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## JOYFOR A Program for Transformation of NJOY Results in MATXS-Format to the MITRA Input Format

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## Abstract

The program JOYFOR is the connection between the output of the group constant calculation code NJOY in MATXS-format and the testing and formatting program MITRA. Resonance selfshielding factors as well as transfermatrices for elastic and inelastic scattering and for (n,2n)- and (n,3n)-processes, normalized corresponding to the conventions of MITRA, are calculated by JOYFOR from the NJOY results and are written in MIGROS-format on an external file and on the standard output unit. Also the group cross-sections for infinite dilution, the 1/v-values and the fission spectrum are written out in the same format as in MIGROS. KERMA-factors are handled by JOYFOR in the same way as group crosssections. The output data of JOYFOR may be tested by MITRA and transformed into input for the GRUBA management program GRUMA. The present version of JOYFOR handles group constants for neutron reactions only. Extension of the program to photon reactions is being planned.

## JOYFOR - Ein Programm zur Transformation von NJOY Ergebnissen im MATXS-Format in das MITRA Eingabe Format

## Zusammenfassung

Das Programm JOYFOR stellt die Verbindung zwischen der Ausgabe des Gruppenkonstantenberechnungscodes NJOY im MATXS-Format und dem Testund Formatierungsprogramm MITRA dar. JOYFOR erzeugt aus den NJOY Ergebnissen Resonanzselbstabschirmfaktoren sowie, entsprechend den MITRA Konventionen, normierte Transfermatrizen für elastische und inelastische Streuung und für (n,2n)- und (n,3n)-Prozesse, und schreibt sie in der gleichen Form, wie es das Programm MIGROS tut, auf einen externen File und auf die Standard Ausgabeeinheit. Auch die Gruppenwirkungsquerschnitte für unendliche Verdünnung, die 1/v-Querschnitte und das Spaltspektrum werden entsprechend den MIGROS Konventionen ausgegeben. KERMA-Faktoren werden in JOYFOR verarbeitet wie Gruppenwirkungsquerschnitte. Die Daten des Ausgabefiles von JOYFOR können, wie die des Ausgabefiles von MIGROS, in MITRA geprüft und als Eingabe für das GRUBA Management Programm GRUMA bereitgestellt werden. Die derzeitige Fassung von JOYFOR verarbeitet nur Gruppenkonstanten für Neutronenreaktionen. Eine Erweiterung für Photonengruppenkonstanten ist geplant.

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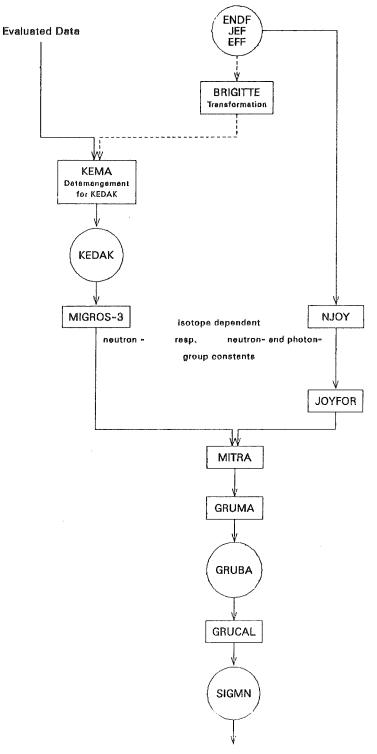
## 1. Introduction

In 1985 the American group constant generation code NJOY was implemented at KfK /1/, /2/ and is presently being extensively used for the testing of the JEF-1 evaluated nuclear data library. Many changes in the original code have to be introduced for a reliable calculation of group constants. This part will be described in another report.

The group constants calculated by NJOY /3/ or THEMIS /4/ are written on an intermediate group constant library, the so-called GENDF-file. This GENDF-file may be transformed to several other formats, so for example by module NMATXS to the MATXS-format, which has been proposed as European standard group constant exchange format. Module NMATXS has been implemented into the KfK-version of NJOY and will be provided for implementation into a future version of THEMIS. The standard group constant format at KfK is the GRUBA/5/-format. The program JOYFOR is the connection between the MATXS-output file produced by NJOY (or THEMIS) and the extended program MITRA /6/. (Formerly MITRA was only able to check and prepare the output data of MIGROS /7/ for a transfer to GRUBA. Extensions of the program were necessary for the handling of JOYFOR output as well.) Figure 1 shows the data and program flow from nuclear data files to reactor calculations for data from KEDAK processed by MIGROS-3 and for data from ENDF, JEF or EFF processed by NJOY and JOYFOR.

Based on the experience gained by the present use of JOYFOR, modifications of the code were carried out and will be carried out in the future. Moreover an extension of the program for the handling of photon group constants is being planned.

JOYFOR needs a very small card input, which is explained in 5., and the output file of NJOY in MATXS-format. The output file of JOYFOR will be arranged in the same way as the output file of MIGROS. Also the printed output is carried out as in MIGROS.



Reactor calculations

Figure 1: Flowchart for nuclear data processing at KfK from ENDF and from KEDAK

## 2. Description of the MATXS-Format

The MATXS-file, produced by the module NMATXS, has the following structure (see also /8/, Appendix K).

Record Type	<u>Present if</u>
File identification File control Set hollerith identification File data	Always Always Always Always
Group structures	Always
(Repeat for all data types) Data type control	Always
(Repeat for all materials) Material control	Always
(Repeat for all submaterials) Vector control	N1DB.GT.0
(Repeat for all vector blocks)	N1DB.GT.0
(Repeat for all matrix blocks) Matrix control	N2DB.GT.0
(Repeat for NSBLK sub-blocks) Matrix sub-block	N2DB.GT.0

In the following detailed explanations all variables with names beginning with H are of type REAL\*8 and filled with 6 alpha signs, all variables with names beginning with I, J, K, L, M, or N are of type INTEGER\*4. All other variables are of type REAL\*4.

File identification		
HNAME,(HUSE(I),I = 1,2),IVERS		
HNAME	Hollerith file name MATXS	
HUSE	Hollerith user identification File version number See card 2 in the NMATXS input as given in the KfK NJOY input description	
IVERS	File version number	

## File control

#### NPART, NTYPE, NHOLL

NPART	Number of particles for which group structures are given
ΝΤΥΡΕ	Number of data types present in set
NHOLL	Number of words of length 6 bytes in 'set hollerith identification' record

#### Set hollerith identification

(HSETID(I), I = 1, NHOLL)

HSETID Hollerith identification of set (to be edited out 72 characters per line)

#### <u>File data</u>

(HPRT(JP), JP = 1, NPART), (HTYPE(JT), JT = 1, NTYPE), (NMAT(JT), JT = 1, NTYPE), (NINP(JT), JT = 1, NTYPE), (NING(JT), JT = 1, NTYPE), (NOUTP(JT), JT = 1, NTYPE), (NOUTG(JT), JT = 1, NTYPE), (LOCT(JT), JT = 1, NTYPE), (NGRP(JP), JP = 1, NPART)

HPRT(JP)	Hollerith identification for particle JP (fixed name) NEUT neutron GAMA photon BETA electron	
	• • •	
HTYPE(JT)	Hollerith identification for data type JT (fixed name)NSCATneutron scatteringNGAMAneutron induced gamma productionNGCUPneutron-gamma coupled setGSCATgamma scattering	

•

NMAT(JT)	Number of materials in set for data type JT
NINP(JT)	Number of incident particles associated with data type JT
NING(JT)	Number of incident energy groups associated with data type JT
NOUTP(JT)	Number of outgoing particles associated with data type JT
NOUTG(JT)	Number of outgoing energy groups associated with data type JT
LOCT(JT)	Number of records to be skipped to read data for data type JT (LOCT(1) = 0)
NGRP(JP)	Number of energy groups for particle JP

Group structure : one group structure for each particle

(GPB(IG),IG = 1,NGR),EMIN

NGR = NGRP(JP) (see file data)

GPB(IG) Maximum energy bound for group IG for particle JP

EMIN Minimum energy bound for particle JP

Data type control : the total following input will be repeated for each data type

(HMATNM(IM),IM = 1,NMAT),(NSUBM(IM),IM = 1,NMAT),(LOCA(IM),IM = 1, NMAT),(IINP(JPI),JPI = 1,NINP),(IOUTP(JPO),JPO = 1,NOUTP),NSBLK

NMAT = NMAT(JT) NINP = NINP(JT) NOUTP = NOUTP(JT)

HMATNM(IM) Hollerith identification for material IM

- NSUBM(IM) Number of submaterials for material IM. A submaterial is a temperature-sigma 0-combination. For example: material IM is calculated by NJOY at the 3 temperatures 300K, 900K and 2100K and the 7 standard values for dilution, e.g. 1.E10, 1.E5, 1.E4, 1.E3, 1.E2, 10, 1.E-3. In this case NSUBM(IM) is 21.
- LOCA(IM) Number of records to be skipped to read data for material IM. LOCA(1) = 0

IINP(JPI)	Number of the particle type corresponding to incident particle JPI for data type JT
IOUTP(JPO)	Number of the particle type corresponding to outgoing particle JPO for data type JT
NSBLK	Sub-blocking parameter

<u>Material control</u> : the total following input will be repeated for each material

```
HMAT,AMASS,(TEMP(ISM),SIGZ(ISM),N1DR(ISM),N1DB(ISM),N2DB(ISM),
LOCS(ISM),ISM = 1,NSUBM)
```

NSUBM = NSUBM(IM) (see data type control)

- HMAT Hollerith material identifier
- AMASS Atomic weight ratio
- TEMP(ISM) Temperature for submaterial ISM
- SIGZ(ISM) Dilution factor for submaterial ISM
- N1DR(ISM) Number of vectors for submaterial ISM
- N1DB(ISM) Number of vector blocks for submaterial ISM
- N2DB(ISM) Number of matrix blocks for submaterial ISM
- LOCS(ISM) Number of records to skip to find first block for submaterial ISM. LOCS(1) = 0

<u>Vector control</u> : the total following input will be repeated for each submaterial

(HVPS(IV), IV = 1, N1DR), (IBLK(IV), IV = 1, N1DR), (NFG(IV), IV = 1, N1DR), (NLG(IV), IV = 1, N1DR)

N1DR = N1DR(ISM) (see material control)

HVPS(IV)	IVPS(IV) Hollerith identifier of vector	
	NELAS	neutron elastic scattering
	N2N	(n,2n)
	NNF	second chance fission
	GABS	gamma absorption
IBLK(IV)	Number of blo	ock in which vector IV is located
NFG(IV)	Number of fire	st group in band for vector IV

NLG(IV)Number of last group in band for vector IV(The lowest group number corresponds to the highest energy)

<u>Vector block</u> : will be repeated for each vector block

(VPS(I), I = 1, KMAX)

KMAX Sum over group band for each vector in block IB

VPS(I) Data for group bands for vectors with IBLK(IV) = IB.
 For the first submaterial VPS contains vector data in the energy groups NFG(IV) to NLG(IV) for all vector types HVPS. For all following submaterials VPS contains the differences between the values belonging to submaterial 1 and the values belonging to the actual submaterial, if these differences are greater than 0.1 % of the values of the first submaterial and besides greater 10<sup>-6</sup>. If the conditions given above are not fulfilled, VPS is omitted in order to save storage space.

<u>Matrix control</u> : the total following input will be repeated for each matrix block

HMTX,LONE,LORD,(JBAND(IG),IG = 1,NOUTG),(IJJ(IG),IG = 1,NOUTG)

NOUTG = NOU	ITG(JT)	(see file data)
HMTX	Hollerith ident	tification of block
LONE	Lowest Legend	dre order present
LORD	Number of Leg	gendre orders present

- JBAND(IG) Bandwidth for group IG (number of energy groups out of which particles are scattered into group IG)
- IJJ(IG) Lowest group in band for group IG (Lowest group number corresponding to highest energy.)

(It will be scattered into energy group IG out of JBAND(IG) groups beginning in group IJJ(IG).)

Matrix sub-block : will be repeated for all NSBLK sub-blocks

((SCAT(I,L),I = 1,KMAX),L = 1,LORD)

KMAX Sum over all JBAND in the group range of this sub-block

SCAT(I,L) Matrix data

For the first material SCAT contains data for matrix HMTX e.g. scattering into energy group IG out of JBAND(IG) groups beginning in energy group IJJ(IG) for Legendre order LONE up to Legendre order LORD - LONE + 1. For all following submaterials SCAT contains only the differences between the values belonging to submaterial 1 and the values belonging to the actual submaterial, if these differences are greater than 0.1 % of the values of the first submaterial and besides greater 10<sup>-6</sup> (see VPS in vector block). If the conditions given above are not fulfilled, SCAT is omitted.

## **3.** Description of the calculations carried out in JOYFOR

In the following it is explained in which way the vector and matrix types given on the MATXS-file are handled to get group cross-sections for infinite dilution, 1/v average group values, fission spectra, KERMA-factors, elastic and inelastic scattering probabilities, transfer probabilities for the (n,2n)- and (n,3n)-processes and resonance selfshielding factors as they are needed for MITRA-input.

## 3.1 Vector types

Vector types are group cross-sections for infinite dilution, 1/v group values, fission spectra and KERMA-factors (/3/, Vol. II and /9/). These data are printed out and stored on an external output file in descending order of energy group numbers. (Group number 1 corresponds to the energy group of highest energy.) The energy groups, which could not be treated in NJOY because no data could be found on the ENDF-(or JEF- or EFF-)file, are filled up with zeros, so that for all energy groups from NGRP(JP) to 1, one value is given out.

Special treatment is needed for:

- weighted 1/v average group values: they are multiplied by 10<sup>-2</sup>, because these values have to be converted from sec/m to sec/cm as calculated in MIGROS.
- (n,2n)-cross-sections: if the direct (n,2n)-cross-section (MF = 3,MT = 16 on ENDF-file) is calculated in NJOY, this averaged group cross-section is written with the name N2N on the MATXS output file. If also the (n,2n)-cross-sections for the 1st to 4th excited state (MF = 3,MT = 6, ...,9) were calculated, the types N2N1, N2N2, N2N3 and N2N4 are written on the MATXS-file. JOYFOR adds the present types N2N, N2N1, N2N2, N2N3 and N2N4 and writes this total (n,2n)-group cross-section with the typename N2NSUM additionally on the output units. (For the meaning of the file numbers MF and reaction types MT see /10/ and /3/, Vol. I).

# 3.2 Resonance selfshielding factors and group cross-sections for infinite dilution

JOYFOR calculates and prints out flux-weighted\* resonance selfshielding factors for radiative capture, fission and elastic scattering and the current-weighted resonance selfshielding factors for the total cross-section calculated from effective group cross-sections for all background cross-sections  $\sigma_0$ , all energy groups and all temperatures given in the input of NJOY. The temperature dependent group cross-sections for infinite dilution are also printed out. The currentweighted elastic scattering selfshielding factor, which is calculated in MIGROS (but not in NJOY), is set equal to 1 at present in the JOYFOR output; correspondingly the group cross-section for infinite dilution is set equal to 0.

The selfshielding factors  $f_{x,q}(\sigma_0,T)$  are calculated as follows:

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

x neutron reaction (n,x)

g energy group

T temperature in Kelvin

σ<sub>o</sub> background cross-section in barns

 $\sigma_{x,g}(\sigma_o,T)$  effective cross-section in energy group g for reaction (n,x), temperature T and background cross-section  $\sigma_o$ 

The group cross-sections for infinite dilution and the selfshielding factors depending on background cross-sections are printed out for descending energy group numbers and ascending temperatures.

If a selfshielding factor is greater than 1 and less than or equal to a prescribed number FFP (see input description in 5),  $f_{x,g}(\sigma_0,T)$  is set equal to 1 on output file 3 of JOYFOR without any comment. If a selfshielding factor is greater than FFP,

\*Bondarenko weighting is normally used in NJOY.

 $f_{x,g}(\sigma_0,T)$  is also set equal to 1 on the output file, but a warning is given out on output unit 11. In both cases the original value of  $f_{x,g}(\sigma_0,T)$  will be printed on unit 11.

If a selfshielding factor obtains a negative value (either resulting from the data file or from the processing\*) this  $f_{x,g}(\sigma_0,T)$  will be inter- or extrapolated with the methods of the standard program GRUCAL for the calculation of macroscopic group constants /11/. The interpolation routine is taken out of WIGRUB /12/ and carries out a  $\sigma_0$ -interpolation. On output unit 11 the negative value of  $f_{x,g}(\sigma_0,T)$  and a comment with the interpolated value is printed out; on output file 3 the negative f-factor is replaced by the interpolated one.

## 3.3 Matrix types

Matrix types are the elastic and inelastic scattering matrices and the transfer matrices of the (n,2n)- and (n,3n)-processes. These matrices are printed out and stored on an external file for each Legendre order.

## 3.3.1 The normalized transfer probabilities for inelastic scattering

NJOY calculates individual inelastic scattering matrices for each discrete excitation state of the residual nucleus (MFD = 6,MTD =  $51, \ldots, 90$ ) and for the continuum of excited states (MFD = 6,MTD = 91). (For the meaning of the reaction types MTD see /3/, Vol. I and /10/.)

The meaning of the MFD-numbers, which have to be specified in the input of NJOY, module GROUPR, is different from the meaning of the MF-numbers on the ENDF/B-library; e.g. MFD = 6 means that a neutron-neutron-matrix will be calculated by NJOY. For this calculation normally ENDF-B-data with MF = 4 and MF = 5 will be used. The MTD-numbers, used in module GROUPR of NJOY, essentially have the same meaning as the MT-numbers of the ENDF/B-library. The following table shows the meaning of some of the MFD values as used in the input of module GROUPR of NJOY (see also /3/, Vol. I and /10/).

<sup>\*</sup>Negative selfshielding factors occur especially for cross-sections of fission products in high concentration (small values of  $\sigma_0$ ).

MFD	Meaning
3	Cross-section or derived quantity (e.g. $\overline{\mu}$ )
5	Fission spectrum
6	Neutron-neutron-matrix
16	Neutron-gamma matrix (photon yields given)
17	Neutron-gamma matrix (photon production cross- sections given)

The partial inelastic matrices calculated by NJOY are then contained in the MATXS-file with the names N51, . . . ., N90 for the discrete excitation states and NCN for the continuum. The normalized transfer probabilities for inelastic scattering  $P^{I}_{in,g\rightarrow h}$ , which are needed by MITRA are calculated as the sum of all partial matrices divided by the inelastic group cross-section.

$$P_{in,g \to h}^{l} = \left(\sum_{I=51}^{90} N(I)_{g \to h}^{l} + NCN_{g \to h}^{l}\right) \cdot \frac{1}{NINEL_{g}}$$

N(I)	inelastic scattering matrices for the 1st up to the 40th excited state
NCN	inelastic scattering matrix for the continuum
NINELg	inelastic group cross-section in energy group g
l	Legendre order
$g {\rightarrow} h$	scattering from energy group g to group h

#### 3.3.2 Normalized transfer probabilities for (n,2n)-reactions

For the calculation of the (n,2n)-transfer probabilities it is a pre-condition that the components of the total (n,2n)-cross-section (MFD = 3,MTD = 6,7,8,9 and 16), see 3.1, and the following matrices were calculated by NJOY if these data types are available on the nuclear data library:

MFD = 6,MTD = 6,7,8,9,16,46,47,48,49

MTD = 6,7,8,9	means the (n,2n)-matrices for the 1st to the 4th excited state describing the first neutron. The names of the matrices on the MATXS-file are N2N1, N2N2, N2N3 and N2N4.
MTD = 16	means the (n,2n)-matrix for the direct (n,2n)-process. The name of the matrix on the MATXS-file is N2N.
MTD = 46,47,48,49	means the (n,2n)-matrices for the 1st to the 4th excited state describing the second neutron. The names of the matrices on the MATXS-file are MT46 , MT47, MT48 and MT49.

The normalized total (n,2n)-transfer probabilities  $P_{n,2n,g\rightarrow h}$ , which are needed by MITRA, are calculated by JOYFOR as follows:

$$P_{n,2n,g \rightarrow h}^{l} = \frac{1}{2 \cdot N2NSUM_{g}} \left[ N2N1_{g \rightarrow h}^{l} + N2N2_{g \rightarrow h}^{l} + N2N3_{g \rightarrow h}^{l} + N2N4_{g \rightarrow h}^{l} + N2N_{g \rightarrow h}^{l} + MT - 46_{g \rightarrow h}^{l} + MT - 47_{g \rightarrow h}^{l} + MT - 48_{g \rightarrow h}^{l} + MT - 49_{g \rightarrow h}^{l} \right]$$

$$N2NSUM_{g} \quad \text{is the total (n,2n)-group cross-section in energy group g.}$$

$$N2N \quad 2 \quad \text{is the (n,2n)-matrix for the 1st, 2nd, 3rd and 4th excited state describing the 1st neutron.}$$

$$N2N \quad \text{is the direct (n,2n)-matrix.}$$

46
MT-- 47
47
48
48
49
49

 $g \rightarrow h$  means scattering from energy group g to group h.

is the Legendre order.

l

## 3.3.3 Normalized transfer probabilities for (n,3n)-reactions

A requirement for the calculation of the (n,3n)-transfer probabilities by JOYFOR is that NJOY has calculated the average (n,3n)-group cross-section (MFD = 3,MTD = 17) and the (n,3n)-matrix (MFD = 6,MTD = 17). The normalized (n,3n)-transfer probability  $PI_{n,3n,g\rightarrow h}$ , needed by MITRA, is then calculated as follows:

$$P_{n,3n,g \to h}^{l} = \frac{N3N_{g \to h}^{l}}{3 \cdot N3N_{g}}$$

- $N3N_{g \rightarrow h}^{l}$  means the elements of the (n,3n)-matrix for Legendre order I and energy group g of the incoming neutron and energy group h of the neutron produced in the (n,3n)reaction.
- $N3N_g$  means the (n,3n)-group cross-section in energy group g.

# 3.3.4 The normalized elastic scattering probabilities and the elastic and total group cross-sections

If NJOY has calculated the average group cross-sections (MFD = 3, MTD = 1)

NWT0,NWT1:	flux- and current-weighted components of the library weight function /8/
NTOT0:	flux-weighted total cross-section
NTOT1:	current-weighted total cross-section
NELAS:	elastic scattering cross-section (MFD = 3,MTD = 2)
	average casing of the cost taking angle (in the laboratory system)

MUBAR: average cosine of the scattering angle (in the laboratory system) for elastic scattering (MFD = 3,MTD = 251)

and the elastic scattering matrices NELAS (MFD = 6,MTD = 2), the MATXS-file contains the elastic scattering matrices depending on temperature and the

 $\sigma_{o}$ -values. In the standard case the normalized elastic scattering matrix for the lowest temperature and the highest  $\sigma_{o}$ -value will be stored on GRUBA. For reactor calculations the normalized matrix is multiplied by the elastic scattering cross-section for the actual values of T and  $\sigma_{o}$  /11/.

The normalized elastic scattering probabilities  $Pl_{el,g\rightarrow h}(\sigma_o,T)$  will be calculated in JOYFOR as follows:

$$P_{el,g \rightarrow h}^{l}(\sigma_{o},T) = \frac{1}{NELAS_{g}(\sigma_{o},T)} \cdot NELAS_{g \rightarrow h}^{l}(\sigma_{o},T)$$

- $\begin{array}{ll} \textit{NELAS}_{g}(\sigma_{o},T) & \text{elastic scattering group cross-section in energy} \\ & \text{group g for the selected temperature} \sigma_{o}^{-} \\ & \text{combination} \end{array}$
- $\begin{array}{ll} \textit{NELASl}_{g \rightarrow h}(\sigma_o, T) & \text{elements of the elastic scattering matrix of} \\ & \text{Legendre order I for the selected temperature-} \\ & \sigma_o\text{-combination} \end{array}$
- $g \rightarrow h$  means scattering from energy group g to group h

In addition to the elastic scattering probabilities the elastic group cross-sections, the group averaged cosine for elastic scattering calculated directly from nuclear data and the group averaged cosine for elastic scattering, dependent on the selected temperature- $\sigma_0$ -combination, calculated from the elastic scattering probabilities for Legendre order 1

$$MUBAR(\sigma_o, T) = \sum_{h \ge g} P^1_{el,g \to h}(\sigma_o, T)$$

are given out. Furtheron the group averaged total cross-section and the energy group integrals of the weighting spectrum for the selected temperature- $\sigma_0$ -combination are given out. MUBAR( $\sigma_0$ ,T) as well as the total cross-section and the energy group integrals are only printed out and are not stored on the external output file of JOYFOR (see also 4.6).

4. Arrangement of the unformatted output on file 3

Each kind of output data is preceded by a special label to make possible a unique identification of the data in the subsequent program MITRA. These labels are written as

0 'LABEL---'

- means a blank

'LABEL---' means a 8 byte alphanumerical word. All data records are written in the form  $N_{O}(I)$ , I = 1, N).

N is an INTEGER\*4 word and gives the number of the succeeding 4 byte words in the record. Only the material names are 8 byte alphanumerical words and are counted as two words in N. All other words are of length 4 bytes.

The last record in the unformatted output is

0 'ENDE----'

## 4.1 Group cross-sections for infinite dilution

1st record: 0, 'INFDILUT'

2nd record: N, highest energy group (lowest number), lowest energy group

3rd record: N, material name, name of reaction type (8-byte, alphanumeric)

4th record: N, group constant of the type defined by the 3rd and 4th word in the 3rd record, for all energy groups specified by the 2nd record. The values are ordered with increasing energies and decreasing group numbers.

The records 2 to 4 are repeated for all reaction types.

## 4.2 Fission spectrum

1st record: 0, 'FISSPECT'

- 2nd record: N, material name, energy of the fission-inducing neutron in eV (double precision), number of the lowest energy group (lowest group number corresponds to highest group boundary), number of the highest energy group.
- 3rd record: N, values of the fission spectrum for all groups specified in the 2nd record, arranged with increasing energies.

#### 4.3 1/v group values

1st record: 0, 'ONE/V---'

2nd record: N, 1/V-values for all energy groups, arranged with increasing energies and decreasing group numbers.

# 4.4 Resonance selfshielding factors and group cross sections for infinite dilution

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

2nd record: N, material name, temperature in K, number of the energy group (lowest group number corresponds to lowest group boundaries), lower group boundary in eV, upper group boundary in eV

3rd record: N, SIGMA G, SIGMA N, SIGMA F, SIGMAN1, SIGMAT1

4th record: N, SIGMA 0, FG, FN, FF, FN1, FT1

for all SIGMA 0-values in increasing order.

The records 2, 3, 4 are repeated for all energy groups in increasing group numbers (increasing group boundaries) and for all temperatures in increasing order.

#### 4.5 Inelastic scattering matrices and matrices for (n,2n)- and (n,3n)-processes

1st record: 0, 'MTOTINEL' ('MTOTN2N-', 'MTOTN3N-')

- 2nd record: N, material name, total number of outscattering groups, number of Legendre moments
- 3rd record: N, number of the Legendre moment, number of the outscattering group, elements of the matrices INELI(N2N-I,N3N-I) (I = number of the moment) in the sense, that the first element describes scattering within the group, the second element describes scattering into the neighbouring group etc.

This procedure is repeated for all outscattering groups in decreasing group numbers (increasing group boundaries) for a certain Legendre order repeated for all Legendre moments

## 4.6 Elastic scattering matrices

- 1st record: 0, 'MELASTIC'
- 2nd record: N, material name, number of outscattering groups, number of Legendre moments
- 3rd record: N, number of the outscattering group, group averaged total elastic cross-section NELAS for the selected submaterial, group averaged cosine for elastic scattering MUBAR, group averaged  $\psi_l$ -weighted\* total cross sections NTOT for all Legendre moments

This procedure is repeated for all outscattering groups in increasing group numbers (decreasing group boundaries).

\*Only  $\psi_0$  (flux -) and  $\psi_1$  (current-) weighted total cross-sections are calculated by NJOY; therefore for I  $\geq$  1 current-weighted total cross-sections are given out in JOYFOR.

4th record: N, number of the Legendre moment, number of the outscattering group, matrix elements ELASI (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.

This procedure is repeated for all outscattering groups in increasing group numbers (decreasing group boundaries) for a certain Legendre moment.

This procedure is repeated for all Legendre moments.

## 5. Input description for program JOYFOR

1. card NGRUP FFP	Number of energy groups used in NJOY. Highest value of resonance selfshielding factors which can be tolerated. If $1 < f_{x,g}(\sigma_0,T) \leq FFP$ , $f_{x,g}(\sigma_0,T)$ is set equal to 1 on output file 3 without any comment. For $f_{x,g}(\sigma_0,T) > FFP f_{x,g}(\sigma_0,T)$ is also set equal to 1 but a warning is given out (see 3.2).
2. card	
NMATXS	1: The MATXS-input file will be printed out on unit 6.
	0: The file will not be printed.
3. card	
INP	1: The elastic scattering matrix of submaterial ISM (see card 4) will be prepared for transfer to the group constant library.
	0: The elastic scattering matrix of the first submaterial (smallest
	temperature and largest $\sigma_{\mathbf{o}}$ -value) will be prepared for transfer
	on the group constant library (see also 3.3.4).
4. card (only if INP = 1)	
ISM	Number of the selected submaterial
DD-cards necessary for a start of JOYFOR	

Unit 1 will be reserved for the output data file of NJOY in MATXS-format.

On unit 3 the output file of JOYFOR will be written which may be used as an input file for MITRA.

Unit 9 and 10 are only for internal use.

`

On unit 11 the printout of JOYFOR, corresponding to the printout of MIGROS, will be written. The standard output unit 6 will be used for the print output of the input data in MATXS-format, if on input card 2 NMATXS is set equal to 1. The input of JOYFOR is also printed out on unit 6.

#### Example for a JOYFOR-job

```
// Jobcard with REGION = 2048K
// EXEC F7CG PARM.G = 'SIZE = 2000K'
//C.SYSPRINT DD DUMIMY
//C.SYSIN DD DSN = TSO017.JOYFOR.FORT,DISP = SHR,LABEL = (,,,IN)
//G.FT01F001 DD DSN = ....,DISP = SHR
//G.FT03F001 DD UNIT = DISK,VOL = SER = BAT00C,DSN = ....,
// DISP = (NEW,CATLG),SPACE = (TRK,10)
//G.FT09F001 DD UNIT = SYSDA,SPACE = (TRK,100),DCB = DCB.VBS
//G.FT10F001 DD UNIT = SYSDA,SPACE = (TRK,10),DCB = DCB.VBS
//G.FT11F001 DD SYSOUT = *,DCB = *.FT06F001
//G.SYSIN DD *
69 1.02
0
//
```

## 6. Explanation of the type names used in the JOYFOR output

The names of the group cross-section types are those used in the MATXS-file. New names were introduced for partial KERMA-factors because for them only the MTD-numbers are given on the MATXS-file. In the following list the names of the group cross-sections are explained. In parenthesis the corresponding MFDand MTD-numbers, used in the GROUPR input of NJOY, are indicated.

NWT0,NWT1:	flux- and current-weighted components of the library weight function /8/. Will not be stored on GRUBA.
NTOT0:	flux-weighted total cross-section (MFD = 3,MTD = 1)
NTOT1:	current-weighted total cross-section (MFD = 3,MTD = 1)
NELAS:	elastic scattering cross-section (MFD = $3$ ,MTD = $2$ )
NINEL:	total inelastic scattering cross-section (MFD = $3$ ,MTD = $4$ )
N2N1:	(n,2n)-cross-section for first excited state, describing the first neutron (MFD = 3,MTD = 6)
N2N2:	(n,2n)-cross-section for second excited state describing the first neutron (MFD = 3,MTD = 7)
N2N3:	(n,2n)-cross-section for third excited state describing the first neutron (MFD = 3,MTD = 8)
N2N4:	(n,2n)-cross-section for fourth excited state describing the first neutron (MFD = 3,MTD = 9)
N2N:	direct (n,2n)-cross-section (MFD $=$ 3,MTD = 16)
N2NSUM:	total (n,2n)-cross-section as sum of N2N1, N2N2, N2N3, N2N4 and N2N
N3N:	(n,3n)-cross-section (MFD = 3,MTD = 17)
NFTOT:	total fission cross-section (MFD = $3$ ,MTD = $18$ )
MT46:	(n,2n)-cross-section for first excited state describing the second neutron (MFD = 3,MTD = 46)

(n,2n)-cross-section for second excited state describing the second neutron (MFD = 3,MTD = 47)
(n,2n)-cross-section for third excited state describing the second neutron (MFD = 3,MTD = 48)
(n,2n)-cross-section for fourth excited state describing the second neutron (MFD = 3,MTD = 49)
neutron disappearance (MFD = 3,MTD = 101) (Sum of all cross-sections in which a neutron is not in the exit channel (MTD = 101 is sum of
MTD = 102 through MTD = 114 with MFD = 3,
MTD = 102 : $(n, y)$ radiative capture cross-section,
MTD = 103 : (n,p)-cross-section,
MTD = 104 : (n,d)-cross-section,

NABS:	neutron disappearance (MFD = 3,MTD = 101) (Sum of all cross-sections in which a neutron is not in the exit channel (MTD = 101 is sum of MTD = 102 through MTD = 114 with MFD = 3, MTD = 102 : $(n, \gamma)$ radiative capture cross-section, MTD = 103 : $(n,p)$ -cross-section, MTD = 104 : $(n,d)$ -cross-section, MTD = 105 : $(n,t)$ -cross-section, MTD = 105 : $(n,t)$ -cross-section, MTD = 106 : $(n,He3)$ -cross-section, MTD = 107 : $(n,\alpha)$ -cross-section, MTD = 108 : $(n,2\alpha)$ -cross-section, MTD = 109 : $(n,3\alpha)$ -cross-section, MTD = 110 : not assigned, MTD = 111 : $(n,2p)$ -cross-section, MTD = 112 : $(n,p + \alpha)$ -cross-section, MTD = 113 : $(n,t + 2\alpha)$ -cross-section and
NG: NP:	$(n, \gamma)$ -cross-section (MFD = 3,MTD = 102) (n,p)-cross-section (MFD = 3,MTD = 103)
	$MTD = 107 : (n,\alpha)$ -cross-section, $MTD = 108 : (n,2\alpha)$ -cross-section, $MTD = 109 : (n,3\alpha)$ -cross-section, MTD = 110 : not assigned, MTD = 111 : (n,2p)-cross-section, $MTD = 112 : (n,p + \alpha)$ -cross-section, $MTD = 113 : (n,t + 2\alpha)$ -cross-section and $MTD = 114 : (n,d + 2\alpha)$ -cross-section)) $(n,\gamma)$ -cross-section (MFD = 3,MTD = 102)

- (n,d)-cross-section (MFD = 3,MTD = 104) ND:
- (n,t)-cross-section (MFD = 3,MTD = 105) NT:
- $(n,\alpha)$ -cross-section (MFD = 3,MTD = 107) NA:
- total tritium production (MFD = 3,MTD = 205) N.H3:
- total <sup>4</sup>He production (MFD = 3,MTD = 207) N.HE4:

MT--47:

MT--48:

MT--49:

MUBAR:	average cosine of the scattering angle (in the laboratory system) (MFD = 3,MTD = 251)
XI:	average logarithmic energy decrement for elastic scattering (MFD = 3,MTD = 252)
GAMMA:	average of the square of the logarithmic energy decrement for elastic scattering, divided by twice the average logarithmic decrement for elastic scattering (MFD = 3,MTD = 253)
NHEAT:	total neutron KERMA-factor (eV*barn) (MFD = 3,MTD = 301)
NHEATEL:	elastic KERMA-factor (eV*barn) (MFD = 3,MTD = 302)
NHEATNE:	non elastic KERMA-factor (eV*barn) (MFD = 3,MTD = 303)
NHEATIN:	inelastic KERMA-factor (eV*barn) (MFD = 3,MTD = 304)
NHEATFIS:	fission KERMA-factor (eV*barn) (MFD = 3,MTD = 318)
NHEATDIS:	disappearance KERMA-factor (eV*barn) (MFD = 3,MTD = 401)
NHEATCAP:	radiative capture KERMA-factor (eV*barn) (MFD = 3,MTD = 402)
NDAME:	total damage energy production ( $eV*barn$ ) (MFD = 3,MTD = 444)
NUE:	average total (prompt + delayed) number of neutrons released per fission event (MFD = 3,MTD = 452)

The fission spectrum, 1/v group values, selfshielding factors, inelastic and elastic scattering matrices and the transfer matrices of the (n,2n)- and (n,3n)-processes are given out with the following type names:

CHIS:	fission spectrum (MFD = 5,MTD = 18)
1/V:	1/V group values (MFD = 3,MTD = 259)
SIGMA-G:	(n,y)-cross-section for infinite dilution depending on T (MFD = 3,MTD = 102)
SIGMA-N:	elastic scattering cross-section for infinite dilution depending on T (MFD = 3,MTD = 2)

SIGMA-F:	total fission cross-section for infinite dilution depending on T (MFD = 3,MTD = 18)
SIGMAN1:	current-weighted elastic scattering cross-section for infinite dilution depending on T (set equal 0 by JOYFOR, see 3.2) (MFD = 3,MTD = 2)
SIGMAT1:	current-weighted total cross-section for infinite dilution depending on T (MFD = 3,MTD = 1)
FG:	flux-weighted resonance selfshielding factor for radiative capture (n,y) (see 3.2)
FN:	flux-weighted resonance selfshielding factor for elastic scattering (see 3.2)
FF:	flux-weighted resonance selfshielding factor for fission (see 3.2)
FN1:	current-weighted resonance selfshielding factor for elastic scattering (set equal 1. by JOYFOR, see 3.2) (see 3.2)
FT1:	current-weighted total resonance selfshielding factor (see 3.2)
INELI:	inelastic scattering matrix for Legendre order I (see 3.3.1)
N2N-I:	(n,2n)-transfer probabilities for Legendre order I (see 3.3.2)
N3N-I:	(n,3n)-transfer probabilities for Legendre order I (see 3.3.3)
ELASI:	elastic scattering matrix for Legendre order I (see 3.3.4)

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#### References

- /1/ I. Broeders, B. Krieg Unpublished report
- /2/ I. Broeders, B. Krieg
   Methods and Codes for Group-Constant Generation at KfK
   KTG/ENS-International "State of the Art"-Seminar on "Nuclear Data, Cross Section Libraries and their Application in Nuclear Technology"
   October 1 2, 1985, Bonn, Proceedings, p. 52
- /3/ R. E. MacFarlane, D. W. Muir, R. M. Boicourt The NJOY Nuclear Data Processing System Vol. I, II, IV, LA-9303-M
- /4/ J. Gonnord

Data Generation for Use in Nuclear Technology KTG/ENS-International "State of the Art"-Seminar on "Nuclear Data, Cross-Section Libraries and their Application in Nuclear Technology" October 1 - 2, 1985, Bonn, Proceedings, p. 32

/5/ D. Woll

Aufbau der Gruppenkonstantenbibliothek GRUBA und ihre Verwaltung durch das Programmsystem GRUMA KfK 3745, August 1984

- /6/ H. Huschke, B. Krieg
   MITRA A Program for the Transformation of the Output of MIGROS-2 into an Input for GRUMA
   KfK 1810, Dezember 1973
- I. Broeders, B. Krieg
   MIGROS-3: A Code for the Generation of Group Constants for Reactor
   Calculations from Neutron Nuclear Data in KEDAK Format
   KfK 2388, Februar 1977

/8/ R. E. MacFarlane

TRANXS-CTR: A Code for Interfacing MATXS Cross-Section Libraries to Nuclear Transport Codes for Fusion Systems Analysis LA-9863-MS, February 1984

- /9/ I. Broeders, B. Goel, B. Krieg, E. Stein, E. Wiegner Private communication
- /10/ R. Kinsey

ENDF-102

Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF/B-V BNL-NCS-50496

#### /11/ D. Woll

GRUCAL - Ein Programmsystem zur Berechnung makroskopischer Gruppenkonstanten KfK 2108, Juni 1975

/12/ C. Broeders

Private communication