRIZEN FUE
     1R DIE REMO-KORREKTUR'/)
      IWORK(24)=0
      IWORK(33)=35
      MO=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                                                     300
      IWORK(17)=NLE                                                     310
      IWORK(19)=NJM+1                                                   320
      IWORK(20)=NUJM                                                    330
      WORK(27)=ERR                                                      340
      WORK(32)=-0.1                                                     350
      DO 30 I=1,NG                                                      360
      I1=NG-I+1                                                         370
   30 WORK(M0+I1-1)=ABN(I)                                              380
      WORK(M0+NG)=0.                                                    390
      CALL MASSIN(WORK,WORK(M0))                                        400
      IMAX=IWORK(18)                                                    410
      N0=IWORK(34)+(NLE+1)*IMAX*2                                       420
      IWORK(1)=N0                                                       430
      IF(MATN.EQ.NHID)GOTO 3                                            440
      CALL NIVNUM(MATN,FNEV(1),NIV,WORK(M0+M2-1),WORK(M0+M1),FNW,       450
     1&3,&3,&3)                                                         460
      NIV=NIV+2                                                         470
      GOTO 4                                                            480
    3 NIV=0                                                             490
      ICOS=0                                                            500
      N2=N0                                                             510
      N3=N0                                                             520
      N4=N0                                                             530
      IS=M2-1                                                           540
    4 IWORK(26)=NIV                                                     550
      N1=N0+NIV                                                         560
      IWORK(2)=N1                                                       570
      IF(NIV.EQ.0)GOTO 5                                                580
      NW=1                                                              590
      CALL DATNUM(MATN,FNEV(1),ICOS,NW,1.0,-1.0,&3,&3,&3)               600
      LM=N1+ICOS                                                        610
      IF(LM.GT.L)GOTO 20                                                620
      IF(FNW.GE.WORK(M0+M2-1))GOTO 3                                    630
      IS=ICSOP(FNW,WORK(M0))                                            640
      IF(FNW.EQ.WORK(M0+IS-1))IS=IS-1                                   650
      N2=N1+ICOS                                                        660
      N3=N2+ICOS*NIV                                                    670
      L1=N3+NIV                                                         680
      L2=L1+ICOS                                                        690
      LM=L2+ICOS*NIV                                                    700
      IF(M1.LT.IS)IS=M1                                                 710
      IF(LM.GT.L)GOTO 20                                                720
      CALL KEDLEC(MATN,FNEV(1),NIV,WORK(N0),IWORK(N3),WORK(M0+M2-1),    730
     1WORK(M0+IS),                                                      740
     1WORK(N1),WORK(L1),WORK(L2),WORK(N2),1.0,-1.0,&3,&3,&3)            750
      IWORK(26)=NIV                                                     760
    5 CONTINUE                                                          770
      IWORK(21)=ICOS                                                    780
      IWORK(3)=N2                                                       790
      IWORK(5)=N4                                                       800
      KDAT(1)=1                                                         810
      KDAT(2)=1                                                         820
      LM=N4                                                             830
      DO 6 I=M2,M1                                                      840
      DO 6 J=1,2                                                        850
      CALL DATNUM(MATN,FNEV(J+1),NDAT,NW,WORK(M0+M2-1),WORK(M1+M0),     860
     1&10,&10,&10)                                                      870
      IF(KDAT(J).LT.NDAT)KDAT(J)=NDAT                                   880
      GOTO 6                                                            890
   10 WRITE(NOUT,71)MATN,FNEV(J+1)                                      900
   71 FORMAT(' ***ERROR  9.5 :  FOR  ',A8,'  THERE IS NO  ',A8)         910
    6 CONTINUE                                                          920
      IF(KDAT(2).LT.KDAT(1)) KDAT(2)=KDAT(1)                            930
      N5=N4+KDAT(2)                                                     940
      N6=N5+KDAT(2)                                                     950
      KK=KDAT(2)                                                        960
      IMAX=IWORK (18)                                                   970
    7 N7=N6+KK                                                          980
      N9=N8+ICOS                                                        990
      N10=N9+IMAX*NUJM*(NLE+1)                                         1000
      N11=IMAX*(NLE+1)+N10                                             1010
      N11=N11+1+IMAX                                                   1020
      IWORK(6)=N5                                                      1030
      IWORK(7)=N6                                                      1040
      IWORK(9)=N8                                                      1050
      IWORK(10)=N9                                                     1060
      IWORK(11)=N10                                                    1070
      IWORK(12)=N11                                                    1080
      LM=N11+KDAT(2)                                                   1090
      IF(L.LT.LM)GOTO 20                                               1100
      NZM=1                                                            1110
      DO 9 I=M2,M1                                                     1120
      NZ=NFG(I)*NFI(I)                                                 1130
      NZM=MAXO(NZM,NZ)                                                 1140
    9 CONTINUE                                                         1150
      IZV=IMAX*(NLE+1)                                                 1160
      IZV=MAXO(4,IZV)                                                  1170
      IWORK(13)=N11+NZM*IZV                                            1180
      JJ=2+IMAX*NZM                                                    1190
      JJ=MAXO(JJ,KDAT(2))                                              1200
      LM=IWORK(13)+JJ                                                  1210
   20 CONTINUE                                                         1220
      IF(L.LT.LM)WRITE(NOUT,70)LM                                      1230
   70 FORMAT(' ***ERROR 9.1 : REQUIRED WORKING FIELD',I8,' WORDS')     1240
      IF(L.LT.LM)RETURN                                                1250
      NQ=0                                                             1260
      WRITE(LI)NQ,REM                                                  1270
      NQ=4                                                             1280
      NM1=NLE-NLA+1                                                    1290
      WRITE(LI)NQ,MATN,NG,NM1                                          1300
      CALL REMP(WORK(M0),NFG,NFI,F,E,WORK,IWORK,IS)                    1310
      RETURN                                                           1320
      END                                                              1330
```

```
      SUBROUTINE                                                        10
     1      KEDDAT(NAMIZ,NAMTYP,NW,NW1,FNW,NDAT,FA,FF,EP,EM,*,*,*)     20
      REAL*8 FM(6),NAMIZ,NAMTYP,NGNC,NGIZ                               30
      DIMENSION EA(1),IEA(1),FA(1),FF(1),FAW(1),FFW(1),NWORT(4),NDT(2)  40
      DATA FM(2)/'BEST '/,KERST/0/ ,NGNC/'SGNC '/,NGIZ/'SGIZ '/         50
      KK=1                                                              60
      IF(NAMTYP.EQ.NGNC.OR.NAMTYP.EQ.NGIZ)KK=2                          70
      GOTO 1                                                            80
      ENTRY DATNUM(NAMIZ,NAMTYP,NDAT,NW,EP,EM,*,*,*)                    90
      KK=3                                                             100
      IF(NAMTYP.EQ.NGNC.OR.NAMTYP.EQ.NGIZ)KK=4                         110
      GOTO 1                                                           120
      ENTRY KEDLEC(NAMIZ,NAMTYP,NW1,EA,IEA,EPW,EMW,FA,FF,FAW,FFW,EP,EM,130
     1*,*,*)                                                           140
      KK=5                                                             150
      NW=0                                                             160
      GOTO 1                                                           170
      ENTRY NIVNUM(NAMIZ,NAMTYP,NW1,EPW,EMW,EFR,*,*,*)                 180
      NW=0                                                             190
      KK=6                                                             200
1     IF(KERST.NE.0)GOTO 20                                            210
      L=1                                                              220
      KERST=1                                                          230
 20   FM(1)=NAMIZ                                                      240
      FM(3)=NAMTYP                                                     250
      GOTO (2,3,2,3,3,3),KK                                            260
 2    CONTINUE                                                         270
      NWORT(1)=3                                                       280
      LL=0                                                             290
      CALL NDFLOC(NT,NWORT,FM,N1,N2)                                   300
      IF(NT.EQ.0)RETURN 1                                              310
 22   NDAT=1                                                           320
      IF(FM(4+LL).LE.EM)GOTO 21                                        330
      IF(KK.EQ.3)GOTO 40                                               340
      FA(1)=EM                                                         350
      FF(1)=FM(5+LL)                                                   360
 40   CONTINUE                                                         370
      NDAT=2                                                           380
 21   CONTINUE                                                         390
      IF(KK.EQ.3)GOTO 8                                                400
      FA(NDAT)=FM(4+LL)                                                410
      FF(NDAT)=FM(5+LL)                                                420
 8    NDAT=NDAT+1                                                      430
      CALL NDFNXT(NT,NWORT,FM,N1,N2)                                   440
      IF(NT.EQ.0)GOTO 9                                                450
      IF(FM(4+LL ).LE.EM)NDAT=1                                        460
      IF(KK.EQ.3)GOTO 41                                               470
      FA(NDAT)=FM(4+LL)                                                480
      FF(NDAT)=FM(5+LL)                                                490
 41   CONTINUE                                                         500
      IF(FM(4+LL).GE.EP)GOTO 30                                        510
      GOTO 8                                                           520
 30   IF(LL.EQ.0)RETURN                                                530
      IF(KK.EQ.1.OR.KK.EQ.3)RETURN                                     540
      GOTO 10                                                          550
 9    CONTINUE                                                         560
      IF(KK.EQ.3)GOTO 42                                               570
      FA(NDAT)=EP                                                      580
      FF(NDAT)=FF(NDAT-1)                                              590
 42   CONTINUE                                                         600
      GOTO 30                                                          610
 3    CONTINUE                                                         620
      NWORT(1)=4                                                       630
      LL=1                                                             640
      NW1=0                                                            650
      FM(4)=1.0                                                        660
 23   CALL NDFLOC(NT,NWORT,FM,N1,N2)                                   670
      CALL NDFLOC(NT,NWORT,FM,N1,N2)                                   680
      IF(NT.EQ.0.AND.NW1.EQ.0)RETURN 1                                 690
      IF(NT.EQ.0)GOTO 18                                               700
      IF(KK.EQ.6.AND.NW1.EQ.0)EFR=FM(4)                                710
      NW1=NW1+1                                                        720
      IF(NW.EQ.0.AND.FM(4).GE.EMW)GOTO 24                              730
      IF(NW.EQ.NW1)GOTO 24                                             740
      FM(4)=(1+1.E-6)*FM(4)                                            750
      GOTO 23                                                          760
 24   CONTINUE                                                         770
      IF(KK.GE.7)GOTO 26                                               780
      IF(KK.GE.5)GOTO 25                                               790
      FNW=FM(4)                                                        800
      KK=KK-1                                                          810
      GOTO 22                                                          820
 25   NW=NW1-1                                                         830
      IF(EMW.EQ.FM(4))NW=NW1                                           840
      LZ=0                                                             850
      IF(NW.EQ.0)LZ=1                                                  860
      IF(NW.EQ.0)NW=1                                                  870
      NPN=0                                                            880
      KK=KK+2                                                          890
      GOTO 3                                                           900
 26   FNW=FM(4)                                                        910
      IF(KK.EQ.7)GOTO 22                                               920
      IF(FM(4).GE.EPW)RETURN                                           930
      FM(4)=(1+1.E-6)*FM(4)                                            940
      NW=NW+1                                                          950
      GOTO 23                                                          960
 10   IF(LZ.NE.0)GOTO 88                                               970
      DO 90 I=1,NDAT                                                   980
      FAW(I)=FA(I)                                                     990
 90   FFW(I)=FF(I)                                                    1000
      IEA(1)=NDAT                                                     1010
      EA(1)=EMW                                                       1020
      LZ=2                                                            1030
      NPN=NDAT                                                        1040
 88   CONTINUE                                                        1050
      DO 91 I=1,NDAT                                                  1060
      FAW(I+NPN)=FA(I)                                                1070
 91   FFW(I+NPN)=FF(I)                                                1080
      EA(LZ)=FNW                                                      1090
      IEA(LZ)=NDAT                                                    1100
      NPN=NPN+NDAT                                                    1110
      LZ=LZ+1                                                         1120
```

```
      IF(FNW.GE.EPW)GOTO 89                                          1130
      NW=NW+1                                                        1140
      FM(4)=(1+1.E-6)*FNW                                            1150
      GOTO 23                                                        1160
18    FNW=EPW                                                        1170
      IF(KK.EQ.7)GOTO 88                                             1180
      NW1=NW1+1                                                      1190
      RETURN                                                         1200
89    NW1=LZ-1                                                       1210
      RETURN                                                         1220
      END                                                            1230
```

```
      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(EP.GE.ES(I).AND.EP.LT.ES(I+1))GOTO 2                          70
      GOTO 1                                                           80
 2    J1=I+1                                                           90
      GOTO 11                                                         100
 1    CONTINUE                                                        110
11    CONTINUE                                                        120
      DO 12 I=2,KL                                                    130
      IF(EM.LE.ES(I).AND.EM.GT.ES(I-1))GOTO 13                        140
      GOTO 12                                                         150
 13   J2=I-1                                                          160
      GOTO 14                                                         170
12    CONTINUE                                                        180
14    CONTINUE                                                        190
      RETURN                                                          200
      END                                                             210
```

```
      SUBROUTINE MASSIN(WORK,ABN)                                      10
      REAL*8 MATN                                                      20
      REAL*8 HID                                                       30
      DIMENSION WORK(1),ABN(1),A(6),AC(13)                             40
      DIMENSION FF(6),FA(6)                                            50
      COMMON MATN,IS(2),NOUT,LI,IR(2)                                  60
      DATA A/0.57735,0.774596,0.33998,0.86114,0.53847,0.90618/         70
      DATA HID/'H  H1'/                                                80
      IF(MATN.EQ.HID)GOTO 40                                           90
      CALL KEDDAT(MATN,'ISOT1    ',0,NW1,FNW,NDAT,FA,FF,300.0,1.0,    100
     1&40,&40,&40)                                                    110
      AME=FA(2)                                                       120
      GOTO 41                                                         130
40    CONTINUE                                                        140
```

```
      AME=1.008665                                                      150
   41 CONTINUE                                                          160
      AME=AME/1.008665                                                  170
      DO 10 I=1,6                                                       180
      XA=A(I)**2-1                                                      190
      AC(I+6)=(XA-A(I)*SQRT(XA+AME**2))/AME                             200
   10 AC(I)=(XA+A(I)*SQRT(XA+AME**2))/AME                               210
      AC(13)=-1/AME                                                     220
      XM=(AME+1)**2/2/AME                                               230
      QM=2.0E8                                                          240
      IF(XM.NE.2)QM=XM/(XM-2)                                           250
      QMX=ALOG(QM)                                                      260
      WORK(28)=AME                                                      270
      WORK(29)=QM                                                       280
      WORK(30)=XM                                                       290
      WORK(31)=QMX                                                      300
      CALL IROMES(AC)                                                   310
      I1=IR(1)                                                          320
      I2=IR(2)                                                          330
      IMAX=2                                                            340
      DO 11 I=I2,I1                                                     350
      E=ABN(I+1)/QM                                                     360
      IM=ICSOP(E,ABN(I))                                                370
      IF(IM.GT.IMAX)IMAX=IM                                             380
   11 CONTINUE                                                          390
      CALL IWIN(18,IMAX,WORK)                                           400
      RETURN                                                            410
      END                                                               420
```

```
      SUBROUTINE INTEN(E,SG,SGNC,EA,ICOS)                               10
      DIMENSION SG(1),SGNC(ICOS,1),EA(1)                                20
      NE=0                                                              30
    3 NE=NE+1                                                           40
      IF(E.GT.EA(NE)+EA(NE)*1.0E-4)GOTO 3                               50
      IF(NE.EQ.1)GOTO 5                                                 60
      A=ALOG(EA(NE)/EA(NE-1))                                           70
      B=ALOG(E/EA(NE-1))                                                80
      DO 4 I=1,ICOS                                                     90
    4  SG(I)=(SGNC(I,NE)-SGNC(I,NE-1))/A*B+SGNC(I,NE-1)                100
      RETURN                                                           110
    5 DO 6 I=1,ICOS                                                    120
      SG(I)=0.5                                                        130
    6 CONTINUE                                                         140
      RETURN                                                           150
      END                                                              160
```

```
      FUNCTION FXINT(EP,EM,SGN,ES,FLUX,EFLUX,NSP,NDAT)                  10
      DIMENSION FLUX(1),EFLUX(1)                                        20
      DIMENSION SGN(1),ES(1)                                            30
      FINTP(XA,XB,XC,YA,YC)=YA+(YC-YA)/(XC-XA)*(XB-XA)                  40
      FG(XA,XB,XC,YA,YC)=YA+(YC-YA)/ALOG(XC/XA)*ALOG(XB/XA)             50
      CALL ZWIN(NDAT,EP,EM,ES,J2,J1)                                    60
      Y=0                                                               70
      SGN1=SGN(J1)                                                      80
      SGN2=SGN(J2)                                                      90
      ES1=ES(J1)                                                       100
      ES2=ES(J2)                                                       110
      SGN(J1)=FG(ES(J1),EP,ES(J1-1),SGN(J1),SGN(J1-1))                 120
      SGN(J2)=FG(ES(J2),EM,ES(J2+1),SGN(J2),SGN(J2+1))                 130
      ES(J1)=EP                                                        140
      ES(J2)=EM                                                        150
      J11=J1-1                                                         160
      IF(NSP.EQ.1)GOTO 1                                               170
      CALL ZWIN(NSP,EP,EM,EFLUX,JF2,JF1)                               180
      FF1=FINTP(EFLUX(JF2),EM,EFLUX(JF2+1),FLUX(JF2),FLUX(JF2+1))      190
      GOTO 2                                                           200
    1 FF1=PHI(EM)                                                      210
    2 CONTINUE                                                         220
      DO 16 I=J2,J11                                                   230
      DX=ES(I+1)-ES(I)                                                 240
      IF(NSP.EQ.1)GOTO   3                                             250
      CALL ZWIN(NSP,ES(I+1),ES(I+1),EFLUX,ISG,ISF)                     260
      FF2=FINTP(EFLUX(ISG),ES(I+1),EFLUX(ISG+1),FLUX(ISG),FLUX(ISG+1)) 270
      GOTO 4                                                           280
    3  CONTINUE                                                        290
      FF2=PHI(ES(I+1))                                                 300
    4  Y=Y+DX*(SGN(I)*FF1+SGN(I+1)*FF2)                                310
      FF1=FF2                                                          320
   16 CONTINUE                                                         330
      FXINT=Y/2                                                        340
      ES(J1)=ES1                                                       350
      ES(J2)=ES2                                                       360
      SGN(J1)=SGN1                                                     370
      SGN(J2)=SGN2                                                     380
      RETURN                                                           390
      END                                                              400
```

```
      SUBROUTINE SMORN(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
    END                                                                   140
```

```
    SUBROUTINE SEARCH(NFG,NFI,WORK,IWORK,FLUX,EFLUX,ABN)                   10
    DIMENSION WORK(1),IWORK(1),FLUX(1),EFLUX(1),ABN(1),SGS(4)              20
    REAL*8 MATN                                                            30
    COMMON MATN,MAY(2),NOUT,LI                                             40
    DATA SGS/'SGT ','SGN ','MUEL', 'FLUX'/                                 50
    NDAT=IWORK(25)                                                         60
    N9=IWORK(13)                                                           70
    DO 3 I=1,NDAT                                                          80
 3  WORK(N9+I-1)=1.0                                                       90
    N4=IWORK(7)                                                           100
    NZ=NFG*NFI                                                            110
    N11=IWORK(12)                                                         120
    IW=N11+3*NZ                                                           130
    IG=IWORK(4)                                                           140
    NSP=IWORK(15)                                                         150
    DU=ALOG(ABN(1)/ABN(2))/NFG                                            160
    E1=ABN(2)                                                             170
    DO 20 I=1,NFG                                                         180
    E2=E1*EXP(DU)                                                         190
    DE=ALOG(E2/E1)/NFI                                                    200
    FF=FXINT(E2,E1,WORK(N9),WORK(N4),FLUX,EFLUX,NSP,NDAT)                 210
    EM=E1                                                                 220
    DO 21 J=1,NFI                                                         230
    EP=EM*EXP(DE)                                                         240
    WORK(IW)=FXINT(EP,EM,WORK(N9),WORK(N4),FLUX,EFLUX,NSP,NDAT)/FF        250
    IW=IW+1                                                               260
21  EM=EP                                                                 270
20  E1=E2                                                                 280
    IWORK(22)=N11                                                         290
    NQ=4*NZ+3                                                             300
    J=4*NZ                                                                310
    WRITE(LI)NQ,IG,NFG,NFI,(WORK(N11+I-1),I=1,J)                          320
    WRITE(NOUT,70)IG,NZ,MATN                                              330
    DO 1 M=1,4                                                            340
    WRITE(NOUT,71)SGS(M)                                                  350
    IW=N11+(M-1)*NZ-1                                                     360
 1  WRITE(NOUT,72)(WORK(IW+I),I=1,NZ)                                     370
70  FORMAT(/'_GROUP=',I3,' NUMBER OF FINE INTERVALS=',I5,                 380
   1' MATERIAL',2X,A8)                                                    390
71  FORMAT(' THE VALUES OF ',A4)                                          400
72  FORMAT(' ',1P6E12.4)                                                  410
    RETURN                                                                420
    END                                                                   430
```

```
    SUBROUTINE REMP(ABN,IGR,NFI,FLUX,EFLUX,WORK,IWORK,IS)                  10
    DIMENSION ABN(1),IGR(1),NFI(1),FLUX(1),EFLUX(1),WORK(1),IWORK(1)       20
    REAL*8 MATN                                                            30
    REAL*8 FNEV(4)                                                         40
    COMMON MATN,IIZ(2),NOUT,LI,IL,IM                                       50
    DATA FNEV/'SGNC ','SGT  ','SGN  ','MUEL '/                             60
    NO=IWORK(1)                                                            70
    N2=IWORK(3)                                                            80
    N4=IWORK(5)                                                            90
    N5=IWORK(6)                                                           100
    N6=IWORK(7)                                                           110
    NE=IWORK(26)                                                          120
    NLA=IWORK(16)                                                         130
    NLE=IWORK(17)                                                         140
    N11=IWORK(12)                                                         150
    IMAX=IWORK(18)                                                        160
    AM=WORK(28)                                                           170
    DO 10 IG1=IM,IL                                                       180
    IG=IM+IL-IG1                                                          190
    IWORK(4)=IG                                                           200
    IF(IG-IS)20,20,21                                                     210
20  CONTINUE                                                              220
    IWORK(23)=1                                                           230
    CALL ZWIN(NE,ABN(IG),ABN(IG+1),WORK(NO),JW2,JW1)                      240
    CALL NORM(JW2,JW1,WORK(N2),WORK)                                      250
    GOTO 22                                                               260
21  IWORK(23)=0                                                           270
22   CONTINUE                                                             280
    IWORK(22)=N11                                                         290
    JN=2                                                                  300
    CALL KEDDAT(MATN,FNEV(JN),NW,NW1,FNW,NDAT,WORK(N6),WORK(N4),          310
   1ABN(IG),ABN(IG+1),&2,&3,&4)                                           320
    IWORK(25)=NDAT                                                        330
    CALL SINT(ABN(IG),IGR(IG),NFI(IG),FLUX,EFLUX,WORK,N4,N6)              340
    JN=3                                                                  350
    CALL KEDDAT(MATN,FNEV(JN),NW,NW1,FNW,NDAT,WORK(N6),WORK(N4),          360
   1ABN(IG),ABN(IG+1),&2,&3,&4)                                           370
    JN=4                                                                  380
    CALL KEDDAT(MATN,FNEV(JN),NW,NW1,FNW,NDAT,WORK(N6),WORK(N5),          390
   1ABN(IG),ABN(IG+1),&5,&3,&4)                                           400
 7  CONTINUE                                                              410
    IWORK(25)=NDAT                                                        420
    N4=-N4                                                                430
    CALL SINT(ABN(IG),IGR(IG),NFI(IG),FLUX,EFLUX,WORK,N4,N6)              440
    JN=4                                                                  450
    CALL KEDDAT(MATN,FNEV(JN),NW,NW1,FNW,NDAT,WORK(N6),WORK(N5),          460
   1ABN(IG),ABN(IG+1),&6,&3,&4)                                           470
 8  CONTINUE                                                              480
    CALL SEARCH(IGR(IG),NFI(IG),WORK,IWORK,FLUX,EFLUX,ABN(IG))            490
    CALL ISOFAL(ABN(IG),IGR(IG),NFI(IG),FLUX,EFLUX,WORK)                  500
    DO 16 IQ=NLA,NLE                                                      510
16  CALL SUCHM(IGR(IG),NFI(IG),WORK,IWORK,IQ,ABN)                         520
    GOTO 10                                                               530
 5  ASSIGN  7 TO NNN                                                      540
    GOTO 9                                                                550
 6  ASSIGN 8 TO NNN                                                       560
```

```
9   W=2.0/3.0/AM                                                          570
    DO 15 J=1,NDAT                                                        580
15  WORK(N5+J-1)=W                                                        590
    GOTO NNN,(7,8)                                                        600
10  CONTINUE                                                              610
    RETURN                                                                620
2   WRITE(NOUT,80)MATN                                                    630
    RETURN                                                                640
3   WRITE(NOUT,90)MATN,FNEV(JN)                                           650
    RETURN                                                                660
4   WRITE(NOUT,91)MATN,FNEV(JN)                                           670
    RETURN                                                                680
80  FORMAT(' ***ERROR 9.2 : MATERIAL ',A8,' IS NOT FOUND')                690
90  FORMAT(' ***ERROR 9.3   MATERIAL ',A8,'  TYP  ',A8,                   700
   1'  ARE NOT FOUND')                                                    710
91  FORMAT(' ***ERROR 9.4   MATERIAL ',A8,'  TYP  ',A8,                   720
   1'  ARE NOT FOUND IN LIST')                                            730
    END                                                                   740
```

```
    SUBROUTINE NORM(J2,J1,SC,WORK)                                         10
    REAL*8 ANINT                                                           20
    DIMENSION SC(1),WORK(1)                                                30
    NN=IWO(33,WORK)                                                        40
    NJM=IWO(19,WORK)                                                       50
    NMU=IWO(17,WORK)                                                       60
    KJJ=1                                                                  70
    N5=IWO(2,WORK)                                                         80
    ICOS=IWO(21,WORK)                                                      90
    BL=WORK(N5)                                                           100
    BU=WORK(N5+ICOS-1)                                                    110
    NJ=0                                                                  120
    CALL IWIN(24,NJ,WORK)                                                 130
    DO 1 I=J2,J1                                                          140
    IW=(I-1)*ICOS                                                         150
    ASG=ANINT(BU,BL,1,SC(IW+1),WORK(N5),0.0,ICOS,WORK,WORK(NN),NJM)       160
    NJ=IWO(24,WORK)                                                       170
    IF(NJ.GE.NJM-1)KJJ=2                                                  180
    CALL IWIN(23,KJJ,WORK)                                                190
    NJ=0                                                                  200
    CALL IWIN(24,NJ,WORK)                                                 210
    DO 2 J=1,ICOS                                                         220
2   SC(IW+J)=SC(IW+J)/ASG                                                 230
1   CONTINUE                                                              240
    RETURN                                                                250
    END                                                                   260
```

```
    SUBROUTINE SINT(ABN,NG,NI,FLUX,EFLUX,WORK,N,N4)                        10
    DIMENSION ABN(1),FLUX(1),EFLUX(1),WORK(1)                              20
    N2=IWO(5,WORK)                                                         30
    N3=IWO(6,WORK)                                                         40
    N7=IWO(22,WORK)                                                        50
    N9=IWO(13,WORK)                                                        60
    NSP=IWO(15,WORK)                                                       70
    NDAT=IWO(25,WORK)                                                      80
    IG=1                                                                   90
    L=N                                                                   100
    N=IABS(N)                                                             110
    N2=IABS(N2)                                                           120
    NZ=NI*NG                                                              130
    DO 3 I=1,NDAT                                                         140
    IF(L.LT.0)WORK(N3+I-1)=WORK(N3+I-1)*WORK(N2+I-1)                      150
3   WORK(N9+I-1)=1.0                                                      160
    DU=ALOG(ABN(IG)/ABN(IG+1))/NG                                         170
    E1=ABN(IG+1)                                                          180
    IW=N7                                                                 190
    DO 1 IP=1,NG                                                          200
    E2=E1*EXP(DU)                                                         210
    DDU=ALOG(E2/E1)/NI                                                    220
    EM=E1                                                                 230
    DO 2 IR=1,NI                                                          240
    EP=EM*EXP(DDU)                                                        250
    WORK(IW)=FXINT(EP,EM,WORK(N),WORK(N4),FLUX,EFLUX,NSP,NDAT)            260
    FF=FXINT(EP,EM,WORK(N9),WORK(N4),FLUX,EFLUX,NSP,NDAT)                 270
    IF(L.GT.0)GOTO 4                                                      280
    WORK(IW+NZ)=FXINT(EP,EM,WORK(N3),WORK(N4),FLUX,EFLUX,NSP,NDAT)        290
   1/WORK(IW)                                                             300
4   WORK(IW)=WORK(IW)/FF                                                  310
    EM=EP                                                                 320
2   IW=IW+1                                                               330
    E1=E2                                                                 340
1   CONTINUE                                                              350
    IF(L.LT.0)IW=IW+NZ                                                    360
    CALL IWIN(22,IW,WORK)                                                 370
    RETURN                                                                380
    END                                                                   390
```

```
    SUBROUTINE ISOFAL(ABN,IGR2,NFI1,FLUX,EFLUX,WORK)                       10
    REAL*8 STOFF                                                           20
    REAL*8 DU,DDU                                                          30
    DIMENSION ABN(1),FLUX(1),EFLUX(1),WORK(1)                              40
    IG=1                                                                   50
    N9=IWO(10,WORK)                                                        60
    QQ=WORK(32)                                                            70
    IC=IG                                                                  80
    IGI=IWO(4,WORK)                                                        90
    IF(QQ.GT.0)CALL EGRENZ(ABN(1),ABN,IC,IV,WORK)                         100
    IFI=IGI+IG-1                                                          110
    CALL IWIN(4,IFI,WORK)                                                 120
```

```
      NM1=IWO(17,WORK)+1                                                130
      NJM=IWO(19,WORK)                                                  140
      NUJM=IWO(20,WORK)                                                 150
      AME=WORK(28)                                                      160
      IMAX=IWO(18,WORK)                                                 170
      IX=IWO(11,WORK)                                                   180
      N7=IWO(22,WORK)                                                   190
      DU=ABN(IG)/ABN(IG+1)                                              200
      DU=DLOG(DU)/IGR2                                                  210
    2 IG1=IG+1                                                          220
      E1=ABN(IG+1)                                                      230
      FNW=0.                                                            240
      IF(QQ.GT.0.)FNW=QQ*AME/(AME-1.)                                   250
      NU=NM1*IMAX                                                       260
        DO 15 IP=1,IGR2                                                 270
      E2=E1*DEXP(DU)                                                    280
      DDU=DU/NFI1                                                       290
      EM=E1                                                             300
       DO 5 IR=1,NFI1                                                   310
      EP=EM*DEXP(DDU)                                                   320
      DO 9I=1,NU                                                        330
    9 WORK(N7+I-1)=0.0                                                  340
      IF(EP.LE.FNW)GOTO 7                                               350
      IF(QQ.LE.0)GOTO 6                                                 360
      IF(EM.LE.FNW)EM=FNW                                               370
    6 CALL WAHRS(EP,EM,IMAX,WORK(N7),ABN(IC),NM1,NUJM,FLUX,EFLUX,       380
     1WORK(N9),WORK,WORK(IX))                                           390
      CALL SMORN(WORK(N7),NM1,IMAX,WORK)                                400
    7 CONTINUE                                                          410
      N7=N7+NM1*IMAX                                                    420
    5 EM=EP                                                             430
   15 E1=E2                                                             440
      CALL IWIN(22,N7,WORK)                                             450
      RETURN                                                            460
      END                                                               470
```

```
      SUBROUTINE WAHRS(EP,EM,IMAX,PI,ABN,NM1,NUJM,FLUX,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
      NN=IWO(34,WORK)                                                     80
      IG=1                                                                90
      AM=WORK(28)                                                        100
      Q=WORK(32)                                                         110
      KL=IWO(25,WORK)                                                    120
      N2=IWO(5,WORK)                                                     130
      KJ=IWO(23,WORK)                                                    140
      N3=IWO(6,WORK)                                                     150
      N4=IWO(7,WORK)                                                     160
      N10=IWO(11,WORK)                                                   170
      N10=N10+ 1+IMAX                                                    180
      EZ(1)=EM                                                           190
      IJ=1                                                               200
      JM=1                                                               210
      E=EM/QM                                                            220
      IMAX1=ICSOP(E,ABN)                                                 230
      IF(E.EQ.ABN(IMAX1))IMAX1=IMAX1-1                                   240
      IF(Q.GT.0)CALL EGRENZ(EM,ABN,IK,IMAX1,WORK)                        250
      IMAX1=IMAX1+1                                                      260
      IG=IWO(4,WORK)                                                     270
      NG=IWO(14,WORK)                                                    280
      IT=NG-IG                                                           290
      IT=MINO(IMAX,IT)                                                   300
      IF(Q.GT.0)GOTO 45                                                  310
      DO 42 I=1,IT                                                       320
      EP1=QM*ABN(IT-I+2)                                                 330
      IF(EP1.GE.EP.OR.EP1.LE.EM)GOTO 42                                  340
      IJ=IJ+1                                                            350
      EZ(IJ)=EP1                                                         360
   42 CONTINUE                                                           370
   45 CONTINUE                                                           380
      DO 44 LJ=1,IJ                                                      390
      EZ(IJ+1)=EP                                                        400
      IMAX1=IMAX1-1                                                      410
      CALL ZWIN(KL,EZ(LJ+1),EZ(LJ),WORK(N4),J2,J1)                       420
       J11=J1-1                                                          430
       EM1=EZ(LJ)                                                        440
      DO 44  IK=J2,J11                                                   450
       EP1=WORK(N4+IK)                                                   460
      IF(IK.EQ.J11)EP1=EZ(LJ+1)                                          470
      CALL LMI(EP1,EM1,WORK(N4+IK),WORK(N4+IK-1),WORK(N2+IK),            480
     1WORK(N2+IK-1),WORK(N3+IK),WORK(N3+IK-1),IMAX1,ABN,TE,NM1,NUJ,NUJM, 490
     2FLUX,EFLUX,WORK,WORK(N10),IMAX,WORK(NN))                           500
        IF(Q.GT.0)JM=IWO(26,WORK)                                        510
      IF(IMAX1.GT.1.OR.KJ.GT.0)GOTO 3                                    520
      IF(NM1.LT.3)GOTO 3                                                 530
      TE(3,JM,NUJ)=TE(1,JM,NUJ)/AM/AM/5                                  540
      IF(NM1.LT.5)GOTO 3                                                 550
      TE(5,JM,NUJ)=-TE(1,JM,NUJ)/AM/AM/AM/AM/63                          560
    3 CONTINUE                                                           570
      NJ=IWO(24,WORK)                                                    580
      IF(NJ.GT.0)WRITE(NOUT,70)EP1,EM1                                   590
   70 FORMAT(' ***WARNING 9.2 : FEW MESH POINTS IN ANGLE INTEGRATION',   600
     1P2E12.4)                                                          610
      NJ=0                                                               620
      CALL IWIN(24,NJ,WORK)                                              630
      EM1=EP1                                                            640
      DO 43 J=JM,IMAX1                                                   650
      DO 43 K=1,NM1                                                      660
   43 PI(K,J)=PI(K,J)+TE(K,J,NUJ)                                        670
   44 CONTINUE                                                           680
      RETURN                                                             690
      END                                                                700
```

```
      SUBROUTINE LMI(EP,EM,E1,E2,SG1,SG2,AMU1,AMU2,  IMAX,ABN,TE,
     1NM1,NUJ,NUJM,FLUX,EFLUX,WORK,PER,IMAM,PL)
      REAL*8 PLK,PL(NM1,IMAM)
      REAL*8 ANINT
      DIMENSION ABN(IMAX),WORK(1)
      DIMENSION EFLUX(1),FLUX(1)
      DIMENSION PER(NM1,IMAM),TE(NM1,IMAM,NUJM)
      COMMON MATN(4),NOUT
      EQUIVALENCE(JM,JMI)
      FG(XA,XB,XC,YA,YC)=YA+(YC-YA)/ALOG(XC/XA)*ALOG(XB/XA)
      NJM=IWO(19,WORK)
      AM=WORK(28)
      QM=WORK(29)
      KJ=IWO(23,WORK)
      XM=WORK(30)
      Q=WORK(32)
      NSP=IWO(15,WORK)
      ERR=WORK(27)
      NLA=IWO(16,WORK)
      NLE=IWO(17,WORK)
      JM=1
      IF(Q.GT.0)FNW=Q/AM/(AM+1.)
      IF(Q.GT.0)CALL EGRENZ(EP,ABN,JM,II,WORK)
      ICOS=IWO(21,WORK)
      NNE=IWO(26,WORK)
      N1=IWO(3,WORK)
      N5=IWO(2,WORK)
      NR=IWO(33,WORK)
      N8=IWO(9,WORK)
      NG=IWO(14,WORK)
      N6=IWO(4,WORK)
      NL1=1
      NL2=NLE+1
      IF(NSP.GT.1)CALL ZWIN(NSP,EP,EM,EFLUX,JF2,JF1)
      IF(Q.GT.0)GOTO 9
      NO=IWO(1,WORK)
      IF(KJ.EQ.0)GOTO 9
      CALL ZWIN(NNE,EP,EM,WORK(NO),JW2,JW1)
      JW=JW2+NO-1
      IW=(JW2-1)*ICOS+N1
    9 CONTINUE
      DO 31 I=1,NM1
      DO 31 J=1,IMAX
      PER(I,J)=1.0
      PL(I,J)=0
   31 CONTINUE
      DU =EP-EM
      M1=1
      NUJ=0
      M2=1
      ANS=1.0
      SE=1
      ISEL=IWO(8,WORK)
      JZZ=0
   41 NU1=2**NUJ+1
      DX=DU/(NU1-1)
      DO 21 I=M1,NU1,M2
      E=EM+(I-1)*DX
      IF(Q.GT.0)WORK(8)=E
      IF(ISEL.EQ.1)SE=FG(E1,E,E2,SG1,SG2)
       ASE=FG(E1,E,E2,AMU1,AMU2)
      AZ=(ASE-2.0/3.0/AM)*3/(1.0-3.0/5.0/(AM**2))
      IF(NSP.GT.1)GOTO 2
      FF=PHI(E)
      GOTO 3
    2 DO 22  J=JF2,JF1
      ISG=J-1
      IF(EFLUX(J).GT.E)GOTO 23
   22 CONTINUE
   23 CONTINUE
      FF=(FLUX(ISG+1)-FLUX(ISG))/(EFLUX(ISG+1)-EFLUX(ISG))*(E-
     1EFLUX(ISG))+FLUX(ISG)
    3 CONTINUE
      ANS=0.0
      BU=1.0
      J=JM-1
      IF(KJ.EQ.0)GOTO 62
      CALL INTEN(E,WORK(N8),WORK(IW),WORK(JW),ICOS)
      BL=-1.0
      ANS=ANINT(BU,BL,2,WORK(N8),WORK(N5),AZ,ICOS,WORK,WORK(NR),NJM)
      ANS=ASE-ANS
   62 J=J+1
      BL=-1.0
      IF(J.GE.NG-N6+1)GOTO 30
      IF(IMAX.EQ.1)GOTO 30
       BL=BCM(E,ABN(J+1),WORK)
      IF(BL.LE.-1.0)BL=-1.0
   30 CONTINUE
      DO 8 K=NL1,NL2
      IF(PER(K,J).LT.ERR)GOTO 8
      IF(BL.EQ.BU)GOTO 4
      IF(BL.LT.BU)GOTO 6
      JZZ=1
      BL1=BL
      BU1=BU
      BL=BU
      BU=BL1
    6 CONTINUE
      IF(BL.GE.1)GOTO 4
      PLK=ANINT(BU,BL,K,WORK(N8),WORK(N5),AZ,ICOS,WORK,WORK(NR),NJM)
      PLK=PLK+AKOR(BU,BL,K,AM)*ANS
      GOTO 5
    4 PLK=0.0
    5 CONTINUE
      IF(JZZ.EQ.0)GOTO 66
      JZZ=0
      BL=BL1
       BU=BU1
   66 CONTINUE
      PLK=PLK*FF
      IF(I.EQ.1)PL(K,J)=0.5*PLK*DX*SE
      IF(I.EQ.NU1)PL(K,J)=PL(K,J)+0.5*PLK*DX*SE
```

```
      IF(I.EQ.1.OR.I.EQ.NU1)GOTO 8                                      1130
      PL(K,J)=PL(K,J)+PLK*DX*SE                                         1140
    8 CONTINUE                                                          1150
      BU=BL                                                             1160
      IF(BU.EQ.-1.0)GOTO 20                                             1170
      GOTO 62                                                           1180
   20 CONTINUE                                                          1190
   21 CONTINUE                                                          1200
      IF(NU1.GT.2)GOTO 27                                               1210
      DO 50 J=JM,IMAX                                                   1220
      DO 50 K=NL1,NL2                                                   1230
      TE(K,J,1)=PL(K,J)                                                 1240
   50 PL(K,J)=0                                                         1250
      NUJ=NUJ+1                                                         1260
      M1=2                                                              1270
      M2=2                                                              1280
      IF(IMAX.GT.JM.OR.KJ.GT.0)GOTO 41                                  1290
      IF(NL2.LT.3)GOTO 41                                               1300
      DO 25 J=3,NL2                                                     1310
      PER(J,JM)=0.                                                      1320
      IF(J.NE.5)TE(J,JM,1)=0.                                           1330
   25 CONTINUE                                                          1340
      GOTO 41                                                           1350
   27 LX=0                                                              1360
      DO 26 J=JM,IMAX                                                   1370
      DO 7 K=NL1,NL2                                                    1380
      IF(PER(K,J).LT.ERR)TE(K,J,NUJ+1)=TE(K,J,NUJ)                      1390
      IF(PER(K,J).LT.ERR)GOTO 7                                         1400
      AJ=0.5*TE(K,J,1)+PL(K,J)                                          1410
      AL=TE(K,J,NUJ)                                                    1420
      ZC=1                                                              1430
      DO 52 IB=1,NUJ                                                    1440
      ZC=4*ZC                                                           1450
      AP=(ZC*AJ-TE(K,J,IB))/(ZC-1)                                      1460
      TE(K,J,IB)=AJ                                                     1470
   52 AJ=AP                                                             1480
      TE(K,J,NUJ+1)=AP                                                  1490
      PER(K,J)=ABS(AP)                                                  1500
      IF(ABS(AP).GT.1.E-10)PER(K,J)=ABS((AP-AL)/AP)                     1510
      IF(PER(K,J).GT.ERR)LX=1                                           1520
      PL(K,J)=0                                                         1530
    7 CONTINUE                                                          1540
   26 CONTINUE                                                          1550
      NUJ=NUJ+1                                                         1560
      IF(NUJ.GE.NUJM)GOTO 100                                           1570
      IF(LX.EQ.1)GOTO 41                                                1580
       IF(Q.GT.0)CALL IWIN(26,JMI,WORK)                                 1590
      CALL IWIN(8,ISEL,WORK)                                            1600
      RETURN                                                            1610
  100 CONTINUE                                                          1620
       IF(Q.GT.0)CALL IWIN(26,JMI,WORK)                                 1630
      WRITE(NOUT,71)EP,EM                                               1640
      DO 10 J=JM,IMAX                                                   1650
      DO 10  K=1,NM1                                                    1660
      IF(PER(K,J).LE.ERR)GOTO 10                                        1670
      WRITE(NOUT,70)K,J,TE(K,J,NUJ),PER(K,J)                            1680
   10 CONTINUE                                                          1690
   70 FORMAT(10X,'SCATTERING MATRIX_',2I4, 3X,1PE12.4,  ' ERROR ',      1700
     11PE12.4)                                                          1710
   71 FORMAT(' ***WARNING 9.3 : FEW ENERGY_MESH POINTS BETWEEN '        1720
     11P2E12.4,' EV')                                                   1730
      CALL IWIN(8,ISEL,WORK)                                            1740
      RETURN                                                            1750
      END                                                               1760



      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,MATN,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(' ',1P6E12.4)                                              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 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
      REAL*8 PTL
      DIMENSION SG(1),XL(1),Z(7) ,WORK(1)
      COMMON MAT(4),NOUT
      EQUIVALENCE(MATN,MAT(1))
C     DATA NHD/'H  H1'/
      ANG(XX)=(XX+GAM)/DSQRT(GAM**2+2*XX*GAM+1.0)
      ERR=WORK(27)
      AM=WORK(28)
      GAM=1/AM
      Q=WORK(32)
      IF(Q.LT.0)GOTO 56
      EI=WORK(8)
      GAM=GAM*SQRT(EI/(EI-(AM+1)/AM*Q))
   56 CONTINUE
      IF(AM.LT.1.1)CALL HIDR(BU,BL,K,AXX,&50)
      IF(AM.LT.1.1)GOTO 50
      XM=WORK(30)
      KJ=IWO(23,WORK)
      CALL AMESH(BU,BL,Z,L2,NX,K)
       NU=1
      XA=BL
      YA=ANG(XA)
      YA=PTL(K,YA)
      YA=YA*WINK(XL,SG,KJ,ICOS,AZ,XA)
      AXX=0
      IL=1
   18 CONTINUE
      XA1=XA
      XB=Z(IL+L2-1)
      IF(KJ.NE.2)GOTO 20
      DO 21 I=1,ICOS
      J=I
      IF(XL(I).GT.XA+ERR.AND.XL(I).LT.XB-ERR)GOTO 22
   21 CONTINUE
      GOTO 20
   22 XB=XL(J)
      IL=IL-1
   20 CONTINUE
      YB=ANG(XB)
      IF(YB.EQ.0.AND.(K-2*(K/2)).EQ.0)GOTO 57
      YB=PTL(K,YB)
      GOTO 58
   57 YB=0.0
   58 CONTINUE
      YB=YB*WINK(XL,SG,KJ,ICOS,AZ,XB)
      NJ=0
      AJ=0.5*(YA+YB)*(XB-XA)
      XA1=XA
      YA1=YA
       T(1)=AJ
   10 NJ=NJ+1
      XA=XA1
      YA=YA1
      AI=AJ
      NP=2**NJ+1
      DM=(XB-XA)/(NP-1)
      AJ=0.5*AI
      DO 40 IZ=2,NP,2
      XA=XA+DM
      YA=ANG(XA)
      YA=PTL(K,YA)
      YA=YA*WINK(XL,SG,KJ,ICOS,AZ,XA)
      XA=XA+DM
   40 AJ=AJ+YA*DM
      AK=AJ
      AL=T(NJ)
      ZC=1
      DO 51  IB=1,NJ
      ZC=ZC*4
      AP=(ZC*AK-T(IB))/(ZC-1)
      T(IB)=AK
   51 AK=AP
      T(NJ+1)=AP
      EPS=(AP-AL)/AP
         EPS=10.0*EPS
      IF(NJ.GE.NJM-1)GOTO 28
      IF(ABS(EPS).GT.ERR)GOTO 10
      GOTO 29
   28 CONTINUE
      CALL IWIN(24,NJ,WORK)
   29 CONTINUE
       AXX=AXX+T(NJ+1)
      XA=XB
      YA=YB
      IL=IL+1
      IF(IL.LE.NX)GOTO 18
   50 CONTINUE
      ANINT=AXX
      RETURN
      END
```

```
      FUNCTION WINK(XL,SG,KJ,ICOS,AZ,AM)
      DIMENSION XL(1),SG(1)
      COMMON M(4),NOUT
      IF(KJ)100,101,100
  101 WINK=0.5*(1+AZ*AM)
      RETURN
  100 DO 1 I=2,ICOS
      IF(AM-XL(I))2,2,1
    2 WINK=(SG(I)-SG(I-1))/(XL(I)-XL(I-1))*(AM-XL(I-1))+SG(I-1)
      RETURN
    1 CONTINUE
      WRITE(NOUT,70)AM
      WINK=0.5
   70 FORMAT(' ***WARNING 9.1 : THE ANGLE ',E11.4,' IS OUTSIDE')
      RETURN
      END
```

```
      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(B1,BL,K,AM)                                         10
      ANG(X)=(X+GAM)/SQRT(GAM**2+2*X*GAM+1.)                            20
      Q0(X)=0.75*X*X                                                    30
      Q1(X)=0.5*(X**3)                                                  40
      Q2(X)=3./16.*X*X*(3*X*X-2)                                        50
      Q3(X)=0.75*(X**3)*(X*X-1)                                         60
      Q4(X)=1./32.*((X*X-1.)*(35.*X*X-10)-1)*X*X                        70
      Q5(X)=3./16.*(X**3)*(X*X-1.)*(9*X*X-5)                            80
      GAM=1./AM                                                         90
      IF(GAM.LT.0.99)GOTO 7                                            100
      A1=SQRT((B1+1.)/2)                                               110
      A2=SQRT((BL+1.)/2.)                                              120
      GOTO 8                                                           130
    7 CONTINUE                                                         140
      A1=ANG(B1)                                                       150
      A2=ANG(BL)                                                       160
    8 CONTINUE                                                         170
      GOTO(1,2,3,4,5,6),K                                              180
    1 AKOR=Q0(A1)-Q0(A2)                                               190
      RETURN                                                           200
    2 AKOR=Q1(A1)-Q1(A2)                                               210
      RETURN                                                           220
    3 AKOR=Q2(A1)-Q2(A2)                                               230
      RETURN                                                           240
    4 AKOR=Q3(A1)-Q3(A2)                                               250
      RETURN                                                           260
    5 AKOR=Q4(A1)-Q4(A2)                                               270
      RETURN                                                           280
    6 AKOR=Q5(A1)-Q5(A2)                                               290
      RETURN                                                           300
      END                                                              310
```

```
      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                   40
      INTEGER*2 IHC(2),IMP(2)                                           50
      DIMENSION N(4),E(2),S(2)                                          60
      COMMON MAT,ISTRUK,ISPA,NOUT,LIZ,NANF,NEND,KL                      70
      EQUIVALENCE(IHC(1),HM)                                            80
      DATA IMP/'PU','U '/                                               90
      WRITE (NOUT ,9000)                                               100
 9000 FORMAT(1H0/1H0/' PROGRAMM KENNZIFFER 10')                        110
      WRITE (NOUT ,9001)                                               120
 9001 FORMAT(' PROGRAMM ZUR BERECHNUNG DER THERMISCHEN QUERSCHNITTE'/)  130
      N(1)=3                                                           140
      CALL DOPW (8HBEST    ,FEST(2))                                   150
      CALL DOPW (8HTHERM   ,A)                                         160
      CALL DOPW (8HSGF     ,B)                                         170
      CALL DOPW (8HSGA     ,C)                                         180
      CALL DOPW (8HSGC     ,D)                                         190
      CALL DOPW (8HALPHA   ,P)                                         200
      CALL DOPW (8HETA     ,F)                                         210
      CALL DOPW (8HNUE     ,G)                                         220
      CALL DOPW (8HSGG     ,H)                                         230
      CALL DOPW (8HMUEL    ,Z)                                         240
      HM=MAT  CALL DOPW (8HSGN     ,X)                                 250
      INR=0                                                            260
      SC=0.                                                            270
      LL=0                                                             280
      IF(IHC(1).EQ.IMP(1))  GO TO 802                                  290
      IF(IHC(1).NE.IMP(2))  GO TO 822                                  300
  802 LAR=1                                                            310
      DO 803 JJ=1,NTY                                                  320
      IF(TYP(JJ).EQ.C)  GO TO 805                                      330
      IF(TYP(JJ).NE.B)  GO TO 803                                      340
  805 LL=LL+1                                                          350
      IF(LL-2)803,801,803                                              360
  803 CONTINUE                                                         370
```

```
      IF(LL-2)807,801,807                                                  380
  807 WRITE(NOUT,808) MAT                                                  390
  808 FORMAT(1H0/' ***WARNING 10. 1 : THE GROUP CROSS SECTION SGC CAN NO   400
     1T BE CALCULATED FOR ',A6/' BECAUSE THE REACTION TYPES SGF AND SGA    410
     2ARE NOT SPECIFIED IN THE INPUT')                                     420
      GO TO 801                                                            430
  822 LAR=0                                                                440
      DO 821 JJ=1,NTY                                                      450
      IF(TYP  (JJ).EQ.C)  GO TO 801                                        460
  821 CONTINUE                                                             470
      GO TO 807                                                            480
  801 I=0                                                                  490
      WRITE (LIZ)I,A                                                       500
      FEST(1)=MAT                                                          510
      DO 1 I=1,NTY                                                         520
      KSIK=0                                                               530
      IF(TYP(I).NE.P.AND.TYP(I).NE.F)  GO TO 871                           540
      IF(LAR.EQ.0)  GO TO 875                                              550
      KSIK=1                                                               560
      FEST(3)=H                                                            570
      GO TO 872                                                            580
  875 WRITE(NOUT,876) MAT,TYP(I)                                           590
  876 FORMAT(1H0/' ***WARNING 10. 2 : THE GROUP CROSS SECTION FOR ',2A8,   600
     1' CAN NOT BE CALCULATED BECAUSE THE VALUE OF SGF IS ZERO')           610
      GO TO 1                                                              620
  874 KSIK=2                                                               630
      FEST(3)=B                                                            640
      GO TO 872                                                            650
  879 KSIK=3                                                               660
      FEST(3)=G                                                            670
      GO TO 872                                                            680
  871 FEST(3)=TYP(I)                                                       690
  872 CALL NDFLOC (J,N,FEST,K,K)                                           700
      IF(J)2,2,3                                                           710
    2 WRITE (NOUT,4) TYP(I),MAT                                            720
    4 FORMAT(1H0/' ***WARNING 10. 3 : THE CROSS SECTION TYPE ',A9,' IS N   730
     1OT AVAILABLE IN THE KEDAK LIBRARY FOR MATERIAL ',A9)                 740
      T=0.                                                                 750
      GO TO 890                                                            760
    3 E(1)=FEST(4)                                                         770
      S(1)=FEST(5)                                                         780
      IF(E(1)-0.0253)24,5,6                                                790
    6 WRITE (NOUT,7) TYP(I),MAT                                            800
    7 FORMAT(1H0/' ***WARNING 10. 4 : IN THE KEDAK LIBRARY IS NO ENERGY    810
     1POINT LESS THAN OR EQUAL TO 0.0253'/' AVAILABLE FOR THE CROSS SECT   820
     2ION TYPE ',A9,' FOR MATERIAL ',A9)                                   830
      GO TO 1                                                              840
   24 CALL NDFNXT(J,N,FEST,K,K)                                            850
      IF(J)2,2,8                                                           860
    8 E(2)=FEST(4)                                                         870
      S(2)=FEST(5)                                                         880
      IF(E(2)-0.0253)24,10,11                                              890
   10 E(1)=E(2)                                                            900
      S(1)=S(2)                                                            910
    5 IF(TYP(I).EQ.G.OR.TYP(I).EQ.Z)  GO TO 30                             920
      T=S(1)*0.8862269                                                     930
      GO TO 9                                                              940
   30 T=S(1)                                                               950
      GO TO 9                                                              960
   11 SE=S(1)+(0.0253-E(1))*((S(2)-S(1))/(E(2)-E(1)))                      970
      IF(TYP(I).EQ.G.OR.TYP(I).EQ.Z)  GO TO 31                             980
      T=SE*0.8862269                                                       990
      GO TO 9                                                             1000
   31 T=SE                                                                1010
    9 IF(KSIK.EQ.3)  GO TO 881                                            1020
      IF(KSIK.EQ.2)  GO TO 877                                            1030
      IF(KSIK.EQ.0)  GO TO 890                                            1040
      TT=T                                                                1050
      GO TO 874                                                           1060
  877 TT=TT/T                                                             1070
      IF(TYP(I).EQ.F)  GO TO 879                                          1080
      T=TT                                                                1090
      GO TO 890                                                           1100
  881 T=T/(1.+TT)                                                         1110
  890 WRITE (NOUT,12) MAT,TYP(I),NE                                       1120
   12 FORMAT(1H /1H ,A9,A9,I10)                                           1130
      WRITE (NOUT,13) T                                                   1140
   13 FORMAT(E16.8)                                                       1150
      K=5                                                                 1160
      WRITE(LIZ) K,MAT,TYP(I),NE                                          1170
      K=1                                                                 1180
      WRITE(LIZ) K,T                                                      1190
      IF(TYP(I ).EQ.C)  GO TO 810                                         1200
      IF(TYP(I ).EQ.B)  GO TO 812                                         1210
      GO TO 1                                                             1220
  810 SC=SC+T                                                             1230
      IF(INR.EQ.1)  GO TO 818                                             1240
      INR=1                                                               1250
      GO TO 1                                                             1260
  812 SC=SC-T                                                             1270
      IF(INR.EQ.1)  GO TO 818                                             1280
      INR=1                                                               1290
      GO TO 1                                                             1300
  818 WRITE(NOUT,12) MAT,D,NE                                             1310
      WRITE(NOUT,13) SC                                                   1320
      K=5                                                                 1330
      WRITE(LIZ)K,MAT,D,NE                                                1340
      K=1                                                                 1350
      WRITE(LIZ) K,SC                                                     1360
    1 CONTINUE                                                            1370
      KL=KL+1                                                             1380
      RETURN                                                              1390
      END                                                                 1400
```

VI.77