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A Program for Transformation of Neutron and Photon Group Constants from NJOY Output in MATXS-Format to the MITRA Input Format

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Abstract

The program JOYFOR-90 connects the output of the group constant calculation code NJOY in MATXS-format with the testing and formatting program MITRA. The first version of JOYFOR, which was described in a previous report (KfK 4179), could handle neutron group constants only. Meanwhile the program has been extended to treat also photon group cross-sections. Transfermatrices for neutron reactions, photon production, and photon reactions, normalized corresponding to the conventions of MITRA, are calculated by JOYFOR-90 from NJOY results and are written in MITRA input format on an external file and on the standard output unit. Also the fission spectrum, 1/v values, resonance selfshielding factors, neutron and photon group cross-sections for infinite dilution and KERMA-factors are made available in the MITRA input format. The output data of JOYFOR-90 can be tested by MITRA and transformed into input for the GRUBA management program GRUMA.

JOYFOR-90 - Ein Programm zur Transformation von Neutronen- und Photonengruppenkonstanten von der NJOY Ausgabe im MATXS-Format in das MITRA Eingabeformat

Zusammenfassung

Das Programm JOYFOR-90 verbindet die Ausgabe des Gruppenkonstantenberechnungscodes NJOY im MATXS-Format mit dem Test- und Formatierungsprogramm MITRA. Die erste Version von JOYFOR, die in einem früheren Bericht (KfK 4179) beschrieben wurde, konnte nur Neutronengruppenkonstanten bearbeiten. Inzwischen wurde das Programm erweitert, so daß auch Photonengruppenwirkungsquerschnitte behandelt werden können. JOYFOR-90 erzeugt aus den NJOY Ergebnissen normierte Transfermatrizen für Neutronenreaktionen, Photonenproduktion und Photonenreaktionen, entsprechend den MITRA Konventionen und schreibt sie auf einen externen File und auf die Standard Ausgabeeinheit. Außerdem werden das Spaltspektrum, die 1/v-Querschnitte, Resonanzselbstabschirmfaktoren, Neutronen- und Photonengruppenwirkungsquerschnitte für unendliche Verdünnung und KERMA-Faktoren im MITRA-Eingabeformat verfügbar gemacht. Die Daten des Ausgabefiles von JOYFOR-90 können in MITRA geprüft und als Eingabe für das GRUBA Managementprogramm GRUMA bereitgestellt werden.

Table of Contents

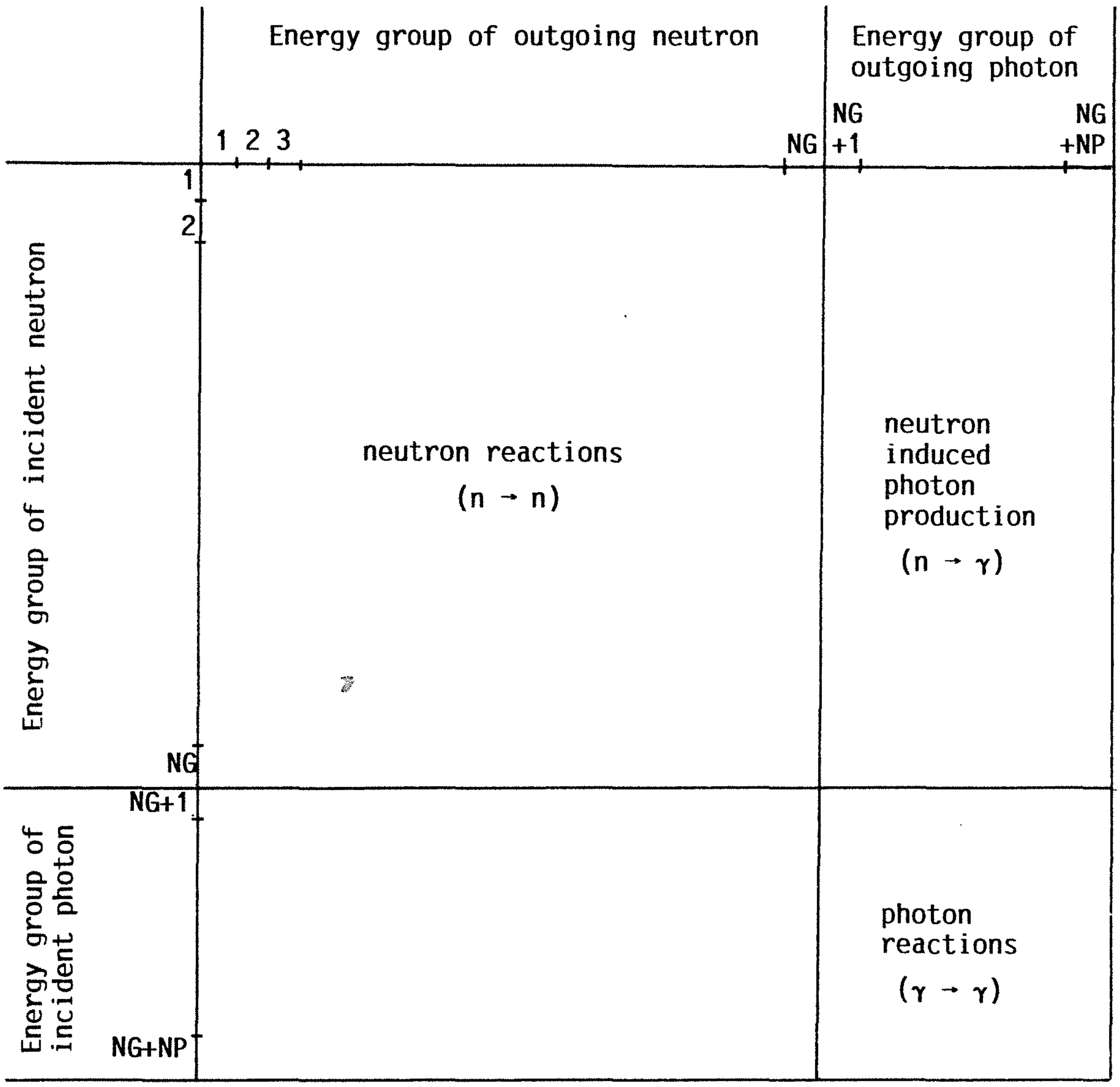
1. Introduction

The group constants calculated by the nuclear data processing system NJOY /1/, /2/, /3/, /4/, /5/ or by THEMIS /6/ 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 MATXSR to the MATXS-format, which has been proposed as European standard group constant exchange format. The MATXS-format is also used as main output format for NJOY calculations at KfK. The standard group constant format at KfK is the GRUBA /7/-format. The program JOYFOR-90 is the connection between the MATXS-output file produced by NJOY and the extended program MITRA /8/. (Formerly MITRA was only able to check and prepare the output data of MIGROS /9/ for a transfer to GRUBA. Extensions of the program were necessary for the handling of JOYFOR-90 output as well.)

The first version of JOYFOR /10/ was restricted to neutron group constants. The extended program, described in the present report, is able to handle neutron and photon group constants.

JOYFOR-90 needs a very small card input, which is explained in chapter 5, and the output file of NJOY in MATXS-format as described in chapter 2. The arrangement of the output file of JOYFOR-90 is explained in chapter 4.

In the output of JOYFOR-90 the following arrangement of neutron and photon energy groups is consistent with the GRUBA-file /7/, /7a/.



NG means number of neutron energy groups

NP means number of photon energy groups

Figure 1

2. Description of the MATXS-Format

The MATXS-file, produced by the module MATXSR, has the following structure (see also /11/, Appendix K).

Record Type	Present if
File identification	Always
File control	Always
Set hollerith identification	Always
File data	Always
(Repeat for all particles)	
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)	
Vector block	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	see card 2 in the MATXSR input as given in the KfK NJOY input description /3/
IVERS	File version number	

File control

NPART,NTYPE,NHOLL

NPART	Number of particles for which group structures are given
NTYPE	Number of data types present in the MATXSR output
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)

File data

(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
GAM	photon
BETA	electron

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HTYPE(JT) Hollerith identification for data type JT (fixed name)

NSCAT	neutron scattering
NGAMA	neutron induced gamma production
GSCAT	gamma scattering
NGCUP	neutron-gamma coupled set

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.
.

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 boundary for group IG for particle JP
EMIN	Minimum energy boundary for particle JP

Data type control: the total following output 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) (see file data)
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

Material control: the following total output 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

Vector control: the following total output 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) Hollerith identifier of vector

NELAS	neutron elastic scattering
N2N	(n,2n)
NFTOT	total fission
GABS	gamma absorption
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.	

IBLK(IV) Number of block in which vector IV is located

NFG(IV) Number of first 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)

Vector block: the vector block output 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^{-30} (or greater EPSV given in the input of module MATXSR in NJOY 87.0 see input description of NJOY 87.0 in /3/). If the conditions given above are not fulfilled, VPS is omitted in order to save storage space.

Matrix control: the following total output will be repeated for each matrix block

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

NOUTG = NOUTG(JT) (see file data)

HMTX Hollerith identification of block

LONE Lowest Legendre order present

LORD Number of Legendre 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: the matrix sub-block output 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^{-8} (or greater EPSM given in the input of module MATXSR in NJOY 87.0 in /3/) (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-90

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 neutron reactions (interactions of neutrons with atomic nuclei), photon production reactions (production of photons induced by neutron reactions), and photon reactions (reactions of photons with atoms) as they are needed for MITRA-input.

3.1 Vector types for neutron reactions

Vector types for neutron reactions are group cross-sections for infinite dilution, 1/v group values, fission spectra and KERMA-factors (/1/). 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^{-2}, because these values have to be converted from sec/m to sec/cm as calculated in MIGROS /9/.

- (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 /12/ and /1/, Vol. I).

3.2 Resonance selfshielding factors and group cross-sections for infinite dilution for neutron induced reactions

For the calculation of neutron group constants and photon production group constants the following weighting function is used in the module GROUPR of NJOY:

$$\Phi_l^i (E, T, \sigma_0) \quad \frac{F(E)}{\left(\sigma_t^i (E, T) + \sigma_0\right)^{l+1}}$$

F (E):	collision density weighting spectrum (has to be specified by input)
$\sigma^i{}_t$ (E, T):	microscopic total cross section of isotope i at energy E and temperature T
$\sigma^i{}_0$:	background cross section (to be specified by input). $\sigma^i{}_0$ is assumed to be constant within the energy group.

Group constants weighted by $\Phi^i{}_0$ (E, T, σ_0) will be called flux weighted in this report, group constants weighted by $\Phi^i{}_1$ (E, T, σ_0) will be called current weighted.

JOYFOR-90 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 σ_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 current-weighted elastic scattering selfshielding factor, which is calculated in MIGROS (but not in NJOY), is set equal to 1 at present in the JOYFOR-90 output; correspondingly the group cross-section for infinite dilution is set equal to 0.

The selfshielding factors $f_{x,g}$ (σ_0,T) are calculated as follows:
(the index i, indicating the isotope, will be omitted in the following formulas)

$$f_{x,g}(\sigma_0,T) = \frac{\sigma_{x,g}(\sigma_0,T)}{\sigma_{x,g}(\sigma_0 \rightarrow \infty,T)}$$

x	neutron reaction (n,x)
g	neutron energy group
T	temperature in Kelvin
σ_0	background cross-section in barns
$\sigma_{x,g}(\sigma_0, T)$	effective cross-section in energy group g for reaction (n,x), temperature T, and background cross-section σ_0

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 the external output file 3 of JOYFOR-90 without any comment. If a selfshielding factor is greater than FPP, $f_{x,g}(\sigma_0,T)$ is also set equal to 1 on the output file, but a warning is given out on print 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 /14/. The interpolation routine is taken out of WIGRUB /15/ and carries out a σ_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 the external output file 3 the negative f-factor is replaced by the interpolated one. (If the interpolated f-factor is less than or equal to 0, this f is set equal to 0.1. If the interpolated f-factor is greater than 1, this f is set equal to 1.)

3.3 Matrix types for neutron reactions

Matrix types for neutron reactions 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.

* Negative selfshielding factors occur especially for cross-sections of fission products in high concentration (small values of σ_0) /13/.

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, ... ,90) and for the continuum of excited states (MFD=6,MTD=91). (For the meaning of the reaction types MTD see /1/, Vol. I and /12/.)

The meaning of the MFD-numbers, which have to be specified in the input of NJOY /3/, module GROUPR, may be 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 ENDF-B-data with MF=4 and MF=5 or MF = 6 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 87.0 /3/.

MFD	Meaning
3	Cross-section or derived quantity (e.g.μ)
5	Fission spectrum
6	Neutron-neutron-matrix
16	Neutron-gamma matrix

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 $P^l_{in,g\rightarrow h}$, which are needed by MITRA, are calculated as the sum of all partial matrices divided by the inelastic group cross-section.

$$P^l_{in,g\rightarrow h} = \left(\sum_{I=51}^{90} N(I)^l_{g\rightarrow h} + NCN^l_{g\rightarrow h} \right) \cdot \frac{1}{NINEL_g}$$

N(I)	inelastic scattering matrices for the 1st up to the 40th excited state
NCN	inelastic scattering matrix for the continuum
$NINEL_g$	inelastic group cross-section in energy group g
l	Legendre order
$g\rightarrow h$	scattering from neutron 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 (of the residual nucleus) 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 MT--46 , MT--47 , MT--48, and MT--49.

The normalized total (n,2n)-tranfer probablities $P^l_{n,2n,g\rightarrow h}$, which are needed by MITRA, are calculated by JOYFOR-90 as follows:

$$P^l_{n,2n,g\rightarrow h} = \frac{1}{2 \cdot N2NSUM_g} \Big[N2N1^l_{g\rightarrow h} + N2N2^l_{g\rightarrow h} + N2N3^l_{g\rightarrow h} + N2N4^l_{g\rightarrow h} + N2N^l_{g\rightarrow h}$$

$$+ MT--46^l_{g\rightarrow h} + MT--47^l_{g\rightarrow h} + MT--48^l_{g\rightarrow h} + MT--49^l_{g\rightarrow h} \Big]$$

$N2NSUM_g$	is the total (n,2n)-group cross-section in energy group g.
N2N 1 N2N 2 N2N 3 N2N 4	is the (n,2n)-matrix for the 1st, 2nd, 3rd, and 4th excited state describing the 1st neutron.
N2N	is the direct (n,2n)-matrix.

	46	
MT--	47	is the (n,2n)-matrix for the 1st, 2nd, 3rd, and 4th excited
	48	state describing the 2nd neutron.
	49	

l is the Legendre order.

g→h means scattering from neutron energy group g to group h.

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

A requirement for the calculation of the (n,3n)-transfer probabilities by JOYFOR-90 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 $P^l_{n,3n,g\to h}$, needed by MITRA, is then calculated as follows:

$$P^l_{n,3n,g\to h} = \frac{N3N^l_{g\to h}}{3 \cdot N3N_g}$$

$N3N^l_{g\to h}$ means the elements of the (n,3n)-matrix for Legendre order l 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

In NJOY transfer matrices for elastic scattering of neutrons are calculated for all temperature- and σ_0-values (submaterials) defined in the input of module GROUPR.

For the calculation of the normalized transfer matrices of elastic scattering the following group constants are needed from the MATXS-file:

NELAS: elastic scattering matrices (MFD = 6,MTD = 2)
NELAS: elastic scattering cross-section (MFD = 3,MTD = 2)

In order to produce the complete output described in this section, which corresponds to the output of module 6 of MIGROS /9/, also the following group constants have to be available in MATXS-format:

NWT0: energy group integral of the flux weighting function /11/:

$$\text{NWT0} = \int_g \frac{F(E)}{\sigma_t(E) + \sigma_0}\, dE\,,$$

F (E): collision density weighting spectrum

σ_t (E): microscopic total cross-section of the isotope for which group constants are to be calculated

$\int_g \ldots dE$: integration over energy group g.

NWT1: energy group integral of the current weighting function

$$\text{NWT1} = \int_g \frac{F(E)}{(\sigma_t(E) + \sigma_0)^2}\, dE$$

NTOT0: flux-weighted total cross-section

NTOT1: current-weighted total cross-section

NWT0, NWT1, NTOT0, and NTOT1 are calculated by NJOY, if MFD = 3,MTD = 1 is specified in the input of the module GROUPR.

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

In the standard case the normalized elastic scattering matrix for the lowest temperature and the highest σ_0-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 σ_0 /14/.

The normalized elastic scattering probabilities $P^l_{el,g\to h}(\sigma_0,T)$ will be calculated in JOYFOR-90 as follows:

$$P^l_{el,g\to h}(\sigma_0,T) = \frac{1}{NELAS_g(\sigma_0,T)} \cdot NELAS^l_{g\to h}(\sigma_0,T)$$

$NELAS_g(\sigma_0,T)$	elastic scattering group cross-section in energy group g for the selected temperature-σ_0-combination
$NELAS^l_{g\to h}(\sigma_0,T)$	elements of the elastic scattering matrix of Legendre order l for the selected temperature-σ_0-combination
$g\to h$	means scattering from neutron energy group g to group h

In addition to the elastic scattering probabilities the elastic group cross-sections NELAS, the group averaged cosine for elastic scattering MUBAR, calculated directly from nuclear data, and the group averaged cosine for elastic scattering, dependent on the selected temperature-σ_0-combination, calculated from the elastic scattering probabilities for Legendre order 1

$$MUBAR(\sigma_0,T) = \sum_{\text{all } h} P^1_{el,g\to h}(\sigma_0,T)$$

are printed out. Furtheron the group averaged flux- and current-weighted total cross-sections and the energy group integrals of the weighting spectrum for the selected temperature-σ_0-combination are printed out. $MUBAR(\sigma_0,T)$ calculated from the elastic scattering probabilities as well as the energy group integrals of the weighting function are only printed out and are not stored on the external output file of JOYFOR-90 (see also 4.6).

3.4 Vector and matrix types for photon production

NJOY calculates photon production matrices for $\sigma_0\to\infty$, for all temperatures T, and all Legendre orders l specified in the input:

$$M^l_{x,j\to\kappa}(\sigma_0\to\infty, T)$$

with

x: type of reaction generating a photon

j: energy group of the neutron that introduce the reaction x

κ: energy group of the photon generated by reaction x. In general the number and structure of energy groups for neutrons and photons is different, see Figure 1. A neutron in energy group j may produce photons in all photon groups κ even if the energy of group κ is higher than the energy of group j.

l: Legendre order

For the following photon production reactions data are available on JEF-1 /16/ on files 12, 13, 14, and 15.

Type number (MT)	Name on the MATXS-file	Meaning
3	NNONL	Nonelastic matrix (MT=3) = (MT=1) - (MT=2)
4	NINEL	Inelastic matrix
16	N2N	Matrix of the direct (n;2n,γ)-reaction. The total (n;2n,γ)-reaction is the sum of MT=6, 7, 8, 9, and 16. Because JEF-1 does not contain photon production data for MT=6, 7, 8, and 9, the matrix for MT=16 is treated as total (n;2n,γ) photon production matrix.
17	N3N	Matrix of the (n;3n,γ)-reaction
18	NFTOT	Matrix for fission
22	NNA	(n;n'+α,γ) matrix
28	NNP	(n;n'+p,γ) matrix
51 - 91	N51, N52...,N90,NCN	(n;n',γ) matrices for different discrete excitation states of the residual nucleus and for the continuum. (MT=4) = (MT=51)+(MT=52) + (MT=53)+.. (MT=90) + (MT=91)

102	NG	(n;γ) matrix
103	NP	(n;p,γ) matrix
104	ND	(n;d,γ) matrix
105	NT	(n;t,γ) matrix
107	NA	(n;α,γ) matrix
741	MT_741	(n;t,γ) matrix for the first excited state of the residual nucleus. MT = 105 is the sum of MT = 740, 741 . . . 758. From reaction MT = 740 photons will not be generated.
781	MT_781	(n;α,γ) matrix for the first excited state of the residual nucleus. MT = 107 is the sum of MT = 780, 781 . . . 798. From reaction MT = 780 photons will not be generated.

JOYFOR-90 calculates photon production cross-sections in each neutron energy group from the above mentioned photon production matrices

$$(n\sigma)_{x,j}(\sigma_0 \rightarrow \infty, T) = \sum_{\kappa} M^{l=0}_{x,j\rightarrow\kappa}(\sigma_0 \rightarrow \infty, T)$$

$(n\sigma)_{x,j}$: photon production cross-section multiplied by the number of produced photons (multiplicity) n

x : reaction type

j : energy group of the neutron, that starts the reaction.

These data are printed out and stored on an external output file in descending order of energy group numbers. The energy groups, which could not be treated in NJOY because no data were found on the nuclear data file, are filled up with zeros, so that for all energy groups from NGRP (JP) to 1, one value is given out.

In addition JOYFOR-90 calculates normalized transfer matrices for photon production

$$P^{l}_{x,j\rightarrow\kappa} = \frac{M^{l}_{x,j\rightarrow\kappa}(\sigma_0 \rightarrow \infty, T)}{(n\sigma)_{x,j}(\sigma_0 \rightarrow \infty, T)} = \frac{M^{l}_{x,j\rightarrow\kappa}(\sigma_0 \rightarrow \infty, T)}{\sum_{\kappa} M^{l=0}_{x,j\rightarrow\kappa}(\sigma_0 \rightarrow \infty, T)}$$

For each Legendre order l these elements are printed out and stored on an external output unit in ascending order of neutron energy group numbers j and descending number of photon group numbers κ.

In the case that the partial inelastic data MT=51, 52, . . . 90, 91 are stored on the nuclear data file instead of the total inelastic scattering data MT=4, the inelastic scattering photon production cross-section is calculated as

$$(n\sigma)_{inel,j}(\sigma_0 \rightarrow \infty, T) = \sum_{I=51}^{90} \sum_{\kappa} M^{l=0}_{N(I),j\rightarrow\kappa}(\sigma_0 \rightarrow \infty, T) + \sum_{\kappa} M^{l=0}_{NCN,j\rightarrow\kappa}(\sigma_0 \rightarrow \infty, T)$$

N(I): Index indicating inelastic scattering to the first up to the 40th excited state

NCN: Index indicating inealstic scattering to the continuum

The same procedure is used, if instead of the (n,t) reaction type MT=105 the partial types MT=741 . . . 758 or instead of the (n,α) reaction type MT=107 the partial types MT=781 . . . 798 are stored on the nuclear data library:

$$(n\sigma)_{(n,t),j}(\sigma_0 \rightarrow \infty, T) = \sum_{I=MT741}^{MT758} \sum_{\kappa} M^{l=0}_{I,j\rightarrow\kappa}(\sigma_0 \rightarrow \infty, T)$$

or

$$(n\sigma)_{(n,\alpha),j}(\sigma_0 \rightarrow \infty, T) = \sum_{I=MT781}^{MT798} \sum_{\kappa} M^{l=0}_{I,j\rightarrow\kappa}(\sigma_0 \rightarrow \infty, T) \quad ,$$

respectively.

For the (n,t)- and the (n,α)-reaction the partial photon production group cross-sections as well as the summed group cross-sections with the names NTS or NAS, respectively, are given out on the print output and on the external output unit.
The normalized matrix elements for photon production for the summed up data types are calculated as follows:

$$P^{l}_{inel,j\rightarrow\kappa} = \frac{\sum\limits_{I=51}^{90} M^{l}_{N(I),j\rightarrow\kappa}(\sigma_0\rightarrow\infty,T) + M^{l}_{NCN,j\rightarrow\kappa}(\sigma_0\rightarrow\infty,T)}{(n\sigma)_{inel,j}(\sigma_0\rightarrow\infty,T)}$$

$$P^{l}_{(n,t),j\rightarrow\kappa} = \frac{\sum\limits_{I=MT741}^{MT758} M^{l}_{I,j\rightarrow\kappa}(\sigma_0\rightarrow\infty,T)}{(n\sigma)_{(n,t),j}(\sigma_0\rightarrow\infty,T)}$$

$$P^{l}_{(n,\alpha),j\rightarrow\kappa} = \frac{\sum\limits_{I=MT781}^{MT798} M^{l}_{I,j\rightarrow\kappa}(\sigma_0\rightarrow\infty,T)}{(n\sigma)_{(n,\alpha),j}(\sigma_0\rightarrow\infty,T)}$$

For the (n,t)- and the (n,α)-reaction the partial normalized matrices for photon production as well as the summed up matrices with the names PNTS or PNAS respectively are given out on the print output and on the external output unit.

In addition photon production group cross-sections NCAPT and normalized matrix elements PNCAPT for neutron disappearance are calculated in JOYFOR-90 as sum of all photon reaction types MT = 102 to MT = 114 i.e. the reactions (n,γ), (n,p), (n,d), (n,t), (n,He3), (n,α), (n,2α), (n,3α), (n,2p), (n,p + α), (n,t + 2α), and (n,d + 2α).

$$(n\sigma)_{capt,j}(\sigma_0\rightarrow\infty,T) = \sum_{I=MT102}^{MT114} \sum_{\kappa} M^{l=0}_{I,j\rightarrow\kappa}(\sigma_0\rightarrow\infty,T)$$

$$P^{l}_{capt,j\rightarrow\kappa} = \frac{\sum\limits_{I=MT102}^{MT114} M^{l}_{I,j\rightarrow\kappa}(\sigma_0\rightarrow\infty,T)}{(n\sigma)_{capt,j}(\sigma_0\rightarrow\infty,T)}$$

For the calculation of $(n\sigma)_{capt}$ and P^{l}_{capt} it is considered that type MT = 105 and/or MT = 107 may not be found directly on the nuclear data file but only the partials. In principle the (n,p) reaction type MT = 103 may also be stored as partials MT = 701 to MT = 718, the (n,α) reaction type MT = 104 as partials MT = 721 to MT = 738, and the (n,He-3) reaction type MT = 106 as partials MT = 761 to MT = 778. In these cases the partial photon production group cross-sections and matrices for the (n,p)-, (n,d)-, and (n,He-3)-reactions are entered into $(n\sigma)_{capt}$ and P^{l}_{capt} and are printed out and stored on the external output unit but the summed types are not explicitly calculated.

As no photons are produced by elastic scattering of neutrons, the total photon production group constants are identical to the nonelastic group constants for photon production:

$$M^{l}_{NNONL,j\to\kappa} = \sum_{x} M^{l}_{x,j\to\kappa} \left[= M^{l}_{tot,j\to\kappa} \right] .$$

Here $\sum_{x}$ means the summation for all reactions except nonelastic.

$M^{l}_{x,j\to\kappa}$ is the photon production matrix as calculated in NJOY.

On the JEF-1 library the nonelastic photon production cross-section (MT=3) is not given in the entire energy range for all isotopes. Therefore, two additional total group cross-sections, SUM and SUM1, are calculated in JOYFOR-90 from partial photon production cross-sections

$$(n\sigma)_{SUM,j}(\sigma_0\to\infty, T) = (n\sigma)_{NNONL,j}(\sigma_0\to\infty, T)$$

in those energy groups j with

$$(n\sigma)_{NNONL,j}(\sigma_0\to\infty, T) > 0 \quad ;$$

otherwise

$$(n\sigma)_{SUM,j}(\sigma_0\to\infty, T) = \sum_{x} (n\sigma)_{x,j}(\sigma_0\to\infty, T)$$

for all reactions x except nonelastic

and

$$(n\sigma)_{SUM1,j}(\sigma_0\to\infty, T) = \sum_{x} (n\sigma)_{x,j}(\sigma_0\to\infty, T)$$

for all reactions x except nonelastic.

The corresponding normalized photon production matrices are

$$P^{l}_{SUM,j\to\kappa} = \frac{M^{l}_{NONL,j\to\kappa}(\sigma_0\to\infty, T)}{(n\sigma)_{NNONL,j}(\sigma_0\to\infty, T)}$$

in those energy groups j with

$$\sum_{\kappa} M^{l}_{NNONL,j\rightarrow\kappa}(\sigma_0\rightarrow\infty, T) > 0 \quad ,$$

otherwise

$$P^{l}_{SUM,j\rightarrow\kappa} = \frac{\sum_{x} M^{l}_{x,j\rightarrow\kappa}(\sigma_0\rightarrow\infty, T)}{(n\sigma)_{SUM,j}(\sigma_0\rightarrow\infty, T)}$$

and

$$P^{l}_{SUM1,j\rightarrow\kappa} = \frac{\sum_{x} M^{l}_{x,j\rightarrow\kappa}(\sigma_0\rightarrow\infty, T)}{(n\sigma)_{SUM1,j}(\sigma_0\rightarrow\infty, T)}$$

for all reactions x except nonelastic. In these group constants too it is considered that the reaction types MT=4, 103, 104, 105, 106, and 107 may not be stored directly on the nuclear data file but may be described by partial types. The user has to decide in the input of program MITRA, in which energy groups the total photon production group constants are described by type NNONL, SUM or SUM1 respectively.

3.5 Resonance selfshielding factors and group cross-sections for photon production for infinite dilution

For the calculation of macroscopic composition dependent group constants for photon production it is necessary to have resonance selfshielding factors for photon production from fission-(MT=18), from (n,γ)-(MT=102), and from nonelastic reactions (MT=3). The photon production selfshielding factors for fission- and (n,γ)-reactions correspond to the selfshielding factors for neutron reactions. Only the selfshielding factors for the nonelastic reaction have to be calculated additionally in JOYFOR-90.

$$f_{(MT=3),j}(\sigma_0, T) =$$

$$\frac{\sigma_{(MT=1),j}(\sigma_0\rightarrow\infty, T) * f_{(MT=1),j}(\sigma_0, T) - \sigma_{(MT=2),j}(\sigma_0\rightarrow\infty, T) * f_{(MT=2),j}(\sigma_0, T)}{\sigma_{(MT=1),j}(\sigma_0\rightarrow\infty, T) - \sigma_{(MT=2),j}(\sigma_0\rightarrow\infty, T)}$$

where $\sigma_{(MT=1),j}(\sigma_0 \rightarrow \infty, T)$ is the total group cross-section

$\sigma_{(MT=2),j}(\sigma_0 \rightarrow \infty, T)$ is the elastic group cross-section

$f_{(MT=1),j}(\sigma_0, T)$ is the total flux-weighted selfshielding factor

$f_{(MT=2),j}(\sigma_0, T)$ is the flux-weighted selfshielding factor for elastic scattering

The nonelastic group cross-section for infinite dilution is calculated as the difference between the total and the elastic group cross-section

$$\sigma_{(MT=3),j}(\sigma_0 \rightarrow \infty, T) = \sigma_{(MT=1),j}(\sigma_0 \rightarrow \infty, T) - \sigma_{(MT=2),j}(\sigma_0 \rightarrow \infty, T)$$

3.6 Group constants for reactions induced by photons (photon interactions)

The basic data for the calculation of photon interaction group constants are stored on a photon interaction file, actually the DLC99/HUGO file which is distributed by the N.E.A. Data Bank. From this file the NJOY module GAMINR calculates photon interaction group cross-sections - independent of dilution and temperature - and photon interaction matrices.
DLC99/HUGO contains photon interaction data for the following reactions:

MT=501 : total photon interaction cross-section.
MT=502 : cross-section for coherent photon scattering.

In the coherent scattering process the photon interacts with a tightly bound electron of the atomic shell. The photon exchanges energy and momentum with the atom as a whole, the atom stays in the ground state. The kinetic energy of the photon remains practically unchanged, the direction of the photon may be changed (see e.g. /17/, /18/, /19/). Coherent scattering is elastic scattering of the photon by the atom.
The energy loss of the photon will be discussed in the following paragraph.

MT=504 : cross-section for incoherent photon scattering. In the incoherent scattering reaction (Compton Effect) the photon exchanges momentum and energy with an electron of the atomic shell. The atom is trans-

formed into an excited state, the kinetic energy of the photon may be considerably reduced. Incoherent scattering is inelastic scattering of the photon by the atom.
The energy hv of a photon scattered by a free electron is given in /18/ by the following formula

$$hv = \frac{hv_0}{1 + 2\,\frac{hv_0}{m_0 c^2}\,\sin^2(\phi/2)}$$

where

h: Planck's constant

c: velocity of light

hv: energy of the scattered photon

hv_0: energy of the photon before scattering

m_0: rest mass of the electron

ϕ: scattering angle of the photon

If the binding energy of the electron in the atomic shell is small compared to the kinetic energy of the photon, incoherent scattering is the main photon scattering reaction; the energy loss of the photon can be described by the formula given above. If the kinetic energy of the photon is much smaller than the binding energy of the electron, the photon interacts with the atom as a whole (coherent scattering). In this case m_0 in the formula has to be replaced by the rest mass of the atom, M_0 /17/. The second term in the denominator then becomes very small compared to 1, so that hv is almost equal to hv_0.

Incoherent scattering mainly occurs, when the photon incident energy is high, coherent scattering is predominant at low photon incident energies, especially for heavy atoms.

MT=515 : pair production in the field of the electron shell

MT=516 : pair production (sum of the reactions MT=515 and MT=517)

MT = 517 : pair production in the field of the atomic nucleus

In the pair production reaction an electron-position-pair is generated by the photon. The threshold energy of this reaction is 1.02 MeV (corresponding to twice the electron rest mass). The process of pair production is followed by a second process, in which generally two photons are produced with 0.51 MeV of kinetic energy each, the excess energy is transferred to a nucleus /18/.

MT = 602 : photoelectric effect (a photon is being absorbed; an electron is released from the atomic shell). This reaction will also be called photon absorption in the following.

Figures 2, 3, and 4 show the photon interaction cross sections (coherent scattering, incoherent scattering, photon absorption, and pair production) for Li, Pb, and U, respectively, as a function of the energy of the incident photons. On Fig. 5 the coherent scattering cross section is shown for atoms with different numbers of shell electrons: Li, Fe, Zr, Pb, and U. On Figures 6, 7, and 8 the cross sections for incoherent scattering, photon absorption, and pair production, respectively, are presented in the same way.

JOYFOR-90 reads the group cross-sections for all data types mentioned above (if the initial data are stored on the photon interaction file) from the vector block of the MATXS output file, prints these values, and writes them on the external output unit. The energy groups, which could not be treated in NJOY because no data could be found on the photon interaction file, are filled up with zeros, so that for all photon energy groups one value is given out.

Additionally the number of photons generated by pair production (MT = 515, 517, and 516) and the normalized photon interaction matrices are calculated and given out.

The number $n_{x,\kappa}$ of photons generated by pair production is calculated by the following formula:

$$n_{x,\kappa} = \frac{\sum_{\lambda} M^{l=0}_{x,\kappa\rightarrow\lambda}}{\sigma_{x,\kappa}}$$

where

$\sigma_{x,\kappa}$	:	photon interaction cross-section for reaction x
x	:	reaction type MT=515, MT=517, and MT=516
$M^l_{x,\kappa\rightarrow\lambda}$	:	photon interaction matrix
κ	:	number of the energy group of the photon before the reaction
λ	:	number of the energy group of the photon after the reaction
l	:	Legendre order

(In our test calculations we found $n_{x,\kappa} = 2$)

The normalized photon interaction matrices of all reactions x are calculated in JOYFOR-90 from the elements of the photon interaction matrix as calculated in module GAMINR in NJOY

$$P^l_{x,\kappa\rightarrow\lambda} = \frac{M^l_{x,\kappa\rightarrow\lambda}}{\sum_\lambda M^{l=0}_{x,\kappa\rightarrow\lambda}}$$

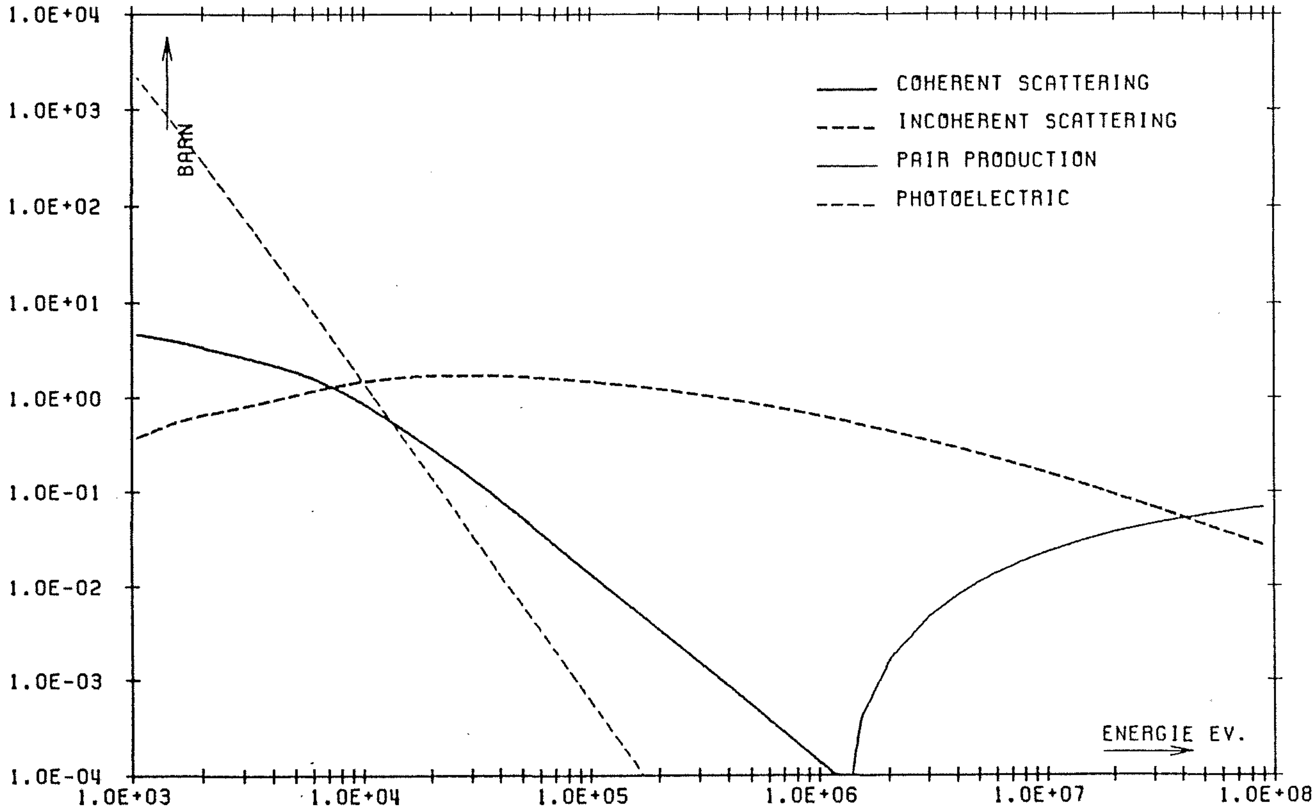

FIG. 2 PHOTON INTERACTION CROSS SECTIONS FOR LI FROM DLC99/HUGO

KfK INR

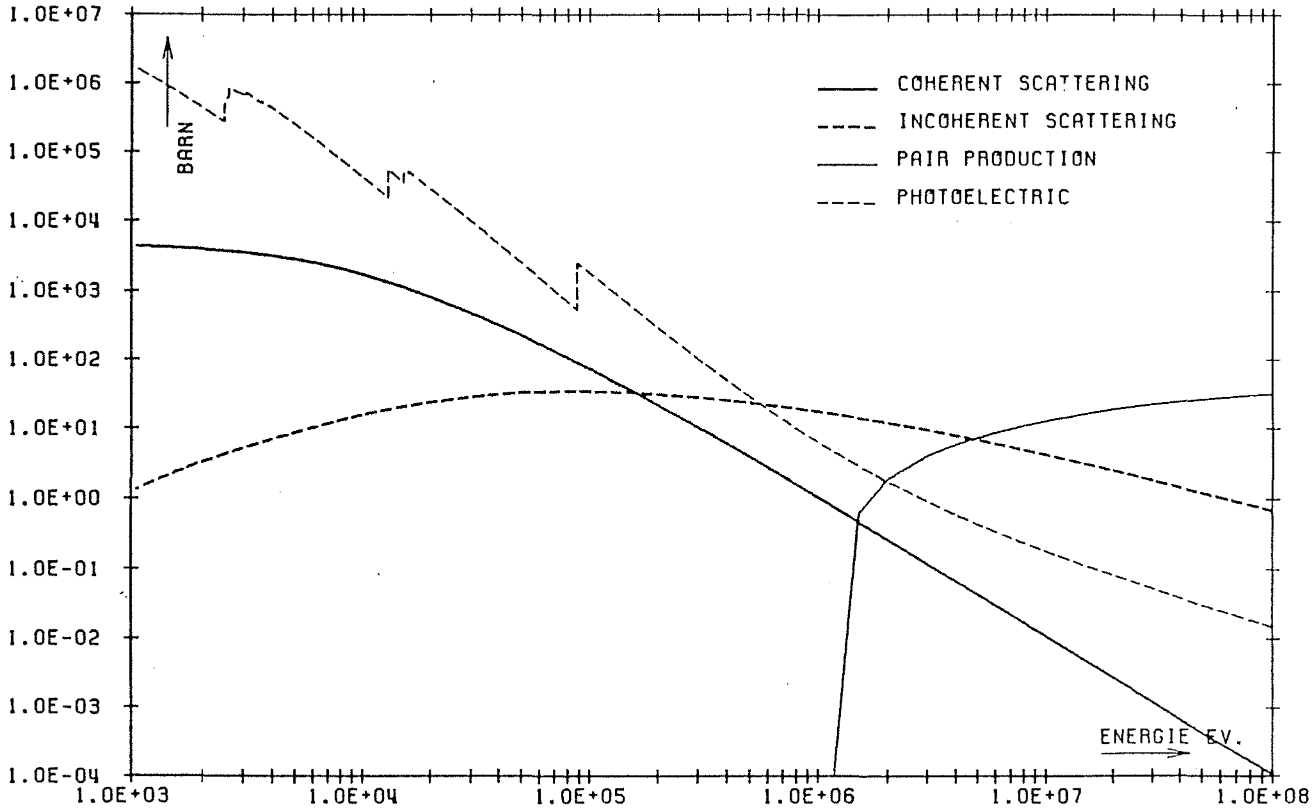

FIG. 3 PHOTON INTERACTION CROSS SECTIONS FOR PB FROM DLC99/HUGO

KfK INR

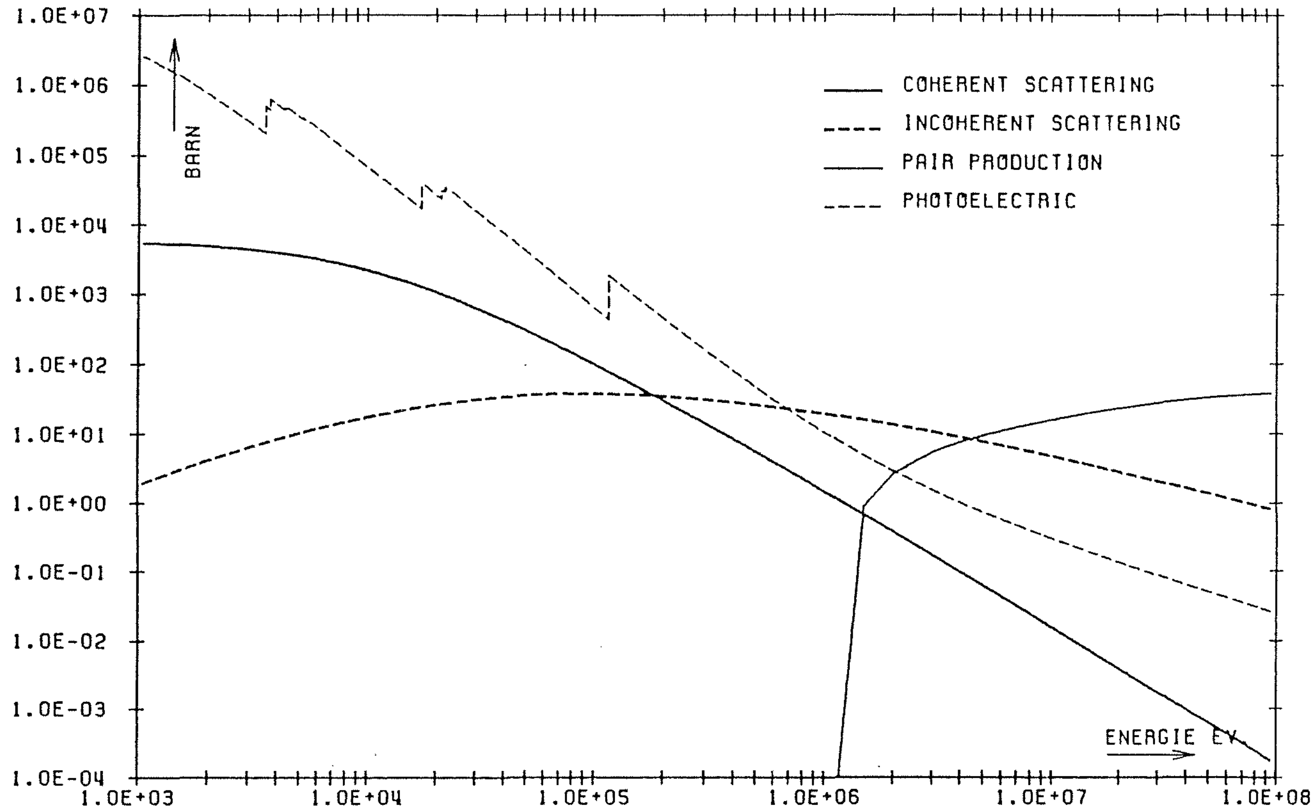

FIG. 4 PHOTON INTERACTION CROSS SECTIONS FOR U FROM DLC99/HUGO

KfK INR

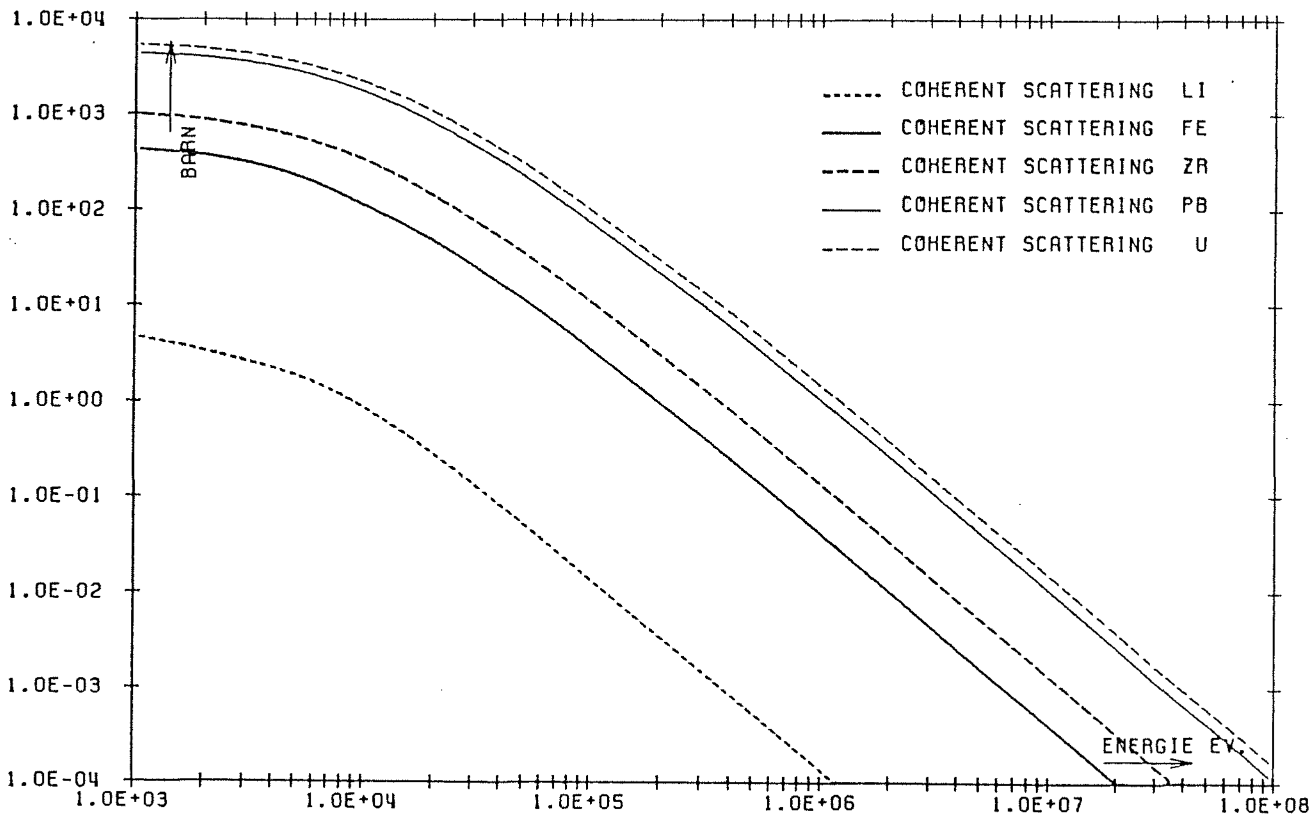

FIG. 5 COHERENT SCATTERING CROSS SECTIONS FROM DLC99/HUGO

KfK INR

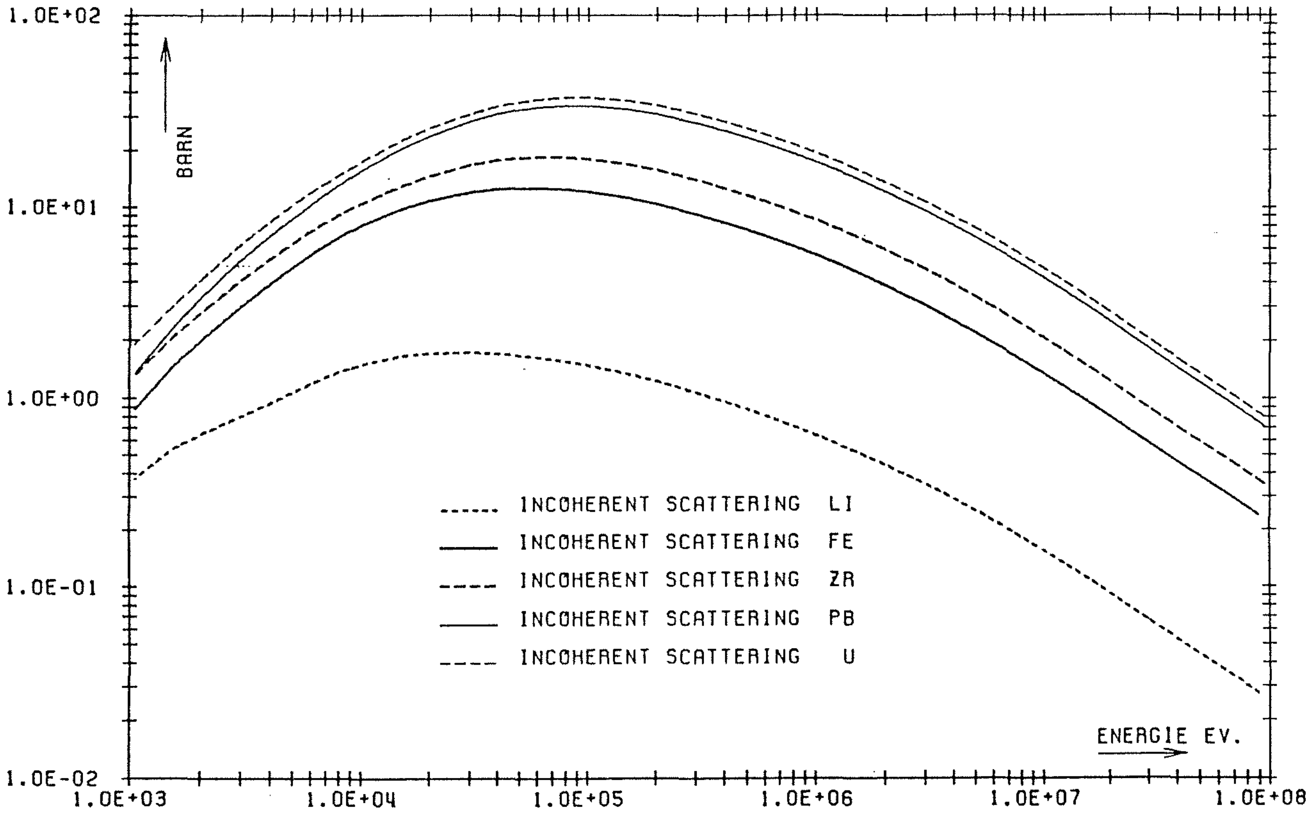

FIG. 6 INCOHERENT SCATTERING CROSS SECTIONS FROM DLC99/HUGO

KfK INR

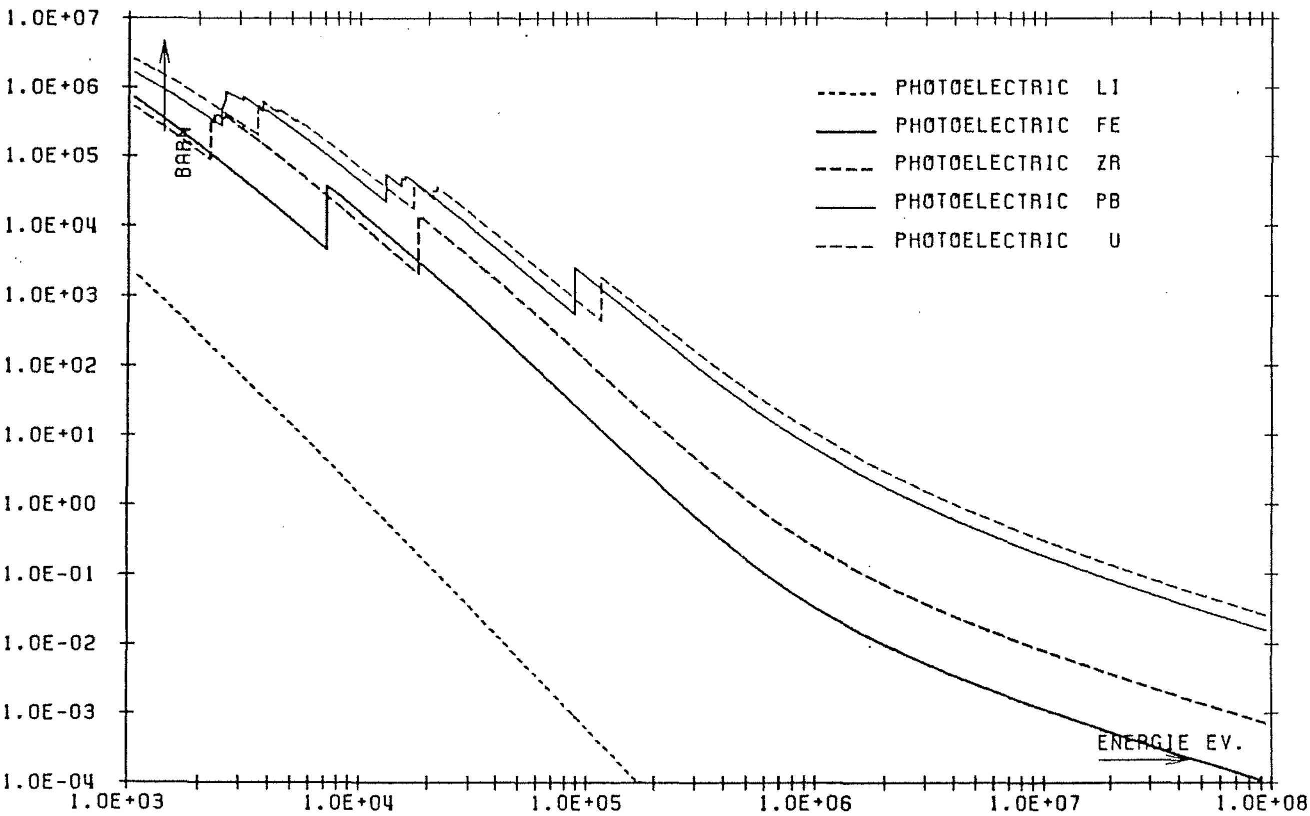

FIG. 7 PHOTOELECTRIC CROSS SECTIONS FROM DLC99/HUGO

KfK INR

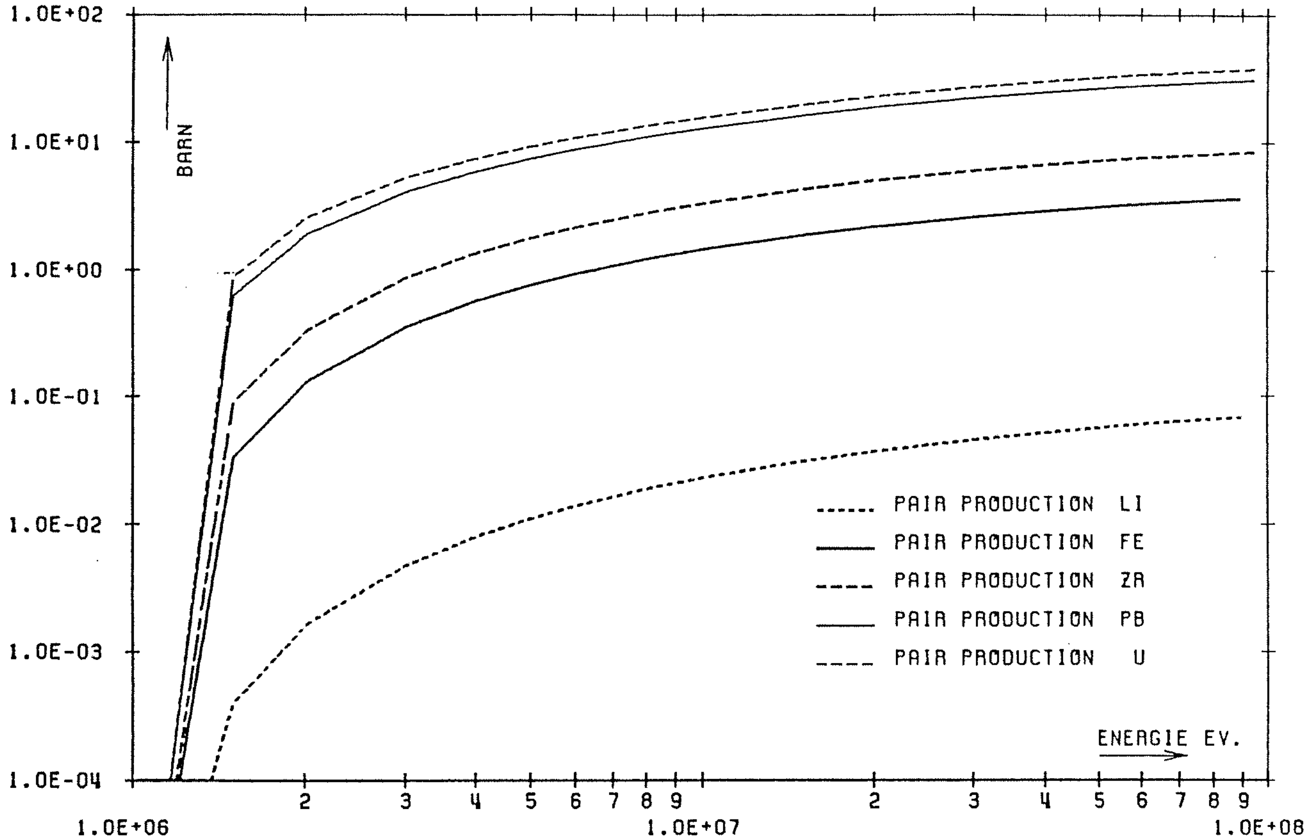

FIG. 8 PAIR PRODUCTION CROSS SECTIONS FROM DLC99/HUGO

KfK INR

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,(D(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 and reaction type 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 for neutron reactions

1st record: 0 , 'INFDILUT'

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

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

4th record: N , neutron group cross-sections of the type defined by the 3rd and 4th word in the 3rd record, for all energy groups specified by the 2nd record at the lowest temperature and highest σ_0-value given in the input of NJOY. 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 group of highest energy), 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 for neutron interaction and photon production

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, SIGMANO

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

. .
. .
. .

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

In this and the following chapters

outscattering group means: energy group of the particle (neutron or photon), that initiates the reaction

and

inscattering group means: energy group of the particle (neutron or photon), that is produced by the reaction.

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 flux weighted total elastic cross-section NELAS for the selected submaterial, group averaged cosine for elastic scattering MUBAR calculated directly from nuclear data, group averaged Φ_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).

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 one Legendre moment.
This procedure is repeated for all Legendre moments.

4.7 Group constants for photon production

1st record: 0, 'GPRODCS_'

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

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

4th record: N, photon production group cross-sections of the type defined by the 3rd and 4th word in the 3rd record at the lowest temperature and infinite dilution. The values are ordered with increasing energies and decreasing group numbers.

* Only Φ_0 (flux-) and Φ_1 (current-) weighted total cross-sections are calculated by NJOY. These data are printed and given out on the external ouput unit. For l > 1 current-weighted total cross-sections are only given out as a list.

5th record:	0,	name of the reaction type with the character 'P' in the first byte (8 byte, alphanumeric)
6th record:	N,	material name, number of neutron outscattering groups, number of photon inscattering groups, number of Legendre moments
7th record:	N,	Legendre order, outscattering group, elements of the photon production matrix in ascending order of inscattering group numbers

The 7th record is repeated for all outscattering groups in ascending order of outscattering group numbers. Records 5 to 7 are repeated for all Legendre orders. Records 1 to 7 are repeated for all reaction types.

4.8 Group cross-sections for photon interactions

1st record:	0,	'GSCAT___'
2nd record:	N,	highest photon energy group (lowest group number), lowest photon energy group (highest group number)
3rd record:	N,	material name, name of the photon interaction reaction type (8 byte, alphanumeric)
4th record:	N,	photon interaction group cross-sections for the above mentioned reaction type in descending order of photon energy group numbers

Records 2 to 4 are repeated for all reaction types.

4.9 Transfer matrices for photon interactions

1st record:	0,	'GSCATM__'

Only in the case of pair production types records 2 to 4

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

3rd record: N, material name, name of the pair production (i.e. NANZ515, NANZ516, NANZ517) (8 byte, alphanumeric)

4th record: N, number of generated photons in each photon energy group in descending order of energy group numbers

5th record: N, material name, name of the photon interaction type with the character 'P' in the first byte and the Legendre order in the eighth byte (8 byte, alphanumeric), number of photon outscattering groups, number of Legendre moments

6th record: N, Legendre order, photon outscattering group, elements of the photon interaction matrix in ascending order of inscattering group numbers

The 6th record is repeated for all photon outscattering groups in ascending order of energy group numbers. Records 2 to 6 or 5 to 6 respectively are repeated for all photon interaction reaction types.

5. Input description for program JOYFOR-90

1. card

FFP — 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.

NMATXS — 1: The MATXS input file will be printed out on unit 6.
0: The file will not be printed.

For each material and each data type (data types are e.g. neutron interaction, photon production, and photon interaction, see chapter 2, file control and file data) the following input cards have to be repeated:

2. card

NGRUP — Number of energy groups used in NJOY.

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 σ_0-value) will be prepared for transfer to the group constant library.

4. card (only if INP = 1)

ISM — Number of the selected submaterial.

<u>DD-cards necessary for a start of JOYFOR-90</u>

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 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. Besides a compact list of messages referring to the f-factors is given out on unit 6.

Example for a JOYFOR-90-job

```
// Jobcard with REGION=2048K
// EXEC F7CG PARM.C='DC(LAB)',PARM.G='SIZE=2000K'
//C.SYSPRINT DD DUMMY
//C.SYSIN DD DSN=TSO017.JOYFOR90.FORT,DISP=SHR,LABEL=(,,,IN)
//G.FT01F001 DD DSN= .....,DISP=SHR
//G.FT03F001 DD UNIT=DISK,VOL=SER=BAT00X,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 *
1.02    0
28
 0
28
 0
12
 0
//
```

Comment: This JOYFOR-90 run has to be preceded by an NJOY run preparing 3 data types: neutron interaction group constants in 28 neutron energy groups, group constants for photon production also in 28 neutron energy groups, and group constants for photon interactions in 12 photon energy groups.

6. Explanation of the type names used in the JOYFOR-90 output

The names of the neutron 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 neutron group cross-sections are explained. In parenthesis the corresponding MFD- and MTD-numbers, used in the GROUPR input of NJOY, are indicated.

NWT0,NWT1: flux- and current-weighted components of the library weight function /11/, see also 3.3.4. 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)

NNA: (n,n' + α)-cross-section (MFD = 3,MTD = 22)

NNP: (n,n' + p)-cross-section (MFD = 3,MTD = 28)

MT--46: (n,2n)-cross-section for first excited state describing the second neutron (MFD = 3,MTD = 46)

MT--47: (n,2n)-cross-section for second excited state describing the second neutron (MFD = 3,MTD = 47)

MT--48: (n,2n)-cross-section for third excited state describing the second neutron (MFD = 3,MTD = 48)

MT--49: (n,2n)-cross-section for fourth excited state describing the second neutron (MFD = 3,MTD = 49)

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,γ) radiative capture cross-section,
MTD = 103 : (n,p)-cross-section,
MTD = 104 : (n,d)-cross-section,
MTD = 105 : (n,t)-cross-section,
MTD = 106 : (n,He3)-cross-section,
MTD = 107 : (n,α)-cross-section
MTD = 108 : (n,2α)-cross-section,
MTD = 109 : (n,3α)-cross-section,
MTD = 110 : not assigned,
MTD = 111 : (n,2p)-cross-section,
MTD = 112 : (n,p + α)-cross-section,
MTD = 113 : (n,t + 2α)-cross-section, and
MTD = 114 : (n,d + 2α)-cross-section))

NG: (n,γ)-cross-section (MFD = 3,MTD = 102)

NP: (n,p)-cross-section (MFD = 3,MTD = 103)

ND: (n,d)-cross-section (MFD = 3,MTD = 104)

NT: (n,t)-cross-section (MFD = 3,MTD = 105)

NA: (n,α)-cross-section (MFD = 3,MTD = 107)

* In MIGROS /9/ this type is called capture cross-section (SGC).

N.H3: total tritium production (MFD = 3,MTD = 205)

N.HE4: total ^{4}He production (MFD = 3,MTD = 207)

MUBAR: average cosine of the scattering angle for elastic scattering (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: nonelastic 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 cross-section (eV*barn)(MFD = 3, MTD = 444).NDAME can be used to calculate DPA (displacements per atom)

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 for neutron reactions and for photon production, 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,γ)-cross-section for infinite dilution depending on T (MFD = 3,MTD = 102)

SIGMA-N: neutron elastic scattering cross-section for infinite dilution depending on T (MFD = 3,MTD = 2)

SIGMA-F: total neutron fission cross-section for infinite dilution depending on T (MFD = 3,MTD = 18)

SIGMAN1: current-weighted neutron elastic scattering cross-section for infinite dilution depending on T (set equal 0 by JOYFOR-90, see 3.2) (MFD = 3,MTD = 2)

SIGMAT1: current-weighted neutron total cross-section for infinite dilution depending on T (MFD = 3,MTD = 1)

SIGMANO: flux-weighted nonelastic photon production cross-section for infinite dilution depending on T as difference of the flux-weighted total and the flux-weighted neutron elastic cross-section

FG: flux-weighted resonance selfshielding factor for radiative capture (n,γ) (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-90, see 3.2)

FT1: current-weighted total resonance selfshielding factor (see 3.2)

FNON: flux-weighted selfshielding factor for nonelastic photon production (see 3.5)

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)

The photon production group cross-sections and normalized photon production matrices are given out with the following type names (all photon production cross-sections are multiplied by the number of photons produced by the reactions, see 3.4):

NNONL, SUM, SUM1:

nonelastic (total) photon production cross-section (see 3.4)

PNNONL_I, PSUM___I, PSUM1__I:

total photon production matrix for Legendre order I (see 3.4)

NINEL: photon production cross-section for inelastic neutron scattering

PNINEL_I: photon production matrix for the neutron inelastic scattering for Legendre order I (see 3.4)

N2N: photon production cross-section for the (n,2n)-reaction

PN2N___I: photon production matrix for the (n,2n)-reaction for Legendre order I

N3N: photon production cross-section for the (n,3n)-reaction

PN3N___I: photon production matrix for the (n,3n)-reaction for Legendre order I

NFTOT: photon production cross-section for fission

PNFTOT_I: photon production matrix for fission for Legendre order I

NNA: photon production cross-section for the (n,n' + α)-reaction

PNNA___I: photon production matrix for the (n,n' + α)-reaction for Legendre order I

NNP: photon production cross-section for the (n,n' + p)-reaction

PNNP___I: photon production matrix for the (n,n' + p)-reaction for Legendre order I

NG:	photon production cross-section for the (n,γ)-reaction
PNG____I:	photon production matrix for the (n,γ)-reaction for Legendre order I
NP:	photon production cross-section for the (n,p)-reaction
PNP____I:	photon production matrix for the (n,p)-reaction for Legendre order I
ND:	photon production cross-section for the (n,d)-reaction
PND____I:	photon production matrix for the (n,d)-reaction for Legendre order I
NT:	photon production cross-section for the (n,t)-reaction
PNT____I:	photon production matrix for the (n,t)-reaction for Legendre order I
NHE3:	photon production cross-section for the (n,He-3)-reaction
PNHE3__I:	photon production matrix for the (n,He-3)-reaction for Legendre order I
NA:	photon production cross-section for the (n,α)-reaction
PNA____I:	photon production matrix for the (n,α)-reaction for Legendre order I
NCAPT:	photon production cross-section for neutron disappearance as sum of the reaction types MT = 102 to MT = 114 (see also the definition of type NABS above in this section)
PNCAPT_I:	photon production matrix for neutron disappearance for Legendre order I

MT_701 to MT_718:	photon production cross-sections for the partial (n,p)-reactions
PMT_701I to PMT_718I:	photon production matrices for the partial (n,p)-reactions for Legendre order I
MT_721 to MT_738:	photon production cross-sections for the partial (n,d)-reactions
PMT_721I to PMT_738I:	photon production matrices for the partial (n,d)-reactions for Legendre order I
MT_741 to MT_758:	photon production cross-sections for the partial (n,t)-reactions
PMT_741I to PMT_758I:	photon production matrices for the partial (n,t)-reactions for Legendre order I
NTS:	photon production cross-section for the sum reaction MT_741 to MT_758 (instead of NT) (see 3.4)
PNTS___I:	photon production matrix for the sum reaction MT_741 to MT_758 for Legendre order I (instead of PNT____I) (see 3.4)
MT_761 to MT_778:	photon production cross-sections for the partial (n,He-3)-reactions
PMT_761I to PMT_778I:	photon production matrices for the partial (n,He-3)-reactions for Legendre order I
MT_781 to MT_798:	photon production cross-sections for the partial (n,α)-reactions
PMT_781I to PMT_798I:	photon production matrices for the partial (n,α)-reactions for Legendre order I
NAS:	photon production cross-section for the sum reaction MT_781 to MT-798 (instead of NA) (see 3.4)
PNAS___I:	photon production matrix for the sum reaction MT_781 to MT_798 for Legendre order I (instead of PNA____I) (see 3.4)

The photon interaction group constants are given out with the following type names:

GTOT0:	total group cross-section for photon interaction (MFD = 23,MTD = 501)
GCOH:	group cross-section for coherent scattering of photons (MFD = 23,MTD = 502)
GINCH:	group cross-section for incoherent scattering of photons (MFD = 23,MTD = 504)
MT_515:	group cross-section for pair production in the electron field (MFD = 23,MTD = 515)
GPAIR:	group cross-section for total pair production (MFD = 23,MTD = 516)
MT_517:	group cross-section for pair production in the nuclear field (MFD = 23,MTD = 517)
GABS:	group cross-section for photon absorption (photoelectric reaction) (MFD = 23,MTD = 602)
GHEAT:	total photon KERMA-factor (eV * barn) (MTD = 23,MFD = 621)
NANZ515:	number of photons generated by pair production in the electron field (MFD = 26,MTD = 515)
NANZ516:	number of photons generated by total pair production (MFD = 26,MTD = 516)
NANZ517:	number of photons generated by pair production in the nuclear field (MFD = 26,MTD = 517)
PGCOH__I:	normalized transfer matrix for coherent photon scattering for Legendre order I (MFD = 26,MTD = 502)
PGINCH_I:	normalized transfer matrix for incoherent photon scattering for Legendre order I (MFD = 26,MTD = 504)

PMT_515I: normalized transfer matrix for pair production in the electron field for Legendre order I (MFD=26,MTD=515)

GPAIR__I: normalized transfer matrix for total pair production for Legendre order I (MFD=26,MTD=516)

PMT_517I: normalized transfer matrix for pair production in the nuclear field for Legendre order I (MFD=26,MTD=517)

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