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SOKRATOR MANUAL

FORMAT OF THE RECOMMENDED NUCLEAR DATA LIBRARY  
FOR REACTOR CALCULATIONS

V.E. Kolesov and M.N. Nikolaev

Translated by the IAEA  
August 1977

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Note

This complete format description of the SOKRATOR library (Soviet Library of Evaluated Nuclear Data) is a translation from a Russian original ("Format of the Recommended Nuclear Data Library for Reactor Calculations" by V.E. Kolesov and M.N. Nikolaev, *Jadernye Konstanty* No. 8, part 4, 1972, p. 3) and its Supplement ("Changes in and Additions to the Format of the SOKRATOR Evaluated Nuclear Data Library" by M.N. Nikolaev, extract from *Jadernye Konstanty* No. 16, 1974). The translation of the supplement had already been published separately as INDC(CCP)-69 (1975).

Previous incomplete versions of the format description have been:

INDC(CCP)-24 (1972)  
INDC(CCP)-13 (1970)  
INDC(FR)-2 (1971) (comparison with the UKNDL format).

These are superseded by the present document.



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## FORMAT OF THE RECOMMENDED NUCLEAR DATA LIBRARY FOR REACTOR CALCULATIONS

V.E. Kolesov and M.N. Nikolaev

At present, most nuclear reactor calculations are performed by means of multigroup methods, and it is most likely that this practice will continue for a fairly long time to come. Until recently the preparation of multigroup constants required such a large expenditure of effort and time that the only practical possibility was to use systems of constants with fixed neutron energy ranges depending on the type of reactor being calculated. At the same time such an approach has a number of obvious disadvantages, arising from the non-universal nature of the systems of constants obtained as well as the technical difficulties involved in introducing changes.

The development of computer techniques has allowed a considerable degree of automation to be introduced into the process of converting a point set of recommended nuclear data into group constants with arbitrary energy divisions, and enables this process to be linked directly with multigroup programmes for reactor calculation. The basis for such an information processing system is a library of recommended nuclear data. Existing library formats for recommended nuclear data [1-4] allow storage of large volumes of different types of information in a form convenient for practical use. In particular, these formats allow the inclusion in the library of data on neutron and photon interactions with nuclei of different materials, as well as data on photon generation. This information makes it possible to solve on a computer a wide range of problems connected with neutron and photon transport.

The same nuclear-physical constants may be represented in various ways. Thus, in the resonance region for example, cross-sections may be represented as a detailed energy variation, as resonance parameters, or in sub-group form, with different numbers of sub-groups. The differential cross-sections for elastically scattered neutrons can also be specified in various ways: as an angular dependence or as expansions in Legendre polynomials. Here too a sub-group representation of the data is possible.

The choice of one or other type of data presentation is governed in practice by a number of different factors: the nature of the problem, considerations of convenience, the programmes available, etc. It is therefore desirable to design the library in such a way that information can be stored in different formats. For this purpose it is convenient to introduce into the storage system a special characteristic - namely a format type number.

This report discusses formats for the storage of recommended nuclear data for reactor calculations. These formats represent a generalization and extension of the English formats described in Ref. [2], which are used in a

number of laboratories abroad. An important feature of the formats proposed here is the introduction of a special classification of the information according to the type of representation. This makes the system of nuclear data storage more flexible and allows the capabilities of modern computers to be more fully utilized.

The present format for storing recommended nuclear data is a development of that proposed in Ref. [6].

#### Translator's note

The following identifier code equivalents have been used in this translation:

ИЯН	=	NIN
НТН	=	RTN
НОК	=	GCN
НЧК	=	PCN
НТН	=	FTN
БНФ	=	LFN
ИНТ	=	INT

### I. CLASSIFICATION OF NUCLEAR DATA

Nuclear data contained in the library are classified according to three criteria: the composition of the substance, the type of reaction, and the term of the data presentation.

First, the data entering the library are sub-divided according to the substances to which they refer. Each data set for a material of specific composition is characterized by a "nuclear identification number" (NIN) and represents a more or less independent body of information. Data having a particular NIN are further classified according to the types of reactions which can take place in the material and are assigned specific "reaction type numbers" (RTN). Finally, nuclear data with a given RTN are classified according to the way they are represented in the library, for which purpose they are given "form type numbers" (FTN).

#### I.1 Nuclear Identification Number (NIN)

Each NIN may comprise data on a given isotope, element, chemical compound, mixture, etc. Classification by NIN also makes it possible to include in the library various data sets for one and the same substance. These may be data from different compilations, or data obtained from basic library data by means of different processing programmes. When such data are entered into the library, they are assigned new NINs. In this way, the NIN characterizes the various systems of library data for different substances as well as for the same substance.

We have adopted the following NIN structure. NIN is a nine-figure integer,  $NIN = m_1m_2m_3m_4m_5m_6m_7m_8m_9$ , the last three places of which,  $m_7m_8m_9$ , are used for recording the atomic number of the isotope A, and places  $m_5$  and  $m_6$  for recording the charge number Z. If the data set relates to a natural mixture of isotopes, zeros are entered in places  $m_7m_8m_9$ . If it relates to a chemical compound, zeros are entered in  $m_5$  and  $m_6$ , and places  $m_7$ ,  $m_8$  and  $m_9$  are used for recording the serial number of the chemical compound.

The first four places are used to denote the serial number of the data set in the evaluated data library (library file number - LFN).

It was decided to keep the first thousand numbers in reserve. The second thousand numbers (from 1000 to 1999) are assigned to data sets relating exclusively to individual reactions, or data relating to limited energy ranges. This information is similar to that stored in the American ENDF/A library and is used to prepare the complete data sets required for reactor physics calculations. The second thousand numbers are allocated to the numbering of such data sets.

The numbers for data sets relating to different isotopes, elements or chemical compounds cannot be identical. Thus there can never be two sets of data with the same first four NIN digits (even if the subsequent digits differ). Thus the last five NIN places are used only for convenient identification of a data set, whereas the first NIN digit determines the type of data ( $m_1 = 1$  is an incomplete set,  $m_1 = 2$  is a complete data set; the meaning of the other possible values of  $m_1$  has not yet been fixed).

## I.2 Reaction Type Number (RTN)

Data which have the same NIN are sub-divided according to the reactions which occur in the material. The Reaction Type Number (RTN) is a five-digit decimal number divided into two parts: a two-digit "general classification number" (GCN) and a three-digit "particular classification number" (PCN).

The construction of the RTN from GCN and PCN give this nuclear reaction data classification system great flexibility. By means of the RTN, it is possible for example to combine into a single set, with a given NIN, both neutron data and data on photon production and photon interactions with matter. In practice, however, it is often more convenient to store these three types of data under three different NINs, especially since their energy ranges do not usually coincide.

Thus, with the NIN and the RTN, it is possible to have various arrangements of the data in the library. This possibility will be further extended by the introduction of the form type number (FTN).

### I.3 General Classification Number (GCN)

Classification by GCN divides data with a given NIN into groups according to type. The following GCNs are used for neutron data:

- 01 - neutron cross-sections
- 02 - angular distributions of secondary particles
- 03 - energy distributions of secondary particles
- 04 - energy-angular distributions in thermal-neutron scattering
- 05 - special quantities for neutrons ( $\bar{v}, \alpha, \eta, \beta_i$  etc.)

No further GCN assignments have yet been made. In particular, no GCNs have been assigned for photon interaction constants because we do not have any recommended data.

### I.4 Particular Classification Number (PCN)

The particular classification numbers specify nuclear interaction processes. Each PCN identifies one of the processes that may occur when neutrons or photons collide with matter. The table that follows lists the PCN assignments for neutrons and is based on the English classification system.

001	total
002	elastic scattering
003	nonelastic
004	inelastic scattering ( $n, n'$ )
005-014	inelastic scattering with excitation of the $i$ -th level of the target nucleus ( $i = 1, 2, \dots, 10$ )
015	inelastic scattering with excitation of other ("unresolved") levels of the target nucleus
016	( $n, 2n$ )
017	( $n, 3n$ )
018	fission [ $(n, f) + (n, n'f) + (n, 2nf) + \dots$ ]
019	( $n, f$ )
020	( $n, n'f$ )
021	( $n, 2nf$ )
022	( $n, n'\alpha$ )
023	( $n, n'3\alpha$ )
024	( $n, 2n\alpha$ )
025	( $n, 3n\alpha$ )
026	( $n, 2n$ ) isomeric state
027-100	reserved for other possible reactions leading to the production of secondary particles of the same type as the primary particles
101	total absorption (all reactions which do not lead to the emission of incident-type particles)

102	(n, $\gamma$ )
103	(n,p)
104	(n,d)
105	(n,t)
106	(n, $^3\text{He}$ )
107	(n, $\alpha$ )
108	(n, $2\alpha$ )
109-150	reserved for other possible reactions which do not lead to the production of secondary particles of the same type as the primary particles
151-200	in the English library these PCNs are used for classifying information on resolved and statistical resonances. The detailed meaning of the PCNs is directly related to the form of the data. We have not yet used these PCNs
201-999	reserved for a variety of other data which may be needed or which may occur in the future

It can be seen that a large number of PCNs have been left unassigned to allow for the future needs of the recommended nuclear data library.

In the English classification, PCNs 201-208 are used to identify such characteristics as transport and removal cross-sections,  $\bar{v}\bar{\sigma}_f$ , and a number of other derived quantities. PCNs 301 to 450 are assigned to parameters such as  $(\bar{\sigma}_k \bar{E}_k)$  which define the rate of energy release ( $\bar{E}_k$  is the average energy released in reaction k). These quantities are also derived from those defined by PCNs 001 to 150; the corresponding reaction is identified by subtracting 300 from this PCN. Thus 301 denotes the total rate of energy production whilst 302 denotes the energy released in elastic scattering.

Derived quantities are usually not contained in a library of recommended nuclear data, but can easily be obtained with the help of special programmes. It is therefore natural not to assign PCNs to these quantities (at least for the time being). It is probably more convenient to include such quantities in a group-constant library to be compiled from the detailed data library considered in this report by means of special processing programmes.

The reaction specification is such that the PCN enables the final product to be uniquely determined. Thus for  $^{12}\text{C}$ , the  $^{12}\text{C}(n,n')3\alpha$  reaction has PCN = 023 whilst the reaction  $^{12}\text{C}(n,n')^{12*}\text{C}(\gamma)^{12}\text{C}$  has PCN = 5 if the 4.43 MeV first excited state is considered. Similarly, for  $^{238}\text{U}$ , PCN = 016 indicates that  $^{237}\text{Np}+2n$  are the final products. Thus for any nuclear transmutation we can use the PCN to determine both the state of the residual nucleus and the type of particle emitted.

### Examples of Reaction Type Numbers

- 01001 - total neutron cross-section
- 01002 - elastic cross-section for neutrons
- 02018 - angular distributions of prompt fission neutrons
- 03016 - energy distribution of neutrons from the (n,2n) reaction
- 05018 - average number of neutrons per fission,  $\bar{\nu}$

### I.5 Form Type Number (FTN)

Since data can be represented in the library in a number of ways, the different forms are classified by a form type number (FTN). The use of the FTN allows various types of representation for data with the same FTN and thereby greatly enlarges the potential of the storage system.

The following modes of data representation are included:

- Detailed energy or angular dependence;
- Parametric representation, for example expansion in Legendre polynomials for the angular distributions;
- Sub-group data representation [5] with a variable number of neutron sub-groups.

In the sub-group representation, neutrons with a given energy are divided into N sub-groups. Each such sub-group (n), characterized by its cross-section value  $\sigma_n$ , has a weight  $a_n$  such that

$$\sum_{n=1}^N a_n = 1.$$

The sub-group representation is a convenient method of quoting the data in the region of unresolved resonances. In this case  $a_n$  may be regarded as the probability that the total cross-section will be equal to  $\sigma_n$  for the energy E under consideration. Sub-group representation can also be used for resolved resonances provided that a detailed energy dependence curve for the data in the relevant energy range is not required.

This format assumes that there is complete correlation between the total and partial sub-group cross-sections, i.e. that neutrons of a given sub-group n have not only an identical total cross-section  $\sigma_n$  but also identical partial cross-sections  $\sigma_{nm}$ . If this approximation is not valid, the sub-group method becomes unusable.

For the angular and energy distributions of secondary particles we can use various modes of representation which reflect the type of mechanism involved in the given nuclear reaction. The FTN classification assumes that the angular and energy distributions are constructed in the form of a superposition of these representation modes with the appropriate probability assigned to each.

In addition, the FTN makes possible a more flexible arrangement of the data stored in the library. In particular, it becomes possible to make any desired changes in the number and priority of the variables (parameters) on which the library data depend.

The FTN is designed to allow not only different modes of data presentation in the library (discrete points, parametric representation, etc.) but also different hierarchies among the variables on which the data depend. Generally speaking, the structure of the FTN depends on the RTN and is governed by the GCN. Thus, for any GCN, the FTN is adequately defined by a three-digit number (FTN =  $n_1 n_2 n_3$ ) whose components assume different meanings depending on the GCN. Supplementary information to specify the FTN more exactly is provided in some cases. The identification of the FTN components and the supplementary information will be considered during the discussion of data formats for the appropriate GCN.

### I.6 Presentation of cross-sections by means of resonance parameters

Only the format for Breit-Wigner resonance parameters has so far been defined. Formats for recording the parameters used in other equations will be developed as programmes based on these equations are compiled and used for calculating cross-sections.

Our format is based on that used by the UK Resonance Parameter Library RPL [7], modified to fit the general requirements of the SOKRATOR library format. The modifications, however, are such that the numerical data on resonance parameters can be fully converted from one format to the other with the aid of a simple programme. Unlike RPL, however, the format of the basic SOKRATOR Library does not provide for the storage of auxiliary information (reference to the evaluation report, date and place of the evaluation and other alphabetical information); such information can be put in a library of textual commentaries parallel to the main library.

#### I.6.1 Breit-Wigner formula

Scattering cross-section:

$$\sigma_{nn}(E) = \pi \lambda^2 \sum_{j_1 \pi} g_{j_1} \left[ \sum_{l=0}^{L_{nl}} \left\{ \sin^2 \gamma_{cy} + \sum_{r=1}^N B_r(E) \left[ \Gamma_{rn} \Gamma_{rne} \cos 2 \gamma_{cy} - 2 \Gamma_{rx} \Gamma_{rne} \sin^2 \gamma_{cy} + 2(E-E_r) \Gamma_{rne} \sin 2 \gamma_{cy} \right] \right\} + \sum_{r=1}^N B_r(E) \left[ \Gamma_r \alpha_r - 2(E-E_r) B_r \right] \Gamma_{rn} + \sigma_{nn}^{nab}(E) \right] \quad (1)$$

Reaction cross-section (n,R)

$$\sigma_{nr}(E) = \pi \lambda^2 \sum_{j_1 \pi} g_{j_1} \sum_{r=1}^N \Gamma_{rn} \Gamma_{re} B_r(E) + \sigma_{nr}^{nab}(E) \quad (2)$$

Total cross section

$$\hat{\sigma}_{nr}(E) = \hat{\sigma}_{nn}(E) + \sum_R \hat{\sigma}_{nR}(E). \quad (3)$$

The following notation is used here:

$$B_r(E) = \frac{1}{(E - E_r')^2 + \Gamma_r^2/4}, \quad (4)$$

$$\mathcal{L}_r = \frac{1}{2} \sum_{s \neq r} \frac{\Gamma_{sn}(\Gamma_s + \Gamma_p)}{D_{sr}}, \quad (5)$$

$$\beta_r = \sum_{s \neq r} \frac{\Gamma_{sn}(E_s' - E_r')}{D_{sr}}, \quad (6)$$

$$D_{sr} = (E_s' - E_r')^2 + \frac{1}{4}(\Gamma_s + \Gamma_r)^2, \quad (7)$$

$$\Gamma_{rn} \equiv \Gamma_{rn}(E) = \sum_{\ell=L_1}^{L_2} \Gamma_{rnl}(E) \quad \text{is the total neutron width} \quad (8)$$

$$\Gamma_{rx} \equiv \Gamma_{rx}(E) = \sum \Gamma_{rx}(E) \quad \text{is the width of inelastic interactions} \quad (9)$$

$$\Gamma_r \equiv \Gamma_r(E) = \Gamma_{rn}(E) + \Gamma_{rx}(E) \quad \text{is the total width} \quad (10)$$

Effective resonance energy  $E_r'$ :

$$E_r' = E_r + \frac{1}{2} \sum_{\ell=L_1}^{L_2} \left[ \mathcal{J}_\ell(|E_r|) - \mathcal{J}_\ell(E) \right] \Gamma_{rnl}(|E_r|) / \rho_\ell(|E_r|) + \frac{1}{2} \sum_R \left[ \mathcal{J}_R(|E_r|) - \mathcal{J}_R(E) \right] \cdot \Gamma_{rR}(|E_r|) / \rho_R(|E_r|). \quad (11)$$

For  $\ell = 0$ , the  $S_\ell$  are independent of  $E$ . The  $S_R$  are usually taken to be constant in the other reactions as well. If, as is done here,  $S$  is given for  $E = E_r$ , then  $E_r'(E_r) = E_r$  in all cases, and as a rule  $E_r' = E_r$  for other values of  $E$  as well. The first summation (over  $J$  and  $\pi$ ) is taken over all systems of levels which can contribute to the cross-section.



The summation over  $\ell$  is taken over all the orbital momenta of the neutrons which can form states with the given  $J$  and  $\pi$  :

$$L_1 = \min \left\{ \left| \gamma - \left| I - \frac{1}{2} \right| \right| ; \left| \gamma - I - \frac{1}{2} \right| \right\}, \quad (12)$$

if

$$(-1)^{L_1} = \pi \cdot \pi_I, \quad (13)$$

where  $\pi_I$  is the parity of the ground state of the target nucleus. If the parity condition in expression (13) is not satisfied,  $L_1$  is greater by unity than the value given by expression (12).

$$L_1 = \gamma + I + \frac{1}{2}, \quad (14)$$

if

$$(-1)^{L_1} = \pi \pi_I \quad (15)$$

or smaller by unity if the condition in expression (15) is not satisfied. Owing to the condition for conservation of parity,

$$(-1)^\ell = \pi \cdot \pi_I, \quad (16)$$

the value of  $\ell$  in the sum changes by 2 from one term to the next.

Since usually

$$\Gamma_{rnl} \gg \Gamma_{rn}(L_1 + 2) \gg \dots \gg \Gamma_{rnl_2},$$

(except for high energies, where  $ka \gg 1$ ), it is generally possible to put  $L_2 = L_1$ .

The penultimate term in expression (1) allows for interresonance interference within the Breit-Wigner approximation. This correction is exact if at least one of the following conditions is satisfied:

- (a) The resonances are well separated and interference is unimportant;
- (b) Only one neutron channel is important (only S-neutrons or S-neutrons and neutrons with high values of momentum interact, but the target nucleus spin is  $I = 0$ ).

The phase shift  $\varphi_{\ell J}$  is defined in terms of the channel radius  $a_{\ell J}(E)$ :  

$$\mathcal{Y}_{\ell y} = k a_{\ell y}.$$

Here

$$k = 2,19685 \cdot 10^{-3} \sqrt{E} \frac{M}{M+1,08665} \quad (\text{barn})^{-1/2}$$

where M is the mass of the nucleus (taking the mass of  $^{12}\text{C}$  equal to 12), and

$$a_{\ell J} = a + \Delta a_{\ell J}(E)$$

is the effective radius of the nucleus for the given channel. If  $a_{\ell J}$  shows a strong energy dependence, this dependence is entered in the library for  $a_{\ell J}$  (and not for  $\Delta a_{\ell J}$ ).

The last terms in equations (1) and (2) describe the contributions from distant resonances and also omitted levels. These cross-sections are either represented at discrete points or are calculated from the mean resonance parameters. In equation (1) this term can be correctly allowed for by the effective radius a. For this purpose, however, interresonance interference must be taken into account in defining the resonance parameters. If this is not done,  $\sigma_{\text{RN}}^{\text{SM}}(E)$  will in point of fact describe the result of interference from many levels.

### I.6.2 Approximations to the Breit-Wigner formula

#### (a) Omission of the term describing interresonance interference

This generally leads to the appearance of negative cross-sections between the resonances unless a smooth cross-section is added. As a rule, the resonance parameters are in fact determined in this approximation. Since only the resonance peak regions are considered, however, the parameters found in this approximation are sufficiently accurate. The nuclear radius is not found accurately, however, and must be corrected before these parameters can be used in a precise equation.

#### (b) Approximate allowance for interresonance interference to give positive solutions

This method is employed in the URAN Programme [8]. It consists in replacing  $\varphi_{\ell J}$  at each point E in the neighbourhood of a given resonance r by  $\varphi_{\ell J}^*$ , which is defined so that

$$4 \sin^2 \varphi_{\ell J}^*(E) = 4 \sin^2 \varphi_{\ell J} + \sum_{\substack{s=r-5 \\ s \neq r}}^{r+5} B_s(E) \left[ \Gamma_{sn} \Gamma_{snc} \cos 2 \varphi_{\ell J} - 2 \Gamma_{sx} \Gamma_{snc} \sin^2 \varphi_{\ell J} + 2(E - E_s') \Gamma_{snc} \sin 2 \varphi_{\ell J} \right]$$

The calculation is performed according to equation (1) with the interresonance term omitted but with  $\varphi_{\ell J}^*(E)$  in place of  $\varphi_{\ell J}$  so as to ensure a positive cross-section.

(c) Omission of the shift factors

Since  $S_0(E)$  is a constant, this is important only for  $l > 0$  and only far from a resonance. Therefore, parameters determined in this approximation can be used directly in an exact equation.

(d) Approximations for the low-energy region:

$$\sin^2 \varphi_0 \approx k^2 a^2, \quad \varphi_l = 0 \quad \text{for } l > 0.$$

Once this approximation has been used for determining parameters in the range where it is valid, the parameters are also suitable for use in the general equation.

(e) Omission of the factor  $\frac{M}{M+1.0865}$  in the expression for k

If the parameters are determined in this approximation, the value for M in the initial data must be made sufficiently high so that this factor is close to unity. Then the resulting parameters can also be used in the general equation.

Penetrabilities and phase shifts must be determined by one of three methods.

(1) For neutron channels  $P_2$  and  $S_2$  are calculated for a square well. In particular,

$$\begin{aligned} P_0 &= 1; \\ P_1 &= \frac{(KR)^2}{1+(KR)^2}; \\ P_2 &= \frac{(KR)^4}{9+3(KR)^2+(KR)^4}; \\ P_3 &= \frac{(KR)^6}{225+45(KR)^2+6(KR)^4+(KR)^6}. \end{aligned}$$

For other reactions we take  $P_R(E) = 1$  and  $S_R(E) = 0$ .

(2)  $P_R, S_R, P_P$  and  $S_2$  can be represented in tabular form as functions of neutron energy since they are determined empirically or calculated from some theoretical model (e.g. for reactions in which charged particles are emitted).

(3) Phase shifts and penetrabilities are calculated by an algorithm whose number is indicated in the library data.

## II. REPRESENTATION OF DATA ON PUNCHED CARDS

The nuclear data information contained in the library is assumed to be punched on symbolic cards. Each such card contains a specific amount of basic and service information. The basic information consists of the actual nuclear data in the form of numerical tabulations and auxiliary information coded in numerical form which serves as headings to the data tables. The service information consists of different types of flags distinguishing one card from another. These flags also simplify the computer processing of the stored data.

The symbolic cards are standard 80-column type cards. However, the manner in which the information is distributed on the card varies according to the particular peripheral equipment used. We shall therefore make a few general comments regarding the distribution and the coding of the information on the cards.

In the case where 960 positions (12 rows x 80 col.) are used for coding of information, the layout might be as follows: 6 fields (each 11 columns wide) separated by blank columns, used for the basic information (data fields), and a service (flag) field in columns 73 to 80. This type of layout is used in the UK recommended nuclear data library. If the input devices in the M-20 computer facility are used, it is more convenient to adopt a different scheme. In this case the basic information is coded on the six upper rows, and the service information is coded on the following rows.

These two types of layout are equivalent in the sense that the information punched on the symbolic card, when printed out by the appropriate peripheral device, is the same. In the first case it is the column field and in the second case the row which is the basic information unit. Each field (row) contains a single machine word (one number). Alphabetic coding is not used in the basic library<sup>1/</sup>. The form in which numbers are presented depends on their semantic content. All nuclear data are represented in floating point binary-coded decimal notation.

In the second case it is possible to have a slightly different information distribution on the card. Since the number of significant digits in the numerical data is usually small, the service information can also be stored in parallel with the basic information, by using for instance the three last decimal locations (third address) in each of the six rows containing the basic information. This would allow one standard punched card to accommodate two symbolic cards.

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<sup>1/</sup> It is assumed that, in parallel with the basic library containing the numerical data, there will be a library of textual commentaries for each file. The format for this has yet to be developed.

For a given substance, the data defined by a specific NIN constitute a closed information set in the sense that this information can henceforth be used independently, without recourse to any other information sets which contain analogous data for that same substance. Such a body of information, consisting of a self-contained set of data, will be referred to below as a "file". Each file is assigned a specific library file number (LFN) which is also entered in the first four places of the NIN.

Each file is divided into sections according to the number of reaction-types associated with a material having a given NIN. Each section contains cards with data on a particular type of reaction (RTN). In different files a given reaction type will in general correspond to a different section. The correspondence between the section number and the RTN is established in special "heading cards" located in the zeroth section of each file. Within each section the cards are numbered consecutively. The numbering of sections within each file is autonomous.

The sequence of the neutron data sections depends primarily on the PCN and, for identical PCN, on the GCN.

#### Examples of section numbering

Section number	RTN	Data definition
00	-	Heading information
01	01001	Total neutron interaction cross-section
02	01002	Elastic scattering cross-section for neutrons
03	02002	Angular distribution of elastically-scattered neutrons
04	01003	Nonelastic interaction cross-section
05	01004	Inelastic scattering cross-section
06	01005	Inelastic scattering cross-section with excitation of the first nuclear level
07	02005	Angular distribution of inelastically-scattered neutrons for excitation of first nuclear level
08	03005	Energy distribution of inelastically scattered neutrons for excitation of first nuclear level

Both the content, and the location of the basic information on the cards depends on the RTN (primarily on the GCN) and also on the FTN. This will be considered in more detail below. The service information includes part of the NIN (LFN), the number of the section, the serial number of the card in the section and also the cyclic sum of the information punched in the first eight rows of the card.

In view of the type of card punch and input equipment most widely used at present in the USSR, we have adopted a system of coding by rows.

In the first six rows of the card we enter the basic information, which is always recorded in floating-point binary coded decimal (including integers). The order of presentation of the basic information on the punched cards is described below (section III).

The seventh row carries a nine-digit integer, the last two places of which are the number of the section in which data of the relevant type are located <sup>2/</sup>; the four leading places are used to record the four leading NIN digits (the library file number (LFN)) in the format considered above. The fifth, sixth and seventh places are not used.

In the eighth row we punch the number of the card in the section in floating point form. The numbering of the cards commences anew in each section from card number 1 (which always contains the title information for the section).

The ninth row contains the cyclic sum of the numbers recorded in the first eight rows. This information does not have to be punched for the present format; it is only required in order to simplify the procedure for finding incorrect cards. After the data have been inserted, the check sum can be used to test that the information on each punched card has been read correctly and to reveal any defective cards.

### III. FORMATS OF NUCLEAR DATA IN THE LIBRARY

Since the character of the nuclear data is determined by the type of reaction, the format of these data in the library depends on the RTN, and primarily on the GCN. The formats will also naturally depend on the FTN. Before specific formats for different GCNs are considered, a few general comments are in order.

The energy range for a given RTN is divided as required into a number of intervals. The following points, among others, must be taken into account:

1. In certain energy regions the values will be negligibly small or zero (cross section below the threshold of a reaction, for example)
2. In some energy intervals the data are independent of energy or are represented identically;
3. In some energy intervals the data have different representations or different temperature dependences.

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<sup>2/</sup> The connection between the section number and the RTN is defined in the first heading section of the file.

The division of an energy region into intervals sometimes helps to avoid duplication of results. The number of energy intervals should be kept as small as possible. For different RTNs within a single NIN the number of intervals may be different. For example, the total cross-section and the cross-section of a threshold process will have different numbers of intervals. Wherever possible it is desirable to have identical energy intervals for a total cross-section and its associated partial cross-sections. This makes it easier to locate gross errors by means of special programmes.

Nuclear data are usually given at discrete energy points. If, however, the data are constant over a particular energy interval, they can be represented by a single value for that interval as a whole. Such a treatment is possible with the help of special formats included in the FTN classification.

Where data are quoted for discrete values of the variables on which they depend, the choice of values for the independent variables must satisfy certain conditions. More specifically, the values selected must be such that the values of the function itself, for any intermediate values of the arguments, can be obtained to a sufficient degree of accuracy by interpolating between neighbouring points available in the file. In some cases it is better to interpolate on a log scale (cross-sections, special quantities for neutrons). The method of interpolation, and the order of the interpolation polynomial for particular data sets to be entered in the library, are determined by evaluators who take into account the capabilities of the available processing programmes; this additional information is then entered into the heading of the FTN.

The interpolation law is represented in the library by a nine-digit INT number:

$$\text{INT} \equiv i_1 i_2 i_3 i_1' i_2' i_3' i_1'' i_2'' i_3''.$$

By means of the INT number it is possible to determine the method of interpolation for a function of one, two and three variables.

The last three places,  $i_1' i_2' i_3'$ , determine the interpolation law for the lowest-priority variable; the three places in the middle,  $i_1'' i_2'' i_3''$  that for the next in order; and the first three places  $i_1 i_2 i_3$ , that for the highest priority variable. The order of priority of the variables is determined by the FTN (see below).

In each set of three numbers,  $i_1 i_2 i_3$ , the digit  $i_1$  defines the method of interpolation:  $i_1 = 1$  denotes linear interpolation, and the meaning of other values of  $i_1$  has not yet been fixed. The next two digits define the scale on which interpolation should be performed;  $i_2$  along the ordinate (scale of the interpolated function),  $i_3$  along the abscissa (scale of the argument).

The scale is defined by the following table:

Value of $i_2$ or $i_3$	Scale along corresponding axis
1	Linear
2	Logarithmic
3	Radical
4	Cosine

When  $i_3 = 0$ , then whatever the value of  $i_2$ , the cross-section is taken to be constant with a value of  $\sigma_i$  between  $E_i$  and  $E_{i+1}$ . The first value  $E_i$  must be identical to  $E_M$ .

The meaning of other values of  $i_2$  and  $i_3$  is as yet unfixed.

Examples: 1. Function of a single variable (E).

INT = ++ 09 122 000 000

denotes linear interpolation ( $i_1=1$ ) on a log-log scale ( $i_2 = i_3 = 2$ ). The energy E is here the only and therefore the highest-priority variable.

2. Function of two variables - a secondary-neutron spectrum as a function of the incident neutron energy:  $f(E_0, E)$ .

INT = ++ 09 111 111 000

denotes linear interpolation of f over each of the variables on a linear scale.

3. Function of three variables - superposition of angular distributions:  $f(E, \mu) = \sum_{k=1}^K a_k(E) f_k(E, \theta)$  (the  $a_k(E)$  might for example be energy-dependent sub-group weighting coefficients, and  $f_k$  sub-group angular distributions).

INT = ++ 09 112 112 114

means, in the case where the order of precedence of the variables is a, E and  $\theta$ , that  $a_k(E)$  must be interpolated linearly on graphs of  $a_k$  versus  $\ln E$  ( $i_1=1, i_2=1, i_3=2$ ) and that  $f_k$  must be interpolated similarly for energy ( $i'_1=1, i'_2=1, i'_3=2$ ) and linearly with respect to the cosine of the angle  $\theta$  ( $i''_1=1, i''_2=1, i''_3=4$ ).

4. The cross-section depends on the sub-group number and the energy.

INT = 09 100 100 000

means that the sub-group weighting  $a_p(E)$  and the sub-group cross-sections  $\sigma_p(E)$  are constant in the interval between  $E_i$  and  $E_{i+1}$  and equal to  $a_p(E_i)$  and  $\sigma_p(E_i)$ .



5. If the data are temperature dependent, the relevant temperature value is given. If the dependence can be calculated analytically, the specification of a single temperature is enough. Otherwise the results are given for several different temperatures so that data for any desired temperature can be obtained by interpolation. For example:

INT = ++ 09 113 000 000

denotes that interpolation must be performed linearly on a graph of the cross-section versus  $\sqrt{T}$  ( $i_1 = 1, i_2 = 1, i_3 = 3$ ).

The RTN specification is such that it allows unambiguous identification of the residual nucleus as well as the reaction products of any given nuclear reaction. In particular, the number of secondary particles resulting from a given reaction is uniquely determined. However, since some data, such as experimental data on angular and energy distributions, may not be known for each secondary particle separately, but sometimes only for certain groups of particle products, the formats include a special number identifying the groups of particles for which such data are specified.

The library formats allow information to be stored in separate sets, each of which in turn can contain smaller sets. The distribution of the data into the sets depends on the existence of common features: for instance they may be data having the same RTN or FTN, data belonging to the same energy range, temperature, and so on.

All the data sets are provided with special headings. Each heading contains a description of the set and information about the number and possibly the location of the directly dependent sub-sets. In this way, a general idea of the content of a set can be gained from the heading alone without the need to "unpack" the whole set.

Each heading begins with a new card. The format for any GCN contains the following headings:

- Reaction-type heading
- Energy-range heading
- Temperature heading (for GCN = 01, 04 and 05) or secondary-particle groups (for GCN = 02 and 03)
- Data form heading

The order of the remaining, internal headings is defined by the FTN. Energy headings, neutron sub-groups, etc. fall into this category.

In what follows, we refer to a field or a row as a position. In the description of specific formats the cards are numbered with Roman numerals and the card positions containing basic information with Arabic numerals. Zeros are punched in positions not occupied by information.

### III.1 File heading

The file heading occupies the zeroth section and establishes the correspondence between the section number, the reaction type number and the number of cards in the section. The heading format is as follows:

#### Type of card

- I.
  - 1. NIN
  - 2. Total number of cards in file, including the heading cards
  - 3. Number of cards in the zeroth section
  - 4. Atomic number Z of the element (a zero is used for chemical compounds and mixtures)
  - 5. Atomic or molecular weight A
  - 6. Number of different RTNs that exist for the given substance
  
- II.
  - 1. Number of the section
  - 2. Corresponding RTN
  - 3. Number of cards in the section

If necessary, the information is continued in the following positions of this and subsequent cards in the format of positions 1-3 of the type II card.

### III.2 Neutron cross-sections (GCN = 01)

In the library, the numerical values of the cross-sections are stored together with the corresponding values of the variable on which they depend. This variable may be the energy, the temperature, the sub-group number, etc. Cross-section data are stored in an order determined by the natural sequence of values of the variable; in the case of energy and temperature, this implies a monotonically increasing order. The numbering of sub-groups is in the order of increasing cross-section. In the formats adopted here, the energy is given in MeV, the temperature in degrees K, and the cross-section in barns.

The energy and temperature values are chosen in such a way that the cross-sections can be obtained by interpolation. This interpolation is often done on a logarithmic scale, in which case it is necessary that the cross-section be non-zero at all points, including the end points of the interval.

The RTN classification scheme also enables the cross-section to be given directly for the whole energy interval provided it is constant over that interval.

It is desirable for the total cross-section and its component partial cross-sections to be given at the same energy points. This can facilitate the process of checking the cross-section data for gross errors by means of special programmes.

III.2.1 FTN classification for GCN = 01

The first FTN digit defines the manner in which the cross-section data are given according to the following table:

$n_1$	Cross-section presentation
1	At discrete points as a function of E and T in sub-group form
2	At discrete points as a function of E with parametric representation of the temperature dependence of the sub-group parameters
3	Parametrically by means of resonance equations for resolved resonances
4	Parametrically by means of statistical information for unresolved resonances
5	Temperature and energy dependences of the cross-sections for some (usually all) reactions in the section for the total cross-section

Subsequent  $n_1$  values (6-9) are reserved for new data presentation forms, if and when they are formulated.

The meaning of the low-priority FTN digits ( $n_2$  and  $n_3$ ) generally depends on the  $n_1$  value. For  $n_1 = 1$  they have the following meaning:

$n_2$  - indicates the number of variables or parameters on which the cross-sections may depend

$n_3$  - indicates the internal order of priority of these parameters.

In the case of two parameters (energy E and the sub-group number i), the meaning of the low-priority FTN digits is defined in the following table:

$n_2n_3$	High-priority variable	Low-priority variable
01	-	-
11	E	-
12	i	-
21	E	i
22	i	E

The  $n_2 n_3 = 01$  case means assigning a cross-section value to the whole energy interval at once.

For  $n_1 = 2$  the card format and the classification of  $n_2$  and  $n_3$  have yet to be fixed.

For  $n_1 = 3$  the second FTN digit ( $n_2$ ) determines the type of the resonance equation. In accordance with RPL [7] we take:

$n_2 = 1$  for the Breit-Wigner equation

$n_2 = 2$  for equations based on the reduced R matrix (Reich-Moore equation)

$n_2 = 3$  for the R-matrix Brissenden-Durston equation

$n_2 = 4$  for the S-matrix Adler-Adler equation;

$n_3$  equal to zero means that the resonance parameters are not cited in the section for the given PCN and that they must be taken from the section for the total cross-section (PCN = 001). With  $n_3 = 0$  and  $n_2 = 0$ , the resonance parameters are not given for the relevant value of temperature; they must be taken from the section corresponding to the first temperature value.

In the section for the total cross-section, the values  $n_2 = 0$  and  $n_3 = 0$  for the lowest of the cited temperature, are inadmissible. The remaining values,  $n_3 = 1, 2, \dots, 9$ , denote the number of the approximation to the general equation which is recommended for use in calculations on the given parameters.  $n_3 = 1$  always means that the parameters are intended for use with the general equation. When  $n_2 = 1$ ,  $n_3 = 2$  denotes that the approximation included in the URAN Programme [8] is recommended. The meaning of other values of  $n_3$  has not yet been assigned.

For  $n_1 = 4$  the meaning of  $n_2$  and  $n_3$  is the same as for  $n_1 = 3$ . The data forms for  $n_1 = 5$  and above are recommended for recording the energy variation of the cross-sections in the resonance region. The number of points here is very large and the cross-sections may vary very strongly with temperature. Therefore, the amount of information on the detailed energy and temperature dependences of the cross-sections in this region usually determines the overall volume of the information in the file.

For FTNs with  $n_1 = 1$  and above the energy values for which the cross-sections are given are duplicated where necessary for the cross-sections of all the reactions and for all the temperatures. Moreover, when there is a large number of energy points, the data on the cross-sections for the various temperatures are very widely separated.

The cross-sections for different reactions are even more widely separated. All this involves large amounts of extra machine time for the rearranging of information required to interpolate the cross-sections with

respect to temperature and to calculate average group values for ratios of the type  $\langle \sigma_c / \sigma_t \rangle$  (which are used to express the group constants in the resonance region). The amount of machine time is particularly great on computers which have a small central memory and which cannot process magnetic tape information while carrying out calculations.

The use of FTNs with  $n_1 = 5$  and above enables us to include in the section for the total cross-section information about the energy and temperature behaviour of all the cross-sections, information already put in a predetermined order suitable for calculating the group constants. The volume of stored numerical information is then cut almost in half, since the energy values are not duplicated for each cross-section and each temperature. To a large extent, this compensates for the disadvantage which arises with these representations in the output of information on the detailed variation of a particular reaction at a fixed value of temperature.

For  $n_1 = 5$ ,  $n_2 > 0$  denotes the maximum number of sub-groups used to describe the structure of the cross-sections in the given energy range. In the unresolved resonance region, where the details of cross-section variation are unknown, FTN with  $n_2 > 1$  will almost always be used. Data formats with  $n_2 > 1$  can also be used in the resolved resonance region if it is not necessary to describe the variation in detail.  $n_3 > 0$  denotes the number of temperatures for which the cross-sections are given.  $n_3 = 9$  means that data are given for more than eight temperature values.  $n_3 = 0$  with  $n_2 \neq 0$  means that, for this temperature value, information about the energy and temperature variations of the cross-sections is not given in compact form but can be taken from the section relating to the first temperature value quoted.  $n_2 = 0$  means that the energy and temperature dependence is not given in compact form for a given FTN but can be taken from the section for the total cross-section. Values of  $n_2 = 0$ , and  $n_3 = 0$  for the lowest temperature value, are not permissible in this section.

It should be noted that since FTNs with  $n_1 = 5$  and above enable us to describe the temperature dependence of the cross-sections (as can be done where resonance parameters are used) there is no point in giving the temperature dependence in the form of energy variations at different temperatures, although this is allowed by the format.

### III.2.2 Card format for GCN = 01 when the cross-sections are given at discrete values of E and T ( $n_1 = 1$ )

- I. 1. RTN
2. Number of energy intervals ( E ) for this RTN
3. Q, reaction energy (MeV)
- 4.)
- 5.) Reserved for supplementary information belonging to this RTN
- 6.)

- II.
1.  $E_H$ , lower limit of  $\Delta E$
  2.  $E_B$ , upper limit of  $\Delta E$
  3. Number of cards for presenting cross-sections in this  $\Delta E$ , including the present card
  4. Number of temperature values considered in this  $\Delta E$ . The lowest temperature, if the temperature dependence of the cross-section is defined by the  $R_{TN}$ . Zero, if there is no temperature dependence.
  5.  $INT$  number determining temperature interpolation law. In the absence of any temperature dependence, use  $INT = 09\ 100\ 000\ 000$ .
  6. Conventional indicator  $a$ .  $|a| = 1$  means that the temperature dependence of the cross-sections is determined by the data presentation forms.  $a < 0$  means that the given energy range contains such wide resonances that, in the compilation of the group constants, the detailed variation of the cross-sections is best described by dividing the standard group into several narrower groups.

- III.
1. Temperature  $T$ , at which cross-section is given
  2.  $F_{TN}$  number for cross-sections at this temperature
  3. Number of cards for representing cross-sections at this temperature, including this card
  - 4.)
  - 5.) Reserved for additional information at this  $T$
  - 6.)

The format of subsequent cards depends on the  $F_{TN}$ .

Case\_(1) Cross-section in the given  $\Delta E$  is not energy dependent (one sub-group)

- IV.
1.  $F_{TN} = 101$
  2. Cross-section value
  3. Number of cards for this  $R_{TN} (=1)$

Case\_(2) Cross-section is energy dependent (one sub-group)

- IV.
1.  $F_{TN} = 111$
  2. Number of energy values
  3. Number of cards for this  $F_{TN}$
  4.  $INT$  number determining the law for energy interpolation of the cross-section
  5.  $E_1$
  6.  $\sigma(E_1)$

If necessary, the information is continued on following cards in the format of positions 5 and 6 of card IV.

Case\_(3) Sub-group representation of the cross-section structure for the whole  $\Delta E$

- IV.
1. FTN = 112
  2. Number of sub-groups
  3.  $a_1$
  4.  $\sigma_1$
  5.  $a_2$
  6.  $\sigma_2$

If necessary the information is continued on subsequent cards in the format of positions 3 and 4 of card IV.

Case\_(4) Cross-section is energy dependent  
Sub-group representation of the cross-section structure for fixed E

- IV.
1. FTN = 121
  2. Number of E values
  3. Number of cards used in the representation of the cross-sections by this FTN (including this card)
  4. Number of sub-groups (if it does not depend on E) or zero
  5. INT number determining the energy interpolation law for  $a_i$  and  $\sigma_i$
  6. Number determining which quantity must be averaged

(a) If direct averaging of  $a_i$  and  $\sigma_i$  is possible for certain intervals  $\Delta E$  or  $\Delta U$  falling within the interval  $[E_H, E_B]$ , we enter in this position either the maximum energy-loss interval for which such averaging still permits the sub-group characteristics to be determined with sufficient accuracy (it is assumed that this interval must be less than 2) or the maximum energy interval taken with a minus sign (minus indicating that the interval is given in the energy scale);

(b) If there is a 2 in this position, the transmission functions must be averaged:

$$T_t(t) = \frac{1}{\Delta E} \int_{\Delta E} e^{-\sigma_t(E) \cdot t} \cdot f(E) \cdot dE \quad (\text{if } \sigma \text{ is the total cross-section})$$

$$T_r(t) = \frac{1}{\Delta E} \int_{\Delta E} \sigma_r(E) e^{-\sigma_t(E) \cdot t} \cdot f(E) \cdot dE \quad (\text{if } \sigma = \sigma_R \text{ is a type R reaction cross section})$$

(f(E) is the spectrum with respect to which averaging is performed).

The sub-group parameters for the interval E are then determined from the condition for approximation of  $T_t(t)$  and  $T_r(t)$  as the sum of the minimum number of exponentials providing the requisite accuracy:

$$T_t(t) \approx \sum_{k=1}^p a_k e^{-\delta_{kt}}$$

$$T_r(t) = \sum_{k=1}^p a_k \delta_{kr} e^{-\delta_{kt}}$$

- (c) If there is a 3 in this position, the recommended method of obtaining the sub-group characteristics for the intervals is to calculate the cross-section moments  $\langle \sigma_R \sigma_t^n \rangle$ , where  $R = e, c, f, \dots, R_{max}$  and subsequently to determine the subgroup parameters by solving the following system of algebraic equations:

$$\langle \sigma_R \sigma_t^{n_R} \rangle = \sum_{k=1}^p a_k \sigma_{Rk} \sigma_{tk}^{n_R}$$

$R = e, c, f, \dots, R_{max}$   
 $n_{Rmin}(p) \leq n_R \leq n_{Rmax}(p)$

where  $n_{Rmin}(p)$  and  $n_{Rmax}(p)$  are chosen from the following table:

Sub-group number	Reaction					
	Elast. Scatt.		Radiative Capt.		Other Reactions	
2	-2	0	-2	0	-1	0
3	-3	0	-3	1	-2	0
4	-4	1	-3	2	-3	0

The number of sub-groups p is chosen to ensure some given accuracy  $\epsilon(n)$  in the calculation of the moments  $\langle \sigma_R \sigma_t^{n_{Rmin}-1} \rangle$  and  $\langle \sigma_R \sigma_t^{n_{Rmax}+1} \rangle$

- (d) Positive integers greater than 3 are reserved for other possible methods of calculating the sub-group characteristics for the intervals.

- V.
1. E
  2. Number of sub-groups
  3.  $a_1$
  4.  $\sigma_1$

If necessary, the information is continued on the subsequent positions of this and the following card in the format of positions 3 and 4 of card V.



Generally speaking, this format makes it possible to give different numbers of sub-groups for different values of E. In practice, however, the number of sub-groups for all E within a given  $\Delta E$  will usually be the same.

Case\_(5) Cross-section is energy dependent. Sub-group parameters are energy dependent

- IV. 1. FTN = 122<sup>3/</sup>  
2. Number of sub-groups  
3. Number of cards for this FTN  
4. Reserve  
5. INT number determining the energy interpolation rule  
6. Conventional number determining the method of obtaining the interval (group) sub-group parameters (see pos. 6, card IV for FTN = 121)
- V. 1. Sub-group number (i)  
2. Number of energy values  
3. Reserve  
4. E<sub>1</sub>  
5. a<sub>il</sub>  
6.  $\zeta_{il}$

If necessary the information is continued on subsequent cards in the format of positions 4-6 of card V.

The format of cards for FTNs with  $n_1 = 2$  has not yet been determined.

III.2.3 Format of cards for representing data on resolved resonance parameters \*)

- (a) General information
- I. 1. FTN  
2. Reserve  
3. Number of cards for this FTN  
4-6. Reserve
- II. 1. E<sub>01</sub>, energy of the first resonance, eV  
2. E<sub>0,last</sub>, energy of the last resonance, eV  
3. Number of isotopes  
4-6. Reserve

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<sup>3/</sup> For the information of evaluators: the processing of data presented in RTN = 121 usually involves less machine time than data with RTN = 122.

\*) This format was partly changed, see p. 61-63 (note by editor)

(b) Information on the isotope

- III.
1. Atomic weight of first isotope
  2. Its fractional concentration in natural isotopic mixture
  3. Number of cards for this isotope (including this card)
  4.  $\pm a$ , radius of neutron channel (in Fermis) (with minus sign if the energy dependence of the radius or its dependence on  $\ell$  and  $J$  is given)
  5.  $\pm I$ , parity and spin of the target nucleus. For computers which do not distinguish between +0 and -0, negative parity is noted by punching not only the sign of the number, but also its indicator.
  6. Number of resonances of the isotope for which parameters are given

- IV.
1. Number of reactions for which parameters are given
  2. PCN of elastic scattering reaction = 002
  3. PCN of total radiative capture reaction = 102
  4. PCN of fission reaction (if it occurs) = 019. If there is no fission, then zero is used
  5. PCN of the fourth reaction (if there is one), otherwise zero
  6. PCN of fifth reaction (if there is one), otherwise zero

If necessary, information continues on subsequent cards in the format of positions 5 and 6 of card IV.

- V.
1. Indicator for presence of non-resonance scattering cross-section, nrr:  
  
nrr = 0 if there is no such contribution  
nrr = 1 if it is given as a series of energy points  
nrr = 2 if it has to be calculated from equations on the basis of the mean resonance parameters  
nrr > 2 if it has to be calculated on some other basis
  2. Indicator for the method of calculating penetrabilities and shift factors for the neutron channel, khupn:  
  
khupn = 0 if these factors are calculated by the usual method  
khupn = 1 if they are given at fixed energies  
khupn = 2 if they have to be calculated from certain specific equations
  3. Indicator for the presence of a non-resonance radiative capture cross-section (analogous to the corresponding indicator for scattering), nrz.

4. Indicator for the method of calculating penetrabilities and shift factors for radiative capture, khupz:  
khupz = 0, if these quantities are independent of energy (as they usually are)  
khupz = -1, if they are given at fixed energies independent of  $\ell$   
khupz = +1, if they are given at fixed energies for different values of  $\ell$   
khupz  $\geq$  2, if they have to be calculated from equations
5. Indicator for the presence of a non-resonance fission cross-section (analogous to the corresponding indicator for scattering), nrd.
6. Indicator for the method of calculating penetrabilities and shift factors for fission (analogous to the corresponding indicator for capture), khupd. If, in addition to elastic scattering, capture and fission, other reactions are involved, information on any non-resonance contributions and on the method of calculating penetrabilities and shift factors is recorded on subsequent cards in the format of position 3-4 of card V.

(c) Presentation of neutron channel radii  
(if  $a < 0$ , see card III, position 4)

- VI.
  1. The number of values of  $\ell$  for which  $a_{\ell J}$  are given
  2. The number of energy values for which the radii are given (= 1 if the  $a_{\ell J}$  are independent of E)
  3. The number of cards with information about the radii (including this card)
  4. The INT number defining the energy interpolation law for  $a_{\ell J}$
  - 5-6. Reserve
- VII.
  1. First value of  $\ell$
  2. The number of values of J for which  $a_{\ell J}$  are given for a given  $\ell$
  3. The number of cards with information for this value of  $\ell$
  4. The first (smallest) J value for the given  $\ell$
  5. The second value of J for the given  $\ell$
  6. The third value of J for the given  $\ell$

If the number of J values for a given  $\ell$  is greater than 3, the information is continued on subsequent cards in the format of positions 4-6 of card VII.

- VIII.
  1. E, the energy (=  $E_H$  if the radii are given for one energy)
  2.  $a_{\ell J}(E)$  for the given  $\ell$  and the first value of J
  3.  $a_{\ell J}(E)$  for the given  $\ell$  and the second value of J etc. (this is continued on subsequent cards if the number of J values is greater than 5)

Type VIII cards are repeated for all values of E. Type VII and VIII cards are repeated for all values of  $\ell$ .

(d) \*) Presentation of non-resonance cross-sections (if at least 1 of the indicators nrr, nrv, nrd etc. (see positions 1, 3 and 5 of card V) is non-zero. The format is determined for indicator values equal to 1 and 2)

- IX. 1. PCN for the first reaction for which the non-resonance cross-section is given  
2. The number of energy points  
3. The number of cards with data on this non-resonance cross-section (including this card)  
4. The INT number defining the energy interpolation law for  $\sigma$   
5-6. Reserve
- X. 1. FTN in which the non-resonance cross-section is given. FTN values of 101,111,112,121,122,411 and 412 are permissible

The content of the remaining positions of card X and of subsequent cards with data on the non-resonance cross-section is determined by the format of the corresponding FTN (see III.2.2 and III.2.4). Type IX and X cards are repeated for each reaction for which a non-resonance cross-section is given.

(e) Representation of penetrabilities and shift factors  
(If the penetrabilities and shift factors are represented in the form of tables at fixed energies for at least one reaction)

- XI. 1. PCN  
2. The number of  $l$  for which penetrability energy dependences, etc. are given  
3. Number of cards with data on penetrabilities and shift factors for the reaction of interest  
4. INT defining the type of interpolation over energy used for penetrabilities and shift factors  
5-6. Reserve
- XII. 1.  $l_1$   
2. Number of energy points for given  $l (=l_1)$   
3. Number of cards with data on penetrabilities and shift factors for given  $l$   
4-5. Reserve
- XIII. 1.  $E_1$   
2.  $P_{l_1}(E_1)$   
3.  $S_{l_1}(E_1)$   
4.  $E_2$   
5.  $P_{l_1}(E_2)$   
6.  $S_{l_1}(E_2)$

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\*) See also p. 67 (note by editor)

The information is continued on subsequent cards in the format of card XIII. Type XIII and XIV cards are repeated for all necessary values of  $\ell$ .\*)

Penetrabilities for other reactions not characterized by the orbital momentum of the escaping particle

- XIV. 1. PCN of reaction  
2. Number of energy points  
3. Number of cards with data on penetrabilities and shift factors for this reaction  
4. Indicator showing that data are independent of  $\ell$  ( $=-1$ )  
5-6. Reserve
- XV. 1.  $E_1$   
2.  $P_R(E_1)$   
3.  $S_R(E_1)$   
4.  $E_2$   
5.  $P_R(E_2)$   
6.  $S_R(E_2)$

Information is continued on subsequent cards in the format of card XV. Cards of type XII-XIII or XIV-XV are repeated for all reactions for which energy dependences of the penetrability and shift factors are given. Penetrabilities for reactions characterized by the orbital momentum of the escaping particle are given in the format of cards XII-XIII, where  $\ell'$  is punched instead of  $\ell$ .

(f) Resonance parameters proper

- XVI. 1.  $E_r$ , resonance energy, eV  
2.  $\pm J$ , parity and spin of the compound state. For computers which do not distinguish between +0 and -0, both the sign and the indicator of the number must be punched.  
3.  $\pm \ell$ , lowest orbital angular momentum of neutrons which can form the above state. Printed with minus sign if the state can also be formed by neutrons with a higher orbital momentum. For computers which do not distinguish between +0 and -0, a minus sign must be accompanied by the indicator.  
4.  $\Gamma_{rn1}(E_r)$ , neutron width, eV  
5.  $\Gamma_{r\gamma}$ , radiation width<sup>4/</sup>, eV  
6.  $\Gamma_{rf}$ , fission width<sup>4/</sup>, eV

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<sup>4/</sup> If the penetrability for any reaction is energy dependent, the width is specified for the energy ' $E_r$ '.

\*) should probably read "Type XII and XIII cards" (note by editor)

If  $l < 0$  the next card takes the following form:

- XVII. 1.  $\pm l_2$ , next angular momentum of neutrons which can form the given state (with minus sign - and for computers which do not distinguish between +0 and -0, the indicator - if the  $l$  value is not the maximum possible)
2.  $\Gamma_{rn} l_2(|E_r|)$ , the corresponding neutron width
3.  $\pm l_3$  (if  $l_2 < 0$ ). Otherwise zeroes are printed in positions 3-6
4.  $\Gamma_{rn} l_3(|E_r|)$
5.  $l_4 \overline{5/}$  (if  $l_3 < 0$ ). Otherwise zeroes are printed in positions 5-6
6.  $\Gamma_{rn} l_4(|E_r|)$

If there are reactions other than  $(n,n)$ ,  $(n,\gamma)$  and  $(n,f)$ , we have:

- XVIII. 1. PCN for the first of these reactions
2.  $\Gamma_{rR1}(|E_r|)$ , the corresponding width for  $E = |E_r|$
3.  $l'$ , the orbital momentum of the escaping particle
4. PCN for the second of these reactions
5.  $\Gamma_{rR2}(|E_r|)$ , the corresponding width for  $E = |E_r|$
6.  $l'$ , the orbital momentum of the escaping particle

If necessary, the information is continued on subsequent cards in the form of card XVIII. Type XVI-XVIII cards are repeated for each resonance in ascending order of  $E_r$ . Cards of types III-XVIII are repeated for each isotope.

III.2.4 Card format for data on statistical parameters of unresolved resonances (GCN = 01, n<sub>1</sub> = 4) \*)

(a) General information

- I. 1. FTN
2. Reserve
3. Number of cards for this FTN
- 4-6. Reserve
- II. 1. Number of isotopes
2. Numerical indicator,  $kh_r$ , defining the nature of the variation of the mean resonance parameters:
- $kh_r = 1$ , if these parameters are constant in the interval
- $kh_r = 2$ , if they vary from one point to another
3. The number of energy points or sub-intervals (if  $kh_r = 2$ ) or zero (if  $kh_r = 1$ )
4. INT number defining the type of energy interpolation for  $\overline{D}$ ,  $\overline{\Gamma}$  and  $\nu$
- 5-6. Reserve

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5/ The format does not allow the input of more than 4  $l$  values.

\*) See also p. 67 (note by editor)

(b) Information on the isotope

- III.
1. Atomic weight of the first isotope
  2. Its fractional concentration in a natural isotopic mixture
  3. Number of cards with data on this isotope
  4. Neutron channel radius in Fermis (punched with minus sign if its energy dependence and/or dependence on  $\ell$  and J is given)
  5.  $\pm I$ , the parity and spin of the target nucleus. For computers which do not distinguish between +0 and -0, the minus sign must be supplemented by the indicator.
  6. Reserve
- IV.
1. Number of reactions for which parameters are given
  2. PCN of elastic scattering reaction = 002
  3. PCN of total radiative capture reaction = 102
  4. PCN of fission reaction = 019 (if it occurs) or 0
  5. PCN of fourth reaction (if it exists) or 0
  6. PCN of fifth reaction (if it exists) or 0

If necessary the information is continued on subsequent type IV cards.

- V.
1. Indicator for presence of a non-resonance scattering cross-section, nrr  
  
nrr = 0, if there is no such contribution  
nrr = 1, if it is specified for discrete energies  
nrr > 1, if it has to be calculated from some particular equation
  2. Indicator for the method of calculating penetrabilities and shift factors for the neutron channel, khupn  
  
khupn  $\neq$  0, if these penetrabilities are calculated by the usual method  
khupn = 1, if they are specified for discrete energies  
khupn > 1, if they have to be calculated from some particular equation
  3. Indicators for the presence of a non-resonance radiative capture cross-section, nrz (analogous to the corresponding indicator for scattering)
  4. Indicator for the method of calculating the penetrabilities and shift factors for radiative capture, khupz  
  
khupz = 0, if these quantities are not energy dependent (which is usually the case)  
khupz = 1, if they are given at discrete energies  
khupz > 1, if they have to be calculated from some particular equation
  5. Indicator for the presence of a non-resonance fission cross-section (analogous to the corresponding indicator for scattering), npd

6. Indicator for the method of calculating the penetrabilities and shift factors for fission (analogous to the corresponding indicator for capture), khupd. If, in addition to elastic scattering, capture and fission, there are other reactions, all relevant information on the presence of a non-resonance contribution and the method of calculating penetrabilities and shift factors is recorded on subsequent cards in the format of positions 3-4 of card V.

Representation of the neutron channel radii

(If  $a < 0$ , see card III, position 4)

- VI.
  1. The number of values of  $\ell$  for which  $a_{\ell J}$  are given
  2. The number of energy values for which  $a_{\ell J}$  are given (= 1 if the  $a_{\ell J}$  are independent of E)
  3. The number of cards with information about the radii (including the present card)
  4. INT number defining the energy interpolation law for the  $a_{\ell J}$
  - 5-6. Reserve
- VII.
  1. The first (smallest) value of  $\ell$
  2. The number of J values for which  $a_{\ell J}$  are given for the given  $\ell$
  3. The number of cards with information on the given  $\ell$
  4. The first (smallest) value of J for the given  $\ell$
  5. The second value of J for the given  $\ell$
  6. The third value of J for the given  $\ell$

If the number of J values for the given  $\ell$  is greater than 3, the information about the remaining J values is continued on the subsequent card or cards.

- VIII.
  1.  $E_1$  (equals  $E_H$  if  $a_{\ell J}$  are independent of E)
  2.  $a_{\ell J}(E_1)$  for the given  $\ell$  and the first value of J, etc. (with continuation on subsequent cards if the number of J values is greater than 5)

Type VIII cards are repeated for all values of E. Type VII cards are repeated for all  $\ell$  values up to  $\ell = \ell_M$ .

Representation of non-resonance cross-sections

(If the data on card V, positions 1, 3 and 5, and on similar cards show that there is such a contribution for at least one reaction)

- IX.
  1. PCN of the first reaction for which the non-resonance variation of the cross-sections is given
  2. The number of energy points
  3. The number of cards with data about this non-resonance cross-section
  4. INT number defining the energy interpolation law for the cross-section
  - 5-6. Reserve



- X.    1.     $E_1$   
      2.     $\sigma(E_1)$ , etc.

Where necessary the information is continued on subsequent cards in the format of positions 1 and 2 of card X.

Cards IX and X are repeated for all reactions whose non-resonance cross-sections are given.

Presentation of penetrabilities and shift factors

(If the data on card V, positions 2, 4 and 6 and on similar cards show that these are to be specified for at least one reaction)

- XI.   1.    PCN of the first reaction for which penetrabilities and shift factors are given  
      2.    The number of angular momenta for which they are given  
      3.    The number of cards with data on penetrabilities and shift factors for this reaction  
      4.    INT number defining the energy interpolation for  $P_\ell$  and  $S_\ell$   
      5-6. Reserve

- XII.  1.     $\ell_1$   
      2.    The number of energy points for  $\ell = \ell_1$   
      3.    The number of cards with data on  $P_{\ell_1}$  and  $S_{\ell_1}$   
      4-6. Reserve

- XIII. 1.     $E_1$   
      2.     $P_{\ell_1}(E_1)$   
      3.     $S_{\ell_1}(E_1)$   
      4.     $E_2$   
      5.     $P_{\ell_1}(E_2)$   
      6.     $S_{\ell_1}(E_2)$  etc. with continuation on subsequent cards in the format of card XIII

Cards XII and XIII are repeated for all values of  $\ell$ . Cards XI-XIII are repeated for all reactions for which penetrabilities and/or shift factors are given.

Presentation of average resonance parameters

- XIV.  1.    The first energy value,  $E = E_N$   
      2.    The number of energy levels considered which differ in spin and/or parity of the compound nucleus  
      3.    The number of cards for this value of energy  
      4-6. Reserve

Information for a particular level system

- XV. 1.  $\pm J$ , the spin and parity of the compound nucleus (starting from the smallest value of  $J$ ). For computers which do not distinguish between +0 and -0 the minus sign must be supplemented by the indicator of the number
2.  $N$ , the number of possible  $l$  values for the given  $J$ ,  $\pi$  and  $E$
3. The number of cards for the given set of  $J$ ,  $\pi$  and  $E$
4.  $l_{\min}$ , the smallest value of  $l$  for the given  $J$ ,  $\pi$  and  $E$
5.  $l_{\max}$ , the greatest value of  $l$  for the given  $J$ ,  $\pi$  and  $E$
6.  $D_{J\pi}$ , the average distance between the levels in this system
- XVI. 1. Average radiation width,  $\bar{\Gamma}_{\gamma, J, \pi}$
2. Number of degrees of freedom for this,  $\nu_{\gamma, J, \pi}$   
( $\nu = 0$  means that the width is not subject to fluctuations)
3. Average fission width,  $\bar{\Gamma}_{f, J, \pi}$
4. Average number of degrees of freedom for this,  $\nu_{f, J, \pi}$
5. Average reduced neutron width for  $l = l_{\min}$ ,  $\bar{\Gamma}_{n, J, l_{\min}}^{\circ}$
6. Number of degrees of freedom for this,  $\nu_{n, J, \pi}$

If  $l_{\max} \neq l_{\min}$ , the data on  $\bar{\Gamma}_{n, J, l}^{\circ}$  for  $l > l_{\min}$  and the corresponding degrees of freedom are punched on subsequent cards in the format of positions 5 and 6 of card X.

Data for reactions other than elastic scattering, radiative capture and fission (if these appear in the list on card IV and similar cards)

- XVII. 1. The number of reactions not already considered which would be possible for the given  $J$ ,  $\pi$  and  $E$
- 2-6. Reserve
- XVIII. 1. PCN for the first reaction
2. The number of possible  $l'$ -values for this reaction (= -1, if the reaction is not characterized by the angular momentum of the secondary particles; = 0 if the reaction is impossible for the given values of  $J$ ,  $\pi$  and  $E$ )
3. The number of cards with information on this reaction
4. The first value of  $l'$ . If the reaction being considered is inelastic scattering with excitation of a definite level in the target nucleus, then  $l'$  can be given with a minus sign. This means that the neutron width of the output channel must be calculated from the equation

$$\Gamma_{in, l'} = \mathcal{E}_{j, l}(I', l') \cdot \Gamma_{n, j}^{(l')} \cdot P_{l'}(E - E_x),$$

$$\mathcal{E}_{j, l}(I', l') = \begin{cases} 0, & \text{if neither } j_1 \text{ or } j_2 \text{ satisfy inequality (A);} \\ 1, & \text{if either } j_1 \text{ or } j_2 \text{ satisfies inequality (A);} \\ 2, & \text{if both } j_1 \text{ and } j_2 \text{ satisfy inequality (A)} \end{cases}$$

$$(A) \quad |j - l| \leq j_{1,2} \leq j + l$$

where

$$j_{1,2} = I' \pm 1/2,$$

$I'$  is the spin of the excited level of the target nucleus (see position 6);  $\Gamma_{n,J}^{(e)}$  is the reduced neutron width for the given level system (its value is given on a punched card of type X);

$P_{g'}$  is the penetrability of the output channel;

$E_x$  is the level energy (see position 5)

5. The average reduced width for the given reaction and the given value of  $l'$  when  $l' > 0$ , or  $E_x$ , the energy of the level excited in inelastic scattering if  $l' < 0$
6. The number of degrees of freedom for this reaction for the given value of  $l' > 0$ , or  $\pm 1$ , the spin and parity of the excited level in the target nucleus (if  $l' < 0$ ). In the last case, with computers which do not distinguish between +0 and -0, the minus sign must be supplemented by the indicator of the number.

If the number of  $l'$  values is greater than 1, the information for the other values is punched on subsequent cards in the format of positions 4-6 of card XII. Cards XVIII and subsequent cards are repeated for each reaction.

Cards XV and subsequent cards are repeated for each level system. Cards XIV and subsequent cards are repeated for each energy point (sub-interval) for which average resonance parameters are given. Cards III and subsequent cards are repeated for each isotope.

### III.2.5 Card format for representing data on the temperature and energy dependences of cross-sections of a number of reactions in the section for the total cross-section

(a) General information for the case  $n_2 \neq 0$ ,  $n_3 \neq 0$

1. RTN
2. The number of sub-groups if this is the same for all energies (=  $n_2$ )
3. The number of cards for the given RTN
4. The INT number defining the temperature interpolation law for the cross-sections and sub-group weightings. The interpolation law for all cross-sections must be identical for all the reactions. This law is defined by the three highest-priority digits of INT. The energy interpolation law for the sub-group weightings is defined by the three middle digits of the INT number. The interpolation over temperature of the cross-sections and sub-group weightings must follow the same law, which is given by the last three digits of INT.

5. The number of temperatures if the temperature dependence of the cross-sections is described ( $n_3 > 1$ ) or unity
6. An indicator which defines the recommended algorithm for calculating the average group cross-sections in terms of the subgroup parameters (see RTN = 121, card IV, position 6)

- II.
1. The number of reactions (including the total cross-section) for which cross-sections are given together with the total cross-section. A minus sign is added if the elastic scattering cross-section can be derived as the difference between the total cross-section and the sum of the cross-sections of all the other reactions
  2. PCN of the total cross-section (= 001)
  3. PCN of the first reaction whose cross-section is given
  4. PCN of the second reaction (or 0 if this does not exist) etc., with continuation where necessary onto subsequent cards in the format of positions 3-6 of card II

(b) Presentation of temperature values (if  $n_3 > 1$ )

- III.
1.  $T_1$
  2.  $T_2$  etc., with continuation on subsequent cards if the number of temperatures is greater than 6

(c) Data on cross-sections

The format depends on the RTN and the number of reactions.

Case 1. One sub-group, one temperature ( $n_2=n_3=1$ )

RTN = 511, two reactions

RTN = 511, number of reactions  
greater than 2

IV	1	$E_1.$	IV	1	$E_1.$	
	2	$\sigma_2(E_1).$		2	$\sigma_2(E_1)$	
	3	$\sigma_{21}(E_1).$		3	$\sigma_{21}(E_1)$	
	4	$E_2.$		4	$\sigma_{22}(E_1)$	
	5	$\sigma_2(E_2).$		5	$\sigma_{23}(E_1)$	or reserve
	6	$\sigma_{21}(E_2).$		6	$\sigma_{24}(E_1)$	or reserve

and so on for all values of energy.

Case 2 Several sub-groups, one temperature ( $n_2 > 1, n_3 = 1$ )

Example for FTN = 521 (3 reactions)

Example for FTN = 531 (2 reactions)

- IV
- 1  $E_1$
  - 2 Number of sub-groups for the given energy
  - 3  $a_1(E_1)$ .
  - 4  $\sigma_1^{(1)}(E_1)$ .
  - 5  $\sigma_{21}^{(1)}(E_1)$ .
  - 6  $\sigma_{22}^{(1)}(E_1)$ .

- IV
- 1  $E_1$
  - 2 Number of sub-groups
  - 3  $a_1(E_1)$ .
  - 4  $\sigma_1^{(1)}(E_1)$ .
  - 5  $\sigma_{21}^{(1)}(E_1)$ .
  - 6  $a_2(E_1)$ .

- V
- 1  $a_2(E_1)$ .
  - 2  $\sigma_2^{(2)}(E_1)$ .
  - 3  $\sigma_{21}^{(2)}(E_1)$ .
  - 4  $\sigma_{22}^{(2)}(E_1)$ .
  - 5 } Reserve
  - 6 } Reserve

- V
- 1  $\sigma_1^{(2)}(E_1)$ .
  - 2  $\sigma_{21}^{(2)}(E_1)$ .
  - 3  $a_3(E_1)$ .
  - 4  $\sigma_1^{(3)}(E_1)$ .
  - 5  $\sigma_{21}^{(3)}(E_1)$ .
  - 6 Reserve

and so on for all values of energy.

Case 3 One sub-group, several temperatures ( $n_2 = 1, n_3 > 1$ )

Example for FTN = 513 (3 reactions)

Example for FTN = 514 (2 reactions)

- IV
- 1  $E_1$ .
  - 2  $\sigma_2(E_1, T_1)$ .
  - 3  $\sigma_2(E_1, T_2)$ .
  - 4  $\sigma_2(E_1, T_3)$ .
  - 5  $\sigma_{21}(E_1, T_1)$ .
  - 6  $\sigma_{21}(E_1, T_2)$ .

- IV
- 1  $E_1$ .
  - 2  $\sigma_2(E_1, T_1)$ .
  - 3  $\sigma_2(E_1, T_2)$ .
  - 4  $\sigma_2(E_1, T_3)$ .
  - 5  $\sigma_2(E_1, T_4)$ .
  - 6  $\sigma_{21}(E_1, T_1)$ .

- V
- 1  $\sigma_{21}(E_1, T_3)$ .
  - 2  $\sigma_{22}(E_1, T_1)$ .
  - 3  $\sigma_{22}(E_1, T_2)$ .
  - 4  $\sigma_{22}(E_1, T_3)$ .
  - 5 } Reserve
  - 6 } Reserve

- V
- 1  $\sigma_{21}(E_1, T_2)$ .
  - 2  $\sigma_{21}(E_1, T_3)$ .
  - 3  $\sigma_{21}(E_1, T_4)$ .
  - 4 } Reserve
  - 5 } Reserve
  - 6 }

and so on for all values of energy.

Case 4 Several sub-groups, several temperatures ( $n_2 > 1, n_3 > 1$ )

Example for FTN = 523 (2 reactions)

Example for FTN = 532 (3 reactions)

- IV
- 1  $E_1$
  - 2 Number of sub-groups = 2
  - 3  $a_1(E_1, T_1)$ .
  - 4  $a_1(E_1, T_2)$ .
  - 5  $a_1(E_1, T_3)$ .
  - 6  $\sigma_1^{(1)}(E_1, T_1)$ .

- IV
- 1  $E_1$
  - 2 Number of sub-groups = 3
  - 3  $a_1(E_1, T_1)$ .
  - 4  $a_1(E_1, T_2)$ .
  - 5  $\sigma_1^{(1)}(E_1, T_1)$ .
  - 6  $\sigma_1^{(1)}(E_1, T_2)$ .

- V
- 1  $\sigma_1^{(1)}(E_1, T_2)$ .
  - 2  $\sigma_1^{(1)}(E_1, T_3)$ .
  - 3  $\sigma_{21}^{(1)}(E_1, T_1)$ .
  - 4  $\sigma_{21}^{(1)}(E_1, T_2)$ .
  - 5  $\sigma_{21}^{(1)}(E_1, T_3)$ .
  - 6  $a_2(E_1, T_1)$ .

- V
- 1  $\sigma_{21}^{(1)}(E_1, T_1)$ .
  - 2  $\sigma_{21}^{(1)}(E_1, T_2)$ .
  - 3  $\sigma_{21}^{(1)}(E_1, T_1)$ .
  - 4  $\sigma_{22}^{(1)}(E_1, T_2)$ .
  - 5  $a_2(E_1, T_1)$ .
  - 6  $a_2(E_1, T_2)$ .

- VI
- 1  $a_2(E_1, T_2)$ .
  - 2  $a_2(E_1, T_3)$ .
  - 3  $\sigma_2^{(2)}(E_1, T_1)$ .
  - 4  $\sigma_2^{(2)}(E_1, T_2)$ .
  - 5  $\sigma_2^{(2)}(E_1, T_3)$ .
  - 6  $\sigma_{21}^{(2)}(E_1, T_1)$ .

- VI
- 1  $\sigma_2^{(2)}(E_1, T_1)$ .
  - 2  $\sigma_2^{(2)}(E_1, T_2)$ .
  - 3  $\sigma_{21}^{(2)}(E_1, T_1)$ .
  - 4  $\sigma_{21}^{(2)}(E_1, T_2)$ .
  - 5  $\sigma_{22}^{(2)}(E_1, T_1)$ .
  - 6  $\sigma_{22}^{(2)}(E_1, T_2)$ .

- VII
- 1  $\sigma_{21}^{(2)}(E_1, T_2)$ .
  - 2  $\sigma_{21}^{(2)}(E_1, T_3)$ .
  - 3
  - 4 } Reserve
  - 5 }
  - 6

- VII
- 1  $a_3(E_1, T_1)$ .
  - 2  $a_3(E_1, T_2)$ .
  - 3  $\sigma_2^{(3)}(E_1, T_1)$ .
  - 4  $\sigma_2^{(3)}(E_1, T_2)$ .
  - 5  $\sigma_{21}^{(3)}(E_1, T_1)$ .
  - 6  $\sigma_{21}^{(3)}(E_1, T_2)$ .

- VIII
- 1  $\sigma_{22}^{(3)}(E_1, T_1)$ .
  - 2  $\sigma_{22}^{(3)}(E_1, T_2)$ .
  - 3
  - 4 } Reserve
  - 5 }
  - 6

and so on for all values of energy. The superscript in brackets denotes the sub-group number.

(d) FTN with  $n_1 = 5$  and  $n_2 = 0$  or  $n_3 = 0$

Only one card is required:

1. FTN
2. Reserve
3. Number of cards for this FTN (= 1)
4. } Reserve
5. }
6. }

This card refers for its information to the section dealing with the total cross-section (if  $n_3 = 0$  and  $n_2 \neq 0$ ) or to the section referring to the first temperature (if  $n_2 = 0$ )

### III.3. Angular distributions of secondary particles (GCN = 02)

The angular distribution of secondary particles  $f(\theta)$  is a normalized scattering probability distribution,

$$f(\theta) = \frac{\int \sigma(\theta, \varphi) d\varphi}{\iint \sigma(\theta, \varphi) d\varphi d\theta}$$

which can be given for a whole energy interval as well as at individual energy points. The following normalization condition is assumed:

$$\int_0^\pi f(\theta) \sin \theta d\theta = 1.$$

Provision is made for the specification of angular distributions at discrete points as a function of  $\mu$ , where  $\mu = \cos \theta$ ,  $\theta$  being the scattering angle (the  $\mu$  representation). The second possible representation is parametrical in the form of  $\omega_\ell$  coefficients of the  $f(\theta)$  expansion in Legendre polynomials,  $P_\ell(\cos \theta)$  (the  $\omega$  representation):

$$f(\theta) = \frac{1}{2} \left[ 1 + \sum_{\ell=1}^n \omega_\ell P_\ell(\cos \theta) \right].$$

The  $\mu$  values are given in increasing magnitude from -1 to +1. The scattering angle  $\theta$  can be either in the centre-of-mass system, or in the laboratory system; indication as to which of the two coordinate systems is used for a particular data set is given as additional information in the FTN heading in the form of a numerical indicator,  $co$ , which is 1 if the data are in the CM system, and 2 if the data are in the laboratory system.

The system used depends on the type of reaction. In the case of elastic scattering and inelastic scattering with excitation of individual nuclear levels, where a simple relationship exists between the energies of the primary and secondary particles, it is probably sensible to choose the CM system. For other inelastic processes data are usually given in the laboratory system. In this connection, the following point must be kept in mind. Where a simple analytical expression relating the angular and energy dependences in these two systems of coordinates exists, it is not particularly important which of the two systems is used for data storage. If, however, no such analytical expression exists, the choice of the coordinate system cannot be arbitrary. The decisive factors are then the availability of data in either of the two systems, the users' requirements and the computer processing capabilities.

In the case of a  $\mu$  representation of the data, the choice of E and  $\mu$  values must be such that the probability for any energy and scattering angle can be obtained with sufficient accuracy by interpolation between values stored in the library. In the case of an  $\omega$  representation, the necessary accuracy is guaranteed by specifying a sufficiently large number (n) of expansion coefficients.

Even though an angular distribution is given as a normalized probability function, it is generally impossible to say, in cases where the actual angular distribution in the  $\mu$  representation is roughly approximated, say, by linear intervals, that the resulting representation will be normalized. It may therefore be necessary in some cases to carry out additional normalization of the angular distributions obtained from the data files.

The formats provide for storage of a total angular distribution  $f(\theta)$  in the form of a linear combination of a number of partial distribution functions  $f_i(\theta)$ , each of which has a given weight  $a_i$  such that

$$f(\theta) = \sum_{i=1}^k a_i f_i(\theta).$$

Individual  $f_i(\theta)$  could describe, for example, the angular distributions of the products of some nuclear process which proceeds along different paths and can therefore be described by means of different mechanisms. The present facility also makes it possible to use a sub-group representation to describe the resonance structure of angular distributions. In this case the  $a_i$  are sub-group weighting factors and  $f_i(\theta)$  characterizes the angular distribution of a particular neutron sub-group.

The current formats require that all related partial distribution functions  $f_i(\theta)$  be given in the same representation (either in the  $\mu$  or  $\omega$  form) and in the same coordinate system. However, the FTN structure is such that this restrictive condition can be relaxed if necessary.



In all cases, the total energy range covered by the angular distributions must coincide with that covered by the corresponding integral cross-sections. If, for instance, an elastic scattering cross-section is specified in the energy range 0.001 eV to 14 MeV, then in a point-by-point energy representation, the first angular distribution must be for 0.001 eV and the last for 14 MeV; in the case of a range representation, the lower energy boundary of the first range must be 0.001 eV and the upper boundary of the last range must be 14 MeV. This rule can also help to show up gross errors in the stored data.

III.3.1 FTN classification for GCN = 02 \*)

The manner of presenting angular distribution data is specified by the high-priority FTN digit according to the following table:

$n_1$	Type of angular distribution representation
1	At discrete points as a function of $\mu$ ( $\mu$ representation)
2	Parametrically in the form of coefficients for a series expansion in Legendre polynomials ( $\omega$ representation)

Subsequent  $n_1$  values (3-9) are reserved for any new data representation forms that may be formulated.

The low-priority FTN digits have the following meaning when  $n_1 = 1$  and  $n_1 = 2$ :

- $n_2$  - specifies the number of variables or parameters on which the angular distributions can depend
- $n_3$  - specifies the internal order of priority of these parameters

For two variables (energy E and the probability of the angular distribution or the sub-group weighting coefficient  $a_i$ ), the meaning of the low priority FTN digits is defined by the following table:

$n_2 n_3$	High priority variable	Low priority variable
01	-	-
02	-	-
11	E	-
12	$a_i$	-
21	E	$a_i$
22	$a_i$	E

\*) See also p. 67 (note by editor)

III.3.2 Card format for GCN = 02 \*)

- I. 1. RTN  
2. Number of energy intervals  $\Delta E$  for this RTN  
3. A, atomic weight  
4-6. Reserve
  
- II. 1.  $E_H$   
2.  $E_B$   
3. Number of cards for this  $\Delta E$ , including the present card  
4. Number of groups of secondary particles for which angular distributions are specified in this  $\Delta E$   
5-6. Reserve
  
- III. 1. Indicator identifying the secondary-particle group  
2. Number of F'TNs assigned to angular distributions for this group of particles  
3. Number of cards to represent the angular distributions in this group, including this card  
4. } Reserved for additional information on this group of secondary  
5. } particles  
6. }

The format of subsequent cards depends on the F'TN.

Case (1) Isotropic angular distribution in  $\Delta E$

In this case card IV specifies only the Form Type Number (F'TN = 101 for the  $\mu$  representation, F'TN = 201 for the  $\omega$  representation) and the indicator identifying the coordinate system.

- |                                    |                                    |
|------------------------------------|------------------------------------|
| IV. 1. F'TN = 101                  | IV. 1. F'TN = 201                  |
| 2. Coordinate system indicator, co | 2. Coordinate system indicator, co |

Case (2) Angular distribution for the whole  $\Delta E$

- |  |                                    |
|--|------------------------------------|
| IV. 1. F'TN = 102  | IV. 1. F'TN = 202                  |
| 2. Coordinate system indicator, co   | 2. Coordinate system indicator, co |
| 3. Number of $\mu$ values  | 3. Number of $\omega$ values       |
| 4. INT number determining the method of interpolating $f(\mu)$ with respect to $\mu$ | 4. $\omega_1$                      |
| 5. $\mu_1$   | 5. $\omega_2$                      |
| 6. $f(\mu_1)$  | 6. $\omega_3$                      |

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\*) See also p. 67 (note by editor)

Case\_(3) Angular distributions at fixed E values

- |     |    |  |     |    |   |
|-----|----|--|-----|----|---|
| IV. | 1. | FTN = 111  | IV. | 1. | FTN = 211   |
|     | 2. | Number of E values   |     | 2. | Number of E values  |
|     | 3. | Number of cards for this FTN   |     | 3. | Number of cards for this FTN  |
|     | 4. | Coordinate system indicator, co  |     | 4. | Coordinate system indicator, co   |
|     | 5. | INT number determining the method of interpolating over E and $\mu$              |     | 5. | INT number determining the method of interpolating $\omega_2$ over E                |
|     | 6. | Number of values of $\mu$ , if it is the same for the whole $\Delta E$ , or zero |     | 6. | Number of values of $\omega$ , if it is the same for the whole $\Delta E$ , or zero |
| V.  | 1. | E  | V.  | 1. | E   |
|     | 2. | Number of $\mu$ values   |     | 2. | Number of $\omega$ values   |
|     | 3. | $\mu_1$  |     | 3. | $\omega_1$  |
|     | 4. | $f(\mu_1)$ etc.  |     | 4. | $\omega_2$ etc.   |

Case\_(4) Superposition of angular distributions for the whole  $\Delta E$

- |     |    |   |     |      |                                 |
|-----|----|---|-----|------|---------------------------------|
| IV. | 1. | FTN = 112   | IV. | 1.   | FTN = 212                       |
|     | 2. | Number of a values  |     | 2.   | Number of a values              |
|     | 3. | Number of cards for this FTN  |     | 3.   | Number of cards for this FTN    |
|     | 4. | Coordinate system indicator, co   |     | 4.   | Coordinate system indicator, co |
|     | 5. | INT number determining the method of interpolating $f(\mu)$ with respect to $\mu$ |     | 5-6. | Reserve                         |
|     | 6. | Reserve   |     |      |                                 |
| V.  | 1. | a   | V.  | 1.   | a                               |
|     | 2. | Number of $\mu$ values  |     | 2.   | Number of $\omega$ values       |
|     | 3. | $\mu_1$   |     | 3.   | $\omega_1$                      |
|     | 4. | $f(\mu_1)$ etc.   |     | 4.   | $\omega_2$ etc.                 |

Case\_(5) Superposition of angular distributions for fixed E values <sup>6/</sup>

- |     |    |                                 |     |    |                                 |
|-----|----|---------------------------------|-----|----|---------------------------------|
| IV. | 1. | FTN = 121                       | IV. | 1. | FTN = 221                       |
|     | 2. | Number of E values              |     | 2. | Number of E values              |
|     | 3. | Number of cards for this FTN    |     | 3. | Number of cards for this FTN    |
|     | 4. | Coordinate system indicator, co |     | 4. | Coordinate system indicator, co |

---

<sup>6/</sup> For the information of evaluators: it is preferable, for reasons of convenience, to process information by the use of FTN = 121 or 221, rather than FTN = 122 or 222.

- |   |   |
|---|---|
| <p>5. INT number determining methods of interpolating <math>a(E)</math> with respect to <math>E</math>, <math>f(E, \mu)</math> with respect to <math>E</math> and <math>f(E, \mu)</math> with respect to <math>\mu</math></p> <p>6. Number of values of <math>\mu</math>, if it is the same for the whole <math>\Delta E</math>, or zero</p>  | <p>5. INT number determining methods of interpolating <math>a(E)</math> with respect to <math>E</math> and <math>\omega_2(E)</math> with respect to <math>E</math></p> <p>6. Number of values of <math>\omega</math>, if it is the same for the whole <math>\Delta E</math>, or zero</p>  |
| <p>V. 1. <math>E</math></p> <p>2. Number of <math>a</math> values</p> <p>3. Number of cards for this <math>E</math></p> <p>4-5. Reserve</p> <p>6. Number of <math>\mu</math> values, if it is the same for all <math>a</math> values, or zero</p>   | <p>V. 1. <math>E</math></p> <p>2. Number of <math>a</math> values</p> <p>3. Number of cards for this <math>E</math></p> <p>4-5. Reserve</p> <p>6. Number of <math>\omega</math> values, if it is the same for all <math>a</math> values, or zero</p>  |
| <p>VI. 1. <math>a</math></p> <p>2. Number of <math>\mu</math> values for this <math>a</math></p> <p>3. <math>\mu_1</math></p> <p>4. <math>f(\mu_1)</math> etc.</p>  | <p>VI. 1. <math>a</math></p> <p>2. Number of <math>\omega</math> values for this <math>a</math></p> <p>3. <math>\omega_1</math></p> <p>4. <math>\omega_2</math> etc.</p>  |
| <p><u>Case_(6)</u> Angular distributions with given <math>a</math> at different <math>E</math> values</p>   |   |
| <p>IV. 1. FTN = 122</p> <p>2. Number of <math>a</math> values</p> <p>3. Number of cards for this FTN</p> <p>4. Coordinate system indicator, <math>co</math></p> <p>5. INT number determining the methods of interpolating <math>a(E)</math> with respect to <math>E</math>, <math>f(E, \mu)</math> with respect to <math>E</math> and <math>f(E, \mu)</math> with respect to <math>\mu</math></p> <p>6. Number of values of <math>E</math>, if it is the same for all values of <math>a</math>, or zero</p> | <p>IV. 1. FTN = 222</p> <p>2. Number of <math>a</math> values</p> <p>3. Number of cards for this FTN</p> <p>4. Coordinate system indicator, <math>co</math></p> <p>5. INT number determining the methods of interpolating <math>a(E)</math> with respect to <math>E</math> and <math>\omega_2(E)</math> with respect to <math>E</math></p> <p>6. Number of values of <math>E</math>, if it is the same for all <math>a</math> values, or zero</p> |
| <p>V. 1. <math>a</math></p> <p>2. Number of <math>E</math> values</p> <p>3. Number of cards for this <math>a</math></p> <p>4-5. Reserve</p> <p>6. Number of <math>\mu</math> values, if it is the same for all <math>E</math>, or zero</p>  | <p>V. 1. <math>a</math></p> <p>2. Number of <math>E</math> values</p> <p>3. Number of cards for this <math>a</math></p> <p>4-5. Reserve</p> <p>6. Number of <math>\omega</math> values if it is the same for all <math>E</math>, or zero</p>  |

VI.	1.	E	1.	E
	2.	Number of $\mu$ values	2.	Number of $\omega$ values
	3.	$\mu_1$	3.	$\omega_1$
	4.	$f(\mu_1)$ etc.	4.	$\omega_2$ etc.

In all the above FTNs, to illustrate the formats of the positions containing angular distribution data, we have given the minimum amount of information, i.e. one pair of  $[\mu, f(\mu)]$  and one value of  $\omega$ . It is assumed that, wherever necessary, this information will be continued on subsequent positions of the same card or on subsequent cards in the above formats.

#### III.4 Energy distributions of secondary particles (GCN = 03)

In the majority of cases, either the energy and angular distributions of the secondary particles emitted in a nuclear reaction are connected by a unique relationship in which the secondary-particle energy for a given angle of emission is rigorously fixed or has a definite probability of taking certain values (elastic scattering, inelastic scattering with excitation of a defined level in the target nucleus), or there is no such correlation and the secondary neutron spectra may be taken to be independent of the angle of emission. GCN = 03 is reserved for these two types of energy distribution. If the secondary-particle spectra vary in a complex way with the angle of emission (inelastic scattering of thermal neutrons), the energy and angular distributions must be given in the file sections corresponding to GCN = 04.

The existing format presupposes that information on the secondary particle spectra  $\varphi(E_0, E)$  ( $E_0$  is the initial energy and  $E$  is the final energy) is given by specifying one of the following laws and defining the parameters involved in it.

Law 1. The emission of particles with known discrete energies (for example, the spectrum of delayed fission neutrons):

$$\varphi(E_0, E) = \sum_{n=1}^N P_n \delta(E - E_n) ; \quad \sum_{n=1}^N P_n = 1.$$

with values given for  $P_n$  and  $E_n$ ,  $n=1, 2, \dots, N$ .

Law 2. Decrease in the energy of scattering by one of the fixed magnitudes  $E_{dn}$  ( $n = 1, 2, \dots, N$ ):

$$\varphi(E_0, E) = \sum_{n=1}^N P_n K_n \delta(E - (E_0 - E_{dn})) ; \quad \sum_{n=1}^N P_n = 1.$$

with values given for  $P_n$ ,  $K_n$  and  $E_{dn}$ .

This law can be used, for example, to give the spectrum for inelastic scattering in a group of N levels. The coefficients  $K_n$  make it possible to allow for the average energy loss per recoil of the product nucleus. For isotropic scattering with excitation of the level  $E_x$

$$K = \frac{M^2+1}{(M+1)^2} \quad ; \quad E_d = \frac{M(M+1)}{M^2+1} E_x .$$

where M is the ratio of the mass of the nucleus to the neutron mass. For anisotropic inelastic scattering the algorithm for calculating K and  $E_d$  is more complicated. The inelastic scattering spectrum for excitation of a definite level is defined more completely by Law 10.

Law 3. Continuous normalized fission-neutron spectrum independent of the initial energy (Watt equation):

$$\varphi(E_0, E) = \frac{2 \cdot e^{-ab/4}}{\sqrt{\pi ab}} \cdot e^{-E/a} \cdot \operatorname{sh} \sqrt{bE} .$$

with values given for a and b.

Law 4. Fission neutron spectrum allowing for the energy dependence of the neutrons causing fission and of the properties of the fissioning nucleus, as in UKNDL:

$$\varphi(E_0, E) = d \frac{E}{T^2} \exp\left(-\frac{E}{T}\right) + (1-d) \cdot \left(\frac{2}{\sqrt{\pi}} B^{3/2}\right) \cdot \sqrt{E} \cdot \exp(-E/B),$$

where  $B = a + b \sqrt{\bar{\nu} + 1}$ ,

$$d = (\sigma_{n,n'f} + \sigma_{n,2nf}) / \bar{\nu} (\sigma_{nf} + \sigma_{n,n'f} + \sigma_{n,2nf}),$$

$$T = c \cdot (E_0 - E_f) / (14 - E_f);$$

Here, a, b and c are constants,  $\bar{\nu}$  is the average number of neutrons emitted per fission,  $E_f$  is the threshold for the reaction (n,n'f),  $\sigma_{n,f}$ ,  $\sigma_{n,n'f}$  and  $\sigma_{n,2nf}$  are the cross-sections of the (n,f), (n,n'f) and (n,2nf) reactions.

Values are given for a, b, c and  $E_f$ . This law can be used only if the file contains the cross-sections for the reactions (n,f), (n,n'f) and (n,2nf) and  $\bar{\nu}$ .

Law 5.  $\varphi(E_0, E)$  is an arbitrary function of  $E$  which does not depend on  $E_0$ :

$$\varphi(E_0, E) = \rho(E).$$

Values are given for the pairs of numbers  $\{E_i, \rho_i\}$  ( $i=0, 1, 2, \dots, \kappa$ ).

$$\int_{E_0}^{E_\kappa} \rho(E) dE = 1.$$

Law 6.  $\varphi(E_0, E)$  is an arbitrary function of  $E/\sqrt{E_0}$ . This law is not recommended for use.

Law 7.  $\varphi(E_0, E)$  is an arbitrary function of the ratio  $x = E/E_0$ :

$$\varphi(E_0/E) = \rho(x).$$

Values are given for the pairs of numbers  $\{x_i, \rho_i\}$  ( $i=0, 1, \dots, \kappa$ )

$$\int_x^{x_\kappa} \rho(x) dx = 1.$$

As a rule,  $0 \leq x \leq 1$ . This condition, however, is not a necessary one.

Law 8.  $\varphi(E_0, E)$  is an arbitrary function of the initial and final energies:

$$\varphi(E_0, E) = \rho(E_0, E).$$

Values are given for the numbers  $\{E_{0i}, E_j, \rho_{ij}\}$

$$(i=1, 2, \dots, M, \quad j=0, 1, \dots, \kappa)$$

$$\int_{E_0}^{E_\kappa} \rho(E_0, E) dE = 1 \quad \text{for any } E_0.$$

Law 9. Truncated evaporation spectrum:

$$\varphi(E_0, E) = \begin{cases} \frac{E}{N'(E_0, u, B)} \cdot e^{-E/T(E_0)}, & B \leq E \leq E_0 - u \\ 0 & , E < B \text{ or } E > E_0 - u, \end{cases}$$

where

$$N'(E_0, u, B) = T^2(E_0) \cdot \left[ \left(1 + \frac{E_0 - B}{T(E_0)}\right) e^{-\frac{(E_0 - B)/T(E_0)}{1 + \frac{E_0 - u}{T(E_0)}}} - \left(1 + \frac{E_0 - u}{T(E_0)}\right) \cdot e^{-\frac{E_0 - u}{T(E_0)}} \right], \quad *)$$

---

\*) This formula is incorrect. For the correct normalization factor see p. 71 (Editor's note)

Values are given for B and u (in MeV) and for the pairs of numbers  $\{E_{0i}, T_i\}$  ( $i = 1, 2, \dots, M$ ).

Law 10.\*) The secondary particle spectrum depends on the angle of emission  $\theta$  and is defined uniquely by the initial energy, the angle of emission and the kinematics of the reaction:

$$\varphi(E_0, E) = \sum_{n=1}^N P_n \delta(E - \mathcal{E}_n(E_0, \theta, \vec{a})),$$

where  $\vec{a}$  is the set of reaction parameters which define the neutron energy.

For inelastic scattering with excitation of a particular level, this set contains the ratio of the nuclear mass to the neutron mass M and the excitation energy  $E_x$ :

$$\mathcal{E}_{1,2}(E_0, \theta, M, E_x) = \frac{E_0}{(M+1)^2} \left\{ 2\mu_L^2 + M \left( 1 - \frac{M+1}{M} \frac{E_x}{E_0} \right) - 1 \pm 2\mu_L \sqrt{\mu_L^2 + M^2 \left( 1 - \frac{M+1}{M} \frac{E_x}{E_0} \right)^2} \right\}$$

where  $\mu_L = \cos \theta$  is the cosine of the scattering angle in the laboratory system of coordinates.

The number  $N = 2$ , if  $\frac{M+1}{M} E_x < E_0 < \frac{M}{M-1} E_x$

then  $P_1 = \frac{1}{2} f(\mu_{c1})$ ,  $P_2 = \frac{1}{2} f(\mu_{c2})$ ,

where  $\mu_{c1}$  and  $\mu_{c2}$  are the roots of the equation which relates the cosine  $\mu_c$  of the scattering angle in the centre of mass system to the cosine  $\mu_L$  of the scattering angle in the laboratory system of coordinates.

$\frac{1}{2} f(\mu_c)$  is the angular distribution in the centre of mass system:

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

If  $\mu_{c1} > \mu_{c2}$ , the plus sign is taken for  $\mathcal{E}_1$  and the minus sign for  $\mathcal{E}_2$ . When  $E_0 > \frac{M}{M+1} E_x$ , the connection between  $\mu_c$  and  $\mu_L$  is single valued, so that  $N = 1$ ,  $P_1 = 1$ ,  $P_2 = 0$  and  $\mathcal{E}$  takes only positive value. For elastic scattering  $E_x = 0$ .

Law 11. Maxwellian spectrum:

$$\varphi(E_0, E) = \left( \frac{2}{\pi^{1/2}} T^{3/2} \right) \sqrt{E} e^{-E/T(E_0)}.$$

Values are given for the pairs of numbers  $\{E_{0i}, T_i\}$  ( $i = 1, 2, \dots, M$ ).

---

\*) For changes and additions to law no. 10 see p. 63-64.  
(Note by editor)



Law 12. Spectra of neutrons emitted in the reactions (n,2n) and (n,3n) in accordance with the sequential evaporation model.

(a) In the region below the threshold of the (n,3n) reaction

Spectrum of primary neutrons from the reaction (n,2n):

$$\varphi_{1,2n}^a(E_0, E_1) = \frac{E_1 \cdot e^{-E_1/T(E_0)}}{T_1^2(E_0) \cdot \left[ 1 - \left( 1 + \frac{E_0 - B_1}{T_1(E_0)} \right) \cdot e^{-(E_0 - B_1)/T_1(E_0)} \right]}$$

Spectrum of secondary neutrons from the reaction (n,2n)

$$\varphi_{2,2n}^a(E_0, E_2) = C_2 \cdot E_2 \int_0^{E_0 - B_1} dE_1 \cdot E_1 \cdot e^{-E_1/T_1(E_0)} \cdot e^{-E_2/T_2(E_0 - E_1 - B_1)}$$

or approximately:

$$\varphi_{2,2n}^a(E_0, E_2) = C_2' \cdot E_2 \cdot e^{-\frac{E_2}{T(E_0 - B_1)}} \cdot \frac{\sqrt{E_0 - B_1}}{\sqrt{E_0 - B_1 - E_2}}$$

The normalizing constants  $C_2$  and  $C_2'$  are calculated by numerical integration.

(b) In the region above the threshold of the (n,3n) reaction

Spectrum of primary neutrons from the (n,2n) reaction

$$\varphi_{1,2n}^b(E_0, E_1) = \begin{cases} C_{12} \cdot E_1 \cdot e^{-E_1/T_1(E_0)}, & E_0 - B_1 - B_2 \leq E_1 \leq E_0 - B_1 \\ C_{12} \cdot E_1 \cdot [1 - P_3(E_1)] \cdot e^{-E_1/T_1(E_0)}, & 0 \leq E_1 \leq E_0 - B_1 - B_2 \end{cases}$$

$$\text{where } P_3(E_1) = \frac{\int_0^{E_0 - E_1 - B_1 - B_2} \varphi_{2,2n}^a(E_2) dE_2}{\int_0^{E_0 - E_1 - B_1 - B_2} \varphi_{2,2n}^a(E_2) dE_2},$$

(see above for the equation for  $\varphi_{2,2n}^a(E_2)$ ), and  $C_{12}$  is calculated from the normalization condition

$$\int_0^{E_0 - B_1} I_{12}^b(E_1) dE_1 = 1.$$

Spectrum of secondary neutrons from the (n,2n) reaction

$$\varphi_{2,2n}^b = \begin{cases} C_{22} \cdot E_2 \int_0^{E_0 - B_1} dE_1 \cdot E_1 \cdot e^{-E_1/T_1(E_0)} \cdot e^{-E_2/T_2(E_0 - E_1 - B_1)}, & E_0 - B_1 - B_2 \leq E_2 \leq E_0 - B_1 \\ C_{22} \cdot E_2 \cdot [1 - P_3(E_2)] \int_0^{E_0 - B_1} dE_1 \cdot E_1 \cdot e^{-E_1/T_1(E_0)} \cdot e^{-E_2/T_2(E_0 - E_1 - B_1)}, & 0 \leq E_2 \leq E_0 - B_1 - B_2 \end{cases}$$

or approximately,

$$\varphi_{2,3n}^b = \begin{cases} C'_{22} \cdot E_2 \cdot e^{-\frac{E_2}{T(E_0-B_1)}} \cdot \frac{\sqrt{E_0-B_1}}{\sqrt{E_0-B_1-E_2}}, & E_0-B_1-B_2 \leq E_2 \leq E_0-B_1 \\ C'_{22} \cdot E_2 \cdot [1-q_3(E_2)] \cdot e^{-\frac{E_2}{T(E_0-B_1)}} \cdot \frac{\sqrt{E_0-B_1}}{\sqrt{E_0-B_1-E_2}}, & 0 \leq E_2 \leq E_0-B_1-B_2 \end{cases}$$

where

$$q_3(E_2) = \frac{\int_0^{E_0-B_1-B_2} \varphi_1(E_1) dE_1}{\int_0^{E_0-B_1-E_2} \varphi_1(E_1) dE_1} = \frac{1 - \left(1 + \frac{E_0-B_1-B_2-E_2}{T_1(E_0)}\right) \cdot e^{-\frac{E_0-B_1-B_2-E_2}{T(E_0)}}}{1 - \left(1 + \frac{E_0-B_1-E_2}{T_1(E_0)}\right) \cdot e^{-\frac{E_0-B_1-E_2}{T(E_0)}}}$$

$C_{22}$  and  $C'_{22}$  are determined from the normalization condition

$$\int_0^{E_0-B_1} \varphi_{2,3n}^b(E_2) dE_2 = 1.$$

Spectrum of primary neutrons from the (n,3n) reaction

$$\varphi_{1,3n} = C_{13} \cdot E_1 \cdot e^{-E_1/T_1(E_0)} \cdot P_3(E_1)$$

(see above for the equation for  $P_3(E_1)$ ).  $C_{13}$  is determined from the normalization condition:

$$\int_0^{E_0-B_1-B_2} \varphi_{1,3n}(E_1) dE_1 = 1.$$

Spectrum of secondary neutrons from the (n,3n) reaction

$$\varphi_{2,3n} = C_{23} E_2 \cdot q_3(E_2) \int_0^{E_0-B_1} dE_1 E_1 \cdot e^{-E_1/T_1(E_0) - E_2/T_2(E_0-E_1-B_1)},$$

where  $C_{23}$  is determined from the normalization condition

$$\int_0^{E_0-B_1-B_2} \varphi_{2,3n}(E_2) dE_2 = 1$$

Spectrum of tertiary neutrons from the (n,3n) reaction

$$\varphi_{3,3n} = C_{33} \cdot E_3 \int_0^{E_0-B_1-B_2} E_2 dE_2 \int_0^{E_0-B_1-E_2} E_1 dE_1 \cdot e^{-E_1/T_1(E_0) - E_2/T_2(E_0-B_1-E_1) - E_3/T_3(E_0-B_1-E_2-E_2)}$$

or approximately

$$\psi_{3,3n} = C_{33} \cdot E_3 \cdot e^{-\frac{E_3}{T(E_0 - B_1 - B_2)}} \cdot \frac{\sqrt{E_0 - B_1 - B_2}}{\sqrt{E_0 - B_1 - B_2 - E_3}},$$

where  $C_{33}$  and  $C'_{33}$  are determined from the normalization condition

$$\int_0^{E_0 - B_1 - B_2} \psi_{3,3n}(E_3) dE_3 = 1.$$

Calculation of the spectra from these equations requires that the parameters  $B_1$  and  $B_2$  (the neutron binding energies in the target nucleus and in the product nucleus from the  $(n,2n)$  reaction) and the energy dependences of the temperature,  $T_1(E)$ ,  $T_2(E)$  and  $T_3(E)$ , be given. If an estimate shows that  $T_1(E) = T_2(E) = T_3(E) = T(E)$ , then only  $T(E)$  is given. The decision whether or not to use the approximate equations depends on whether the appropriate processing programmes are available.

Law 13: See p. 65 (Note by editor)

As in the case of angular distributions, the formats for the secondary particle energy distributions require the final distributions to be given as a superposition of a certain number of laws with their individual probabilities. Each law corresponds to one of the possible mechanisms for the nuclear reaction.

This possibility can in principle also be interpreted as a sub-group representation of the secondary-particle energy distribution. The probabilities of the different laws are then equivalent to the sub-group weights and the laws themselves characterize the energy distributions for the corresponding neutron sub-groups. The choice between one interpretation and the other is governed by whether or not the file contains the sub-group representation of the total cross-section and the cross-section of the corresponding reaction for the given energy range and whether or not the sub-group weights given in the section for the total cross-section are equal to the probabilities of the laws.

#### III.4.1 F<sup>2</sup>TN classification for GCN = 03

The manner in which the data on secondary-particle energy distributions are stored is determined by the high-priority F<sup>2</sup>TN digit, according to the following table:

$n_1$	Method of energy-distribution presentation
1	In the form of laws, when the initial energy is not given explicitly
2	In the form of laws, when the initial energy is given explicitly

Subsequent values of  $n_1$  (3-9) are reserved for any other presentation forms that may be used.

The two low-priority FTN digits have the following meaning:

$n_2n_3 = 01-49$  are reserved for specifying the distribution by means of a single law and indicate the number of the corresponding law

$n_2n_3 \geq 50$  are reserved for specifying the distribution in the form of a superposition of laws in the following cases:

$n_2n_3 = 50$ :  $E_0$  is not given explicitly

$n_2n_3 = 51$ : all laws for a given  $E_0$

$n_2n_3 = 52$ : all  $E_0$  for a given law

### III.4.2 Card format for GCN = 03

- I.
  - 1. RTN
  - 2. The number of  $\Delta E$  for this RTN
  - 3-6. Reserve
  
- II.
  - 1.  $E_H$
  - 2.  $E_B$
  - 3. The number of cards for this  $\Delta E$ , including this card
  - 4. The number of secondary-particle groups for which energy distributions are given in this  $\Delta E$
  - 5-6. Reserve
  
- III.
  - 1. Indicator identifying a given secondary-particle group
  - 2. Number of FTNs assigned to the energy distributions for this group of particles
  - 3. Number of cards used to represent the energy distribution of this group, including this card
  - 4-6. Reserve

The format of the following cards depends on the FTN.

- 1. Law 1
  
- IV.
  - 1. FTN = 101
  - 2. N, number of discrete energies with which particles are emitted
  - 3.  $E_{d1}$
  - 4.  $p(E_{d1})$
  - 5.  $E_{d2}$
  - 6.  $p(E_{d2})$

with continuation on subsequent cards if  $N > 2$ .

2. Law 2

- IV. 1. FTN = 102  
2. N, the number of  $\{E_d, K\}$  pairs  
3. Reserve  
4.  $E_{d1}$   
5.  $K_1$   
6.  $p(E_{d1})$

with continuation on subsequent cards if  $N > 1$ .

3. Laws 3 and 4

- IV. 1. FTN = 103  
2. A  
3. B  
4-6. Reserve

- IV. 1. FTN = 104  
2. a  
3. b  
4. c  
5.  $E_f$   
6. Reserve

4. Laws 5, 6 and 7

- IV. 1. FTN = 105 (or 106, or 107)  
2. Number of points in the spectrum  
3. Reserve  
4. INT number, defining the interpolation law for  $p(x)$  with respect to  $x$   
5.  $x_1$   
6.  $p(x_1)$

with continuation on subsequent cards

5. Law 8

- IV. 1. FTN = 208  
2. Number of  $E_0$  values  
3. Number of cards for this FTN  
4. INT number defining the interpolation law for  $p(E_0, E)$  with respect to  $E_0$  and  $E$   
5-6. Reserve

- V. 1.  $E_{01}$   
2. Number of  $E$  values for this  $E_0$   
3.  $E_1$   
4.  $p(E_{01}, E_1)$   
5.  $E_2$   
6.  $p(E_{01}, E_2)$

6. Law 9

- IV. 1. FTN = 209  
2. Number of  $E_0$  values  
3. Number of cards for this FTN  
4. INT number defining the interpolation law for T with respect to  $E_0$   
5. B  
6. u

- V. 1.  $E_{01}$   
2.  $T(E_{01})$ , etc.

7. Law 10

- IV. 1. FTN = 110  
2-6. Reserve

8. Law 11

- IV. 1. FTN = 211  
2. Number of  $E_0$  values. Zero is punched if the temperature of the Maxwellian spectrum is equal to the temperature of the medium  
3. Number of cards for this FTN  
4. INT number defining the interpolation law for T with respect to  $E_0$   
5-6. Reserve

- V. 1.  $E_{01}$   
2.  $T(E_{01})$ , etc.

9. Law 12

- IV. 1. FTN = 212  
2. ITEM number, showing for which temperatures the energy dependences are given I  
ITEM = 111,  $T_1(E) = T_2(E) = T_3(E) = T(E)$ ;  $T(E)$  is given  
ITEM = 123,  $T_1(E)$ ,  $T_2(E)$  and  $T_3(E)$  are given  
ITEM = 122,  $T_1(E)$  and  $T_2(E)$  are given;  $T_3(E) = T_2(E)$   
ITEM = 121,  $T_1(E)$  and  $T_2(E)$  are given;  $T_3(E) = T_1(E)$   
ITEM = 113,  $T_1(E)$  and  $T_3(E)$  are given;  $T_2(E) = T_1(E)$

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I If the (n,3n) reaction is not possible, the lowest-priority digit of the ITEM number is also unimportant and can be taken equal to zero.

3. Number of cards for this FTN
  4. INT number, defining the interpolation law for  $T_1$ ,  $T_2$  and  $T_3$  with respect to E
  5.  $B_1$
  6.  $B_2$  (if the (n,3n) reaction is possible), or zero
- V.
1. The number of  $E_0$  for the first of the given temperatures
  2. Reserve
  3.  $E_{01}$
  4.  $T_1(E_{01})$ , etc.

The data for the energy dependences of the remaining temperatures are given in a similar way.

10. Linear combination of laws \*)

- IV.
1. FTN (= 150, 252) \*\*)
  2. Number of different laws in the combination
  3. Number of cards for this FTN
  - 4-6. Reserve
- V.
1. FTN of the first law
  2. Corresponding probability
  3. FTN of the second law
  4. Corresponding probability

and so on for all the laws in the combination.

Subsequent cards contain information on the laws in the combination, with the format for each law the same as that already described.

III.5 Energy-angular distributions of thermal neutrons (GCN = 04)

The data on energy-angular distributions for thermal-neutron scattering characterize the interaction of neutrons with atomic nuclei in the energy region where the relative motion of the neutron and nucleus as well as atomic interactions (e.g. chemical bond effects etc.) have to be taken into account. Such information may be presented in different ways. At present, the formats provide for the representation of thermal-neutron energy-angular distributions in the form of a matrix of twice differential cross-sections and in the form of a scattering law.

In the first case, a matrix of numerical values is given for the function  $(E_0 \rightarrow E, \Theta)$ , representing the probability of neutrons with initial energy  $E_0$  being scattered through an angle  $\Theta$  and having a final energy E. The discrete values of the variables  $(E_0, E, \Theta)$  on which the probability function for thermal-neutron scattering depends are chosen so that any required values of the function can be obtained quite accurately by interpolating between values contained in the matrix.

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\*) See also p. 66

\*\*) mistake. Should read FTN(=150,250) according to the footnote on p. 66  
(Notes by editor)

When the energy-angular distribution of thermal neutrons is defined by a scattering law, the matrix of  $S(\alpha, \beta)$  values is given for discrete values of the variables.

$$\alpha = [E_0 + E - 2(E_0 E)^{1/2} \cos \theta] / A' kT$$

and

$$\beta = (E - E_0) / kT.$$

Here  $E_0$  is the initial neutron energy,  $E$  the final energy,  $\theta$  the scattering angle in the laboratory system,  $kT$  the temperature in energy units and  $A'$  the nucleus-neutron mass ratio (this definition may be extended to the case of molecules). Thus, the parameters  $\alpha$  and  $\beta$  are related to the momentum and energy transfer resulting from the collision. The choice of values for the variables  $\alpha$  and  $\beta$  must ensure that it is possible to obtain any  $S(\alpha, \beta)$  value to a sufficient degree of accuracy by means of interpolation.

The expression for the cross-section of a process in which a neutron with initial energy  $E_0$  scatters through an angle  $\theta$  in the laboratory coordinate system and has a final energy  $E$ , is

$$\sigma(E_0 \rightarrow E, \theta) dE d \cos \theta = \frac{\sigma_b}{kT} \sqrt{\frac{E}{E_0}} \exp(-\beta/2) S(\alpha, \beta) dE d \cos \theta.$$

Here,  $\sigma_b$  is the cross-section for a bound atom:

$$\sigma_b = \sigma_{fr} \left( \frac{A+1}{A} \right)^2,$$

and  $\sigma_{fr}$  is the cross-section for a free atom.

For a monoatomic gas in which chemical binding effects are not important, the scattering function  $S(\alpha, \beta)$  is defined by the expression

$$S(\alpha, \beta) = \frac{1}{2\sqrt{\pi}d} \exp[-(\alpha^2 + \beta^2)/4d].$$

The gas-model approximation is often used for defining the function  $S(\alpha, \beta)$  in cases where no other information on the thermal-neutron scattering law is available.

When  $S(\alpha, \beta)$  has a  $\delta$ -function singularity at  $\beta = 0$ , it may be represented as follows:

$$S(\alpha, \beta) = S^*(\alpha, \beta) + e^{-\lambda d} \delta(\beta).$$



In this case the place of  $S(\alpha, \beta)$  in the library is occupied by  $S^*(\alpha, \beta)$ , and the value of  $\lambda$  is specified on the FTN heading cards as additional information. The following data are also entered:

- $\sigma_{fr}$  - the cross-section for a free atom (if it is constant);
- $\mathcal{E} = E_{bc}/kT$  - a quantity corresponding to the lower limit of validity of the static elastic-scattering model
- $E_m$  - the upper boundary of the range for which  $\sigma_{fr}$  is a constant: above this value the energy dependence of  $\sigma_{fr}$  must be taken into account (one can take it to be equal, for example, to the elastic scattering cross-section (RTN = 01002) which is available in the library, neglecting the contribution of inelastic scattering because it is so small);
- A' - the effective atom (molecule) - neutron mass ratio; for molecules this value is to some extent arbitrary and is usually chosen from an analysis of experimental results.

### III.5.1 FTN classification for GCN = 04

The method of specifying data on energy-angular distributions of thermal neutrons is given by the high-priority FTN digit in accordance with the following table:

$n_1$	Method of representing energy-angular distributions
1	In the form of the scattering probability matrix
2	In the form of the $S(\alpha, \beta)$ scattering function matrix

The two low-priority FTN digits specify the serial number of the format for a given  $n_1$  value.

### III.5.2 Card format for GCN = 04

- I.
  - 1. RTN
  - 2. The number of temperature considered
  - 3. Reserve
  - 4. INT number defining the law for interpolating  $(E_0, E, \theta, T)$  or  $S(\alpha, \beta, T)$  with respect to temperature T

- II. 1. The temperature to which the data correspond
- 2. The number of FTNs at this temperature
- 3. The number of cards for this temperature, including this card
- 4-6. Reserve

The format of the following cards depends on the FTN.

Case\_(1): FTN = 100

- III. 1. FTN = 100
- 2. The number of  $E_0$  values
- 3. The number of cards for this FTN
- 4. INT number determining the laws for interpolating  $\sigma(E_0, E, \theta)$  with respect to  $E_0$ ,  $E$  and  $\theta$
- 5-6. Reserve
  
- IV. 1.  $E_0$
- 2. The number of  $E$  values at this  $E_0$
- 3. The number of cards for this  $E_0$
- 4-6. Reserve
  
- V. 1.  $E$
- 2. The number of  $\theta$  values at this  $E$
- 3.  $\theta$
- 4.  $\sigma(\theta)$

Case\_(2): FTN = 200

- III. 1. FTN = 200
- 2. The number of  $\beta$  values
- 3. The number of cards for this FTN
- 4.  $\lambda$
- 5.  $\sigma_{fr}$
- 6.  $E$
  
- IV. 1.  $E_m$
- 2.  $A'$
- 3. Reserve
- 4. INT number defining the laws for interpolating  $S(\alpha, \beta)$  with respect to  $\beta$  and  $\alpha$
- 5-6. Reserve
  
- V. 1.  $\beta$
- 2. The number of  $\alpha$  values at this  $\beta$
- 3.  $\alpha_1$
- 4.  $S(\alpha_1)$  etc.

### III.6. Special quantities for neutrons, $\bar{\nu}$ , $\alpha$ , $\eta$ , etc. (GCN = 05)

The following quantities belong in this category:

$n$ , the number of secondary neutrons per collision (elastic and inelastic),

$$\eta = (\sigma_n + \sigma_{n'} + 2\sigma_{2n} + 3\sigma_{3n} + \bar{\nu}\sigma_f + \dots) / \sigma_c$$

$\eta$ , the number of secondary neutrons per inelastic collision event,

$$\eta = (\sigma_{n'} + 2\sigma_{2n} + 3\sigma_{3n} + \bar{\nu}\sigma_f + \dots) / \sigma_x$$

$\alpha$ , capture to fission cross-section ratio,

$$\alpha = \sigma_c / \sigma_f$$

$\bar{\nu}$ , the average number of secondary neutrons per fission

The need to define similar quantities for other data may arise in the future.

The first three values are derived and can therefore be calculated from the appropriate equations; their specification in the library is not necessary in this case. On the other hand,  $\bar{\nu}$  is measured directly by experiment and must be specified for all fissile nuclei.

The methods of representing special neutron quantities are similar to those used to represent cross-sections. Therefore, all specifications given in the description of the formats for GCN = 01 are applicable. It must be remembered, though, that  $\bar{\nu}$  values may be defined at points which do not coincide with points specified for other cross-sections, in particular  $\sigma_f$ . Therefore, it is essential that the extreme energy points (the smallest and the largest) at which  $\bar{\nu}$  and  $\sigma_f$  are given should coincide. We can then find by interpolation the values of  $\bar{\nu}$  and  $\sigma_f$  necessary for calculating the  $\bar{\nu}\sigma_f$  values.

#### III.6.1 The FTN classification for GCN = 05

The FTN classification for special neutron values is similar to the corresponding classification for neutron cross-sections (GCN = 01)

#### III.6.2 Card format for GCN = 05

The card format for representing special neutron quantities is identical to the format for neutron cross-section representation (GCN = 01), except that nothing is punched in position 3 of card I for GCN = 05.

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Translated from Russian

CHANGES IN AND ADDITIONS TO THE FORMAT OF  
THE SOKRATOR EVALUATED NUCLEAR  
DATA LIBRARY

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1. CHANGES IN THE FORMAT FOR THE PRESENTATION OF DATA ON RESOLVED  
RESONANCE PARAMETERS

In the published format of the SOKRATOR library it was proposed that resonance parameters be given separately for each isotope in a natural mixture of isotopes. This kind of data presentation is inconvenient when one is using the data to obtain multigroup constants since one has to arrange the resonances of different isotopes in the order in which the latter are encountered in a natural mixture. It has been decided that, in order to avoid this procedure, the format for the presentation of data on resolved resonance parameters (see Ref. [1], sub-section III, 2, 3) \*\*) shall be changed as follows:

(a) General information

<u>Type</u>	<u>Position</u>	<u>Quantity</u>
I.	1.	FTN
	2.	Reserve
	3.	Number of cards for a given FTN
	4-6.	Reserve
II.	1.	$E_{01}$ - energy of the first resonance (eV)
	2.	$E_{0\Pi}^{*/}$ - energy of the last resonance (eV)
	3.	Number of isotopes
	4.	num - total number of level systems with different spin and parity summed over all isotopes
	5.	Total number of resonances given for all the isotopes
	6.	Reserve

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\* / The second subscript is a Russian " $\Pi$ ", standing for "posledni" = last.

\*\* ) "Ref. [1]" = pages 1-60 of the present document

(b) Information about isotope

- III.      1.      Atomic weight of the  $n^{\text{th}}$  isotope (on  $^{12}\text{C}$  scale)
2.      Its fractional concentration
3.      Number of cards with general information on the isotope; i.e. number of cards of types III-XV
4.       $\pm a$  - radius of the neutron channel (Fermi); the minus sign denotes that the radius is dependent on energy or on  $l$  and  $j$ ; in this case, the value of the radius is given for  $E = 0$ , for the  $n^{\text{th}}$  value of  $l$  and for the value of  $j$  corresponding to the given value of  $l$ .
5.       $\pm I$  - parity and spin of the target nucleus; for computers which do not distinguish between  $+0$  and  $-0$ , the negative parity for  $I=0$  is duplicated by punching the number sign.
6.      Number of resonances given for a given isotope

Cards of types IV-XV keep their format. Cards of types III-XV are repeated for each isotope. Then follow cards with information on level systems, each having the following format:

- XVI.      1.       $\mu$  - number of the level system ( $1 \leq \mu \leq \text{num}$ )
2.       $A$  - atomic number of the isotope
3.       $\pm l_1$  - lowest orbital angular momentum of the neutrons which can form the state indicated. A minus sign is used if the state can also be formed by neutrons having a higher angular momentum. For computers which do not distinguish between  $+0$  and  $-0$ , for  $l_1 = 0$  the minus sign is duplicated by punching the number sign.
4.       $\pm j$  - parity and spin of the compound nucleus. For computers which do not distinguish between  $+0$  and  $-0$ , for  $j = 0$  the minus sign is duplicated by punching the number sign.

5-6. Reserve.

Cards of type XVI are repeated for all level systems. Then follow cards on which the resonance parameters proper are given - in order of rising resonance energy regardless of the number of the level system to which a given resonance relates.

- XVII.
1.  $E_r$  - resonance energy
  2.  $\nu$  - number of the level system
  3. Number of cards for a given resonance
  4.  $\Gamma_{rne}(|E_r|)$  - neutron width (eV) for  $l = l_1(\nu)$
  5.  $\Gamma_{r\gamma}$  - radiation width (eV)
  6.  $\Gamma_{rf}$  - fission width (eV)

Cards of type XVIII (giving  $\Gamma_n$  for orbital momenta  $l > |l_1(\nu)|$  when  $l_1(\nu) < 0$ ) and type XIX (giving the widths of reactions other than scattering, capture and fission - if such reactions occur) agree in format with the corresponding cards described in Ref. [1] (cards XVII and XVIII).

Cards of type XVII and, if necessary, types XVIII and XIX are given for each resonance.

2. CHANGES IN AND ADDITIONS TO THE FORMATS FOR PRESENTING DATA ON THE ENERGY DEPENDENCES OF SECONDARY PARTICLES

(a) Law No. 10

$$Y(E, E_0) = \sum_{n=1}^N \rho_n \delta[E - \varepsilon(E_0, \theta, \bar{a})], \quad (1)$$

is determined in such a way that, with its help, one can describe the energy distributions of secondary particles (other than nucleons) and also of neutrons released as a result of the break-up of an unbound multinucleon particle formed as a result of a reaction (for example, as a result of direct reactions of the type  $D + n \rightarrow$  bineutron +  $p \rightarrow 2n + p$ ;  $D + n \rightarrow$  unbound deuteron +  $n \rightarrow n + p + n$ ). For this purpose, besides the reaction

energy  $Q$  (for endothermal reactions  $Q < 0$ ) and the mass  $M_0$  of the target nucleus, one must add to the vector  $\vec{a}$  of the reaction parameters the mass  $M$  of the secondary particle and the mass of the particle of interest resulting from its break-up:  $m_1 \leq M$ . In this case

$$\begin{aligned} & \mathcal{E}(E_0, \theta, Q, M_0, M, m_0, m, m_1) = \\ & = E_0 \frac{m_0}{m} \frac{m_1}{M} \left[ 1 - \alpha \left( 1 - \frac{M^2}{(m_0 M^2 + M_0 m^2)} \beta \frac{Q}{E_0} - \frac{M_0}{\beta} \sqrt{1 + \frac{(m_0 + M_0)^2}{(m M_0^2 + M m_0^2)}} \frac{Q}{E_0} \right) \right]; \\ & \alpha = \frac{(2m_0 M_0 + M_0^2)(m_0 M^2 + M_0 m^2) - (m M_0^2 + M m_0^2) M^2}{(m_0 + M_0)^2 \cdot (m_0 M^2 + M_0 m^2)}; \quad (2) \\ & \beta = \frac{\alpha (m_0 + M_0)^2}{2 M m_0^2} \sqrt{\frac{M^2 m_0 + M_0 m^2}{m M_0^2 + M m_0^2}}. \end{aligned}$$

Here  $m_0$  is the mass of the incident particle and  $m$  is the mass of the particle resulting from the reaction, where

$$\begin{aligned} \mu_c &= \frac{1}{2K^2} \left[ y \mu_c^2 - \frac{2m_0 K}{m_0 + M_0} \pm \mu_c \sqrt{\mu_c^2 y^2 + K^2 x - \frac{4K y m_0}{m_0 + M_0}} \right]; \\ \mu_c &= \cos \theta; \\ K &= \frac{M}{m_0 + M_0} \sqrt{\frac{m_0 M_0^2 + M m_0^2}{M^2 m_0 + M_0 m^2}} \sqrt{1 + \frac{(m_0 + M_0)^2 m_0}{m M_0^2 + M m_0^2}} \frac{Q}{E_0}; \\ x &= 1 - \alpha \left( 1 - \frac{M^2}{(m_0 M^2 + M_0 m^2)} \frac{Q}{E_0} \right); \\ y &= \frac{\alpha}{\beta} \sqrt{1 + \frac{(m_0 + M_0)^2}{(m M_0^2 + M m_0^2)}} \frac{Q}{E_0}. \quad (3) \end{aligned}$$

With regard to the number of terms in the sum (1) and the use of the minus sign in the formula for  $\mu_c$ , see Ref. [1]. At energies up to 15 MeV, the relativistic effects neglected in expressions (2) make a contribution which does not exceed 1% and as a rule is much lower.

The format of the card for FTN = 110 with data for the 10th law is as follows:

- IV.            1.        FTN = 110
2.        m
- 3-6.    Reserve

$M$  and  $Q$  are given in other parts of the file;  $m_0$  is uniquely determined by the type of reaction. If  $m$  is not specified, it is tacitly assumed that  $m = m_0$ .



- (b) Law No. 13 is introduced - it describes the angular and energy distributions of secondary neutrons formed through the break-up of a nucleus (phase space model):

$$Y(E_0, \theta, Q, E) = C(E_0, Q) \sqrt{E[E_{\max}(E_0, \theta, Q) - E]^{(3n-3)}};$$

(below, M is the mass of the target nucleus in neutron mass units).

$$C(E_0, Q) = \frac{1}{2\pi \int_0^\pi \sin \theta d\theta \int_0^{E_{\max}(E_0, \theta, Q)} \sqrt{E[E(E_0, \theta, Q) - E]^{(3n-3)}} dE}.$$

In a three-particle case, e.g. the reaction  $D(n, 2n)H$ , for  $E_0 \leq -QM/(M-1)$ ,

$$C(E_0) = \frac{2(M+1)^{1/2}}{E_0^2 \pi^2 [a^2(1-\mu_m) + \frac{2}{3}a(1-\mu_m^2) + \frac{2}{9}(1-\mu_m^3)]};$$

for  $E_0 > -QM/(M-1)$ ,

$$C(E_0) = \frac{2(M+1)^{1/2}}{E_0^2 \pi^2 [a^2 - \frac{2}{3}a + \frac{2}{9}]};$$

$$Q = M^2 \left(1 + \frac{M+1}{M} \cdot \frac{Q}{E_0}\right) - 1;$$

$$\mu_m = (M+1) \sqrt{\frac{Q}{E_0} \cdot \frac{M}{M+1} - \frac{M-1}{M+1}};$$

$$E_{\max}(E_0, \theta, Q) = E_0 \left[1 - \frac{2M}{(M+1)^2} \cdot \left(1 - \frac{M+1}{2} \cdot \frac{Q}{E_0} - \mu_c \sqrt{1 - \frac{(M+1)Q}{M E_0}}\right)\right];$$

Q is the reaction energy in MeV (negative for endothermal reactions);  $\mu_c$  is the cosine of the angle of scattering in the centre-of-inertia system. The angular distribution of the reaction products must be assumed to be isotropic in the centre-of-inertia system. The dependence of  $E_{\max}$  on the cosine of the scattering angle in the laboratory system of co-ordinates,  $\mu_c = \cos \theta$ , has the form

$$E_{\max}(E_0, \theta, Q) = \frac{2M_c^2 + Q(\pm) 2M_c \sqrt{M_c^2 + Q}}{(M+1)^2},$$

where the minus sign is used in front of  $\mu_L$  only when  $E_0 < -QM/(M + 1)$  and takes into account the presence of two groups of neutrons having a forward angular distribution.

- (c) In the format description [1]<sup>\*/</sup>, the formats of the cards are determined using a linear combination of laws only for the case where the linear combination coefficients are constant within the energy interval (FTN = 150, 250<sup>\*/</sup>). Below are determined the formats enabling one to describe the energy dependence of the linear combination coefficients (FTN = 151, 251).

- IV.        1.        FTN
2.        Number of energies at which the linear combination coefficients are specified. The first energy must coincide with the lowest and the last with the highest energy in the range  $\Delta E$  for which data are presented.
3.        Number of cards with information for this FTN
4.        Number of laws used
5.        INT determining the law for energy interpolation of the linear combination coefficients (for probability conservation, it is recommended that INT = 111000000 be used in the interpolation process).
6.        Reserve
- V.         1.         $E_1$
2.         $a_1(E)$
3.         $a_2(E)$  etc. until the probabilities of all the laws at the first energy have been given

Cards of type V are repeated for each energy.

On subsequent cards, information is given about the corresponding laws. Each law can be represented by means of only one FTN, which also determines the format. If among these FTNs, there is even one in

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<sup>\*/</sup> In Ref. [1] it is stated that format No. 10 is intended for FTN = 150 and 252. This is a mistake; it is intended for FTN = 150 and 250.

which the dependence on the initial energy is stated explicitly (FTN = 208, 209, 212), then the FTN of the linear combination should be made equal to 251. Otherwise the FTN of the linear combination is 151.

### 3. NEW WAYS OF PRESENTING DATA ON ANGULAR DISTRIBUTIONS

In the earlier format [1], it was intended that the FTN = 121, 221; 122, 222 by means of which angular distributions can be specified in the form of a superposition of partial angular distributions with definite weights should also be used for specifying the sub-group structure of angular distributions.

However, this greatly complicates the treatment of data on angular distributions: in order to decide on the meaning of coefficients  $a$ , one must compare them with the sub-group fractions specified in the zone for the corresponding partial (or total) cross-section. To avoid this difficulty in specifying the sub-group structure of angular distributions, one introduces FTN = 321, 421; 322, 422, the format of which agrees with the format of FTN = 121, 221; 122, 222 respectively. For FTNs where  $n_1 = 3$  or 4, the coefficients  $a$  have the meaning of sub-group fractions and must agree exactly with the sub-group fractions of the cross-sections.

### 4. ALLOWANCE FOR THE STRUCTURE OF CROSS-SECTIONS IN THE REGION OF PARTIALLY RESOLVED RESONANCES

When cross-sections are specified by means of resolved resonance parameters, there are greater possibilities of taking into account the contribution of unresolved levels. In the description of the format [1], this contribution was taken into account only as a non-resonance contribution, it being possible to specify the value of the contribution of unresolved levels with the help of mean resonance parameters (see p. 28 - "Specifying non-resonance cross-sections by representing cross-section data with the help of resolved resonance parameters"; a card of type X is the heading card of the FTN with the help of which the non-resonance cross-section is specified). If this FTN = 411 or 412, one punches 0 in position 2 of this card (see p. 30; card type 1) if the contribution of the unresolved levels can be taken into account as a non-resonance contribution or 1 if the resonance structure of the unresolved levels has to be taken into account.

To allow for the fact that some levels of one or another system of resonances are resolved and taken into account in the resolved resonance parameters, after a card of type XIV (see p. 33) a card of type XIV-A with the following format must be introduced:

- XIV-A.    1.    Ratio of the reduced neutron width corresponding to the resolution threshold to the mean reduced width of the  $n^{\text{th}}$  level system, or 0 if the levels of the given system are completely unresolved.

Similar information for the remaining level systems is punched in the following positions of this card. If necessary, the information is carried over to the next card of the same format.

The introduction of a card of type XIV-A by using a FTN with  $n_1 = 4$  to specify the "non-resonance" contribution in the region of resolved resonances is essential.

5.    LIMITATIONS ON THE POSSIBILITIES OF THE LIBRARY FORMAT DEFINED IN REF. [1]

- (a) In a complete data file, each cross-section must be specified within the entire range of energies covered by the file. This also applies to threshold reactions: below the threshold, the equality of the threshold to zero must be stated explicitly with the help of FTN = 101.
- (b) In the zones for the different reaction cross-sections, the boundaries of energy regions which differ in their type of representation must correspond exactly to the boundaries of the corresponding regions in the zone for the total cross-section, except where the low-energy boundary of the region coincides with the reaction threshold.

Thus, the boundaries of the energy region in the zone for the total cross-section correspond to a change in the type of representation of the cross-section, at least for one reaction.

- (c) In each energy interval, the total cross-section and the cross-section for partial reactions should be specified with equivalent types of representation:

-        A representation by means of resonance parameters must describe the cross-sections for all reactions (some of them can be specified only in the form of a non-resonance

contribution in the format envisaged for specifying such a contribution by describing cross-sections by means of resonance parameters);

- A point-by-point representation can only be general for specifying cross-sections of all types. The energies at which the values of the partial cross-sections are specified can be chosen only from the set of energy values at which the total cross-section is specified;
  - The sub-group representation can only be general for reactions of all types (non-resonance cross-sections are specified by means of equal values of sub-group cross-sections).
- (d) The laws of cross-section interpolation by energy can, generally speaking, be different for different cross-sections. It is recommended, however, that one use a linear-linear or a linear-logarithmic interpolation guaranteeing that the sum of the partial cross-sections will remain equal to the total cross-section.
- (e) When one uses FTNs which enable one to describe the energy dependences of the cross-sections for all reactions in the zone for the total cross-section, an external temperature cycle is not permitted; the temperature dependence of the cross-sections must be specified as envisaged by the format of the corresponding FTN. When the energy dependence of cross-sections is specified by means of resonance parameters, the data are presented for only one temperature - 0°K.
- An external temperature cycle is retained for specifying cross-sections in FTN = 111, 112, 121, 122.
- There is no provision for specifying the temperature dependence of energy and angular distributions.
- (f) Angular distributions cannot be specified by means of resonance parameters. Even if cross-sections are specified by means of resonance parameters which also define the angular distributions, the latter must nevertheless be specified in explicit form.
- (g) There is no provision for taking into account the resonance structure of the parameters of energy distributions (temperature in laws Nos 9, 11 and 12; transition probabilities in law No. 8) by

means of a sub-group representation.

The influence of resonance self-shielding on the shape of the angular distributions in the region of unresolved resonances can be taken into account only by describing the sub-group structure of the cross-sections for reactions characterized by different secondary-neutron energy distributions.

- (h) The cross-sections may be specified by means of no more than three types of representation. If several types of representation are used, the FTNs must follow one another in order of seniority.

The most senior ones are representations using resonance parameters (FTN =  $n_1, n_2, n_3$  beginning with  $n_1 = 3$  (region of resolved resonances) or  $n_1 = 4$  (region of unresolved resonances)).

The next in seniority are point-by-point representations ( $n_1 = 5, n_2 = 1$  or  $n_1 = 1, n_1 + n_2 < 3$ ).

The least senior are sub-group representations ( $n = 1, n_1 + n_2 \geq 3$  or  $n_1 = 5, n_3 > 1$ ).

- (i) When cross-sections and energy and angular distributions are specified, the FTN heading card must indicate the maximum number of parameters (sub-group fractions; values of  $\mu$  or  $\omega$ ).

In particular, when cross-sections are specified by means of FTN = 121, on the FTN heading card (card of type IV) the maximum number of sub-groups must be indicated in position 4 (in the format described in Ref. [1] there is provision for punching zero if the number of sub-groups changes from energy to energy).

When angular distributions are specified by means of FTN = 111 or 211; 121 or 221; 321 or 421, on the FTN heading card (card of type IV) the maximum number of values of the cosine of the scattering angle or the maximum number of Legendre polynomial expansion terms must be indicated in position 6. When using FTN = 122 or 222, 322 or 422, such information must be presented in position 6 of the card of type V following the FTN heading card.

6. ERROR IN THE DESCRIPTION OF LAW No. 9

Ref. [1] contains an error in the description of law No. 9 concerning the energy distribution of secondary neutrons. The normalization factor for this law is

$$N(E_0, u, B) = T^2(E_0) \left[ \left(1 + \frac{B}{T(E_0)}\right) e^{-B/T(E_0)} - \left(1 + \frac{E_0 - u}{T(E_0)}\right) e^{-\frac{E_0 - u}{T(E_0)}} \right].$$

REFERENCES

- [1] KOLESOV, V.E., NIKOLAEV, M.N., Format of the library of recommended data for reactor calculations (in Russian), in "Jadernye konstanty", issue 8, No. 4, p. 3, Moscow, TsNIIATOMINFORM (1972).