International Atomic Energy Agency

INDC(CCP)-24/G

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

FORMAT OF THE EVALUATED NUCLEAR DATA LIBRARY FOR REACTOR CALCULATIONS

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Translated by the IAEA
April 1972

INDC(CCP)-24/G

This is the English translation
of a paper published in the Russian
language in the Proceedings of the
IAEA Panel on Neutron Nuclear Data Evaluation,
Vienna, 30 August - 3 September 1971.

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Introduction

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, which lie in the non-universal character of the constants obtained as well as in the technical difficulties of correcting the data.

The development of calculational techniques allows a considerable degree of automatic processing of recommended pointwise nuclear data sets into group constants with arbitrary energy divisions, and this process can be directly linked with multigroup codes for reactor calculation. The basis for such a system of information processing is a library of recommended nuclear data [1]. Present library formats for recommended nuclear data [2, 3, 4] allow storage of large volumes of various 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 a wide range of problems connected with neutron and photon transport by means of computers.

The same nuclear-physical constants may be represented in various ways. In the resonance region, the cross-sections may be represented pointwise to describe a detailed energy behaviour, or 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 by different methods - as angular dependences or as Legendre polynomials. Here too the sub-group representation of data is possible.

The choice of one or other type of data representation depends in practice on various considerations: on the nature of the problem, on considerations of convenience, on the codes available, etc. Therefore, it is desirable to

design the library in such a way that information can be stored in different representations. For this purpose it is convenient to introduce into the storage system a special characteristic - namely a representation type number.

This report discusses formats for the storage of recommended nuclear data for reactor calculations. They constitute generalizations and a further development of the English formats described in Ref. [2], which are used in a number of foreign laboratories. 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 implemented.

This format for storing evaluated nuclear data represents a further development of that proposed in Ref. [6].

Translator's note

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

ИЯН = NIN

НТР = RTN

НОК = GCN

НЧК = PCN

НТП = FTN

БНФ = LFN

ИНТ = INT

I. CLASSIFICATION OF NUCLEAR DATA

Nuclear data contained in the library is classified according to substance, composition, reaction type and data form (or representation).

First, all data entered into the library are classified 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 their manner of representation 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 the same substance. These may be data from different compilations, or data from basic data libraries which have been processed by different (computer) codes. When such data are entered into the library, they are assigned new NINs. In this manner, the NIN characterizes 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-place integral number, 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 places 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 for denoting the index number of the data set in the evaluated data library. 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 numbers of data sets relating to different isotopes, elements or chemical compounds cannot coincide. Thus there can never be two sets of data with the same first four digits, even if the subsequent digits differ. Thus the last five NIN places are used only for convenient identification of a set of data, whereas the first NIN digit determines the type of data ($m_1 = 1$ is an incomplete set, $m_1 = 2$ is a complete set of data; the meaning of the remaining possible values of m_1 is not yet fixed).

I.2. Reaction Type Number (RTN)

Data which have the same NIN are sub-divided according to the reactions which can occur in the material. The Reaction Type Number (RTN) is a five-digit number sub-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 GCNs and PCNs give this nuclear reaction data classification system great flexibility. With the RTN, it is possible to combine into one set, with a given NIN, both neutron data and data on photon production and their interaction with matter. In practice, however, it is often more practical to store these three types of data under three different NINs, especially since their energy ranges do not usually coincide.

Thus we have, with the NIN and the RTN, the possibility of various groupings of data in the library. This possibility will be further broadened by introducing the form type number (FTN).

I.3. General Classification Number (GCN)

Classification by GCN sub-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 distribution of secondary particles
03 - energy distribution of secondary particles
04 - energy-angular distributions in thermal neutron scattering
05 - special quantities for neutrons ($\bar{\nu}, \alpha, \eta, \beta_i$ etc.)

So far no further GCN assignments have been made. In particular, those GCNs which define photon interaction constants have been omitted because we have no evaluated data for them.

I.4. Particular Classification Number (PCN)

The Particular Classification Numbers specify nuclear interactions. Each PCN identifies one of the processes that may occur as a result of neutron or photon interaction with matter. The table that follows lists the PCN assignments for neutrons, based on the English classification system.

001 Total
002 Elastic
003 Non-elastic (= total - elastic)
004 Total (n,n') = total inelastic scattering summed over all final states
005 (n,n') to 1st excited state
006 (n,n') to 2nd excited state

007 (n,n') to 3rd excited state

008 (n,n') to 4th excited state

009 (n,n') to 5th excited state

010 (n,n') to 6th excited state

011 (n,n') to 7th excited state

012 (n,n') to 8th excited state

013 (n,n') to 9th excited state

014 (n,n') to 10th excited state

015 (n,n') to continuum. This includes that part of the (n,n') reaction not covered by PCNs 5-14 and the use of "continuum" is a little loose

016 (n,2n) or $(\gamma,2\gamma)$ - pair production

017 (n,3n)

018 Fission = (n,f) + (n,n'f) + (n,2nf) + ...

019 (n,f) - no pre-fission evaporation or direct interaction neutrons

020 (n,n'f)

021 (n,2nf)

022 (n,n')α

023 (n,n')3α

024 (n,2n)α

025 (n,3n)α

026 (n,2n) isomeric state

027-100 reserved for other possible reactions which lead to the production of secondary particles of the same type as the primary particles

101 total absorption (all reactions which do not lead to emission of primary particles)

102 (n,γ) or (γ,e^-)

103 (n,p)

104 (n,d)

105 (n,t)

106 $(n,{}^3He)$

107 (n,α)

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 the classification of resolved and statistical resonance information. The detailed meaning of the PCNs is closely 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 in the future

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

In the English classification PCNs 201-208 are used to identify characteristics such as transport and removal cross-sections, $\bar{\nu}\sigma_f$, and a number of other derived quantities. PCNs 301 to 450 are reserved for 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 the PCN. Thus 301 denotes the total energy release rate parameter whilst 302 denotes the energy release from elastic scattering.

Derived quantities are usually not contained in a library of evaluated nuclear data, but can easily be obtained with the help of special (computer) programmes. It is therefore reasonable 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 built up later, from the detailed data library considered in this report, by means of special processing (computer) programmes.

The reaction specification is such that the PCN enables the final product nuclei to be uniquely determined. Thus for ^{12}C the $^{12}C(n,n')3\alpha$ reaction has PCN = 023 whilst the reaction $^{12}C(n,n')^{12*}C(\gamma)^{12}C$ has PCN = 5 if the 4.43 MeV first excited state is considered. Similarly, for ^{238}U PCN = 016 indicates that ^{237}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 the particles emitted.

Examples of Reaction Type Numbers

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

I.5. Form Type Number (FTN)

Since data can be presented in the library in a number of ways, they are classified according to a form type number (FTN). The FTN allows various input modes for data having the same RTN and thereby enlarges the potential of our storage system.

The following modes of data representation may be indicated:

- Detailed energy or angular dependence;
- Parametric representation, in the form of resonance parameters for neutron cross-sections or in the form of Legendre coefficients for angular distributions;
- Groupwise data representation [5] with optional numbers of neutron sub-groups.

In sub-group representation, neutrons with a given energy are shared out among N sub-groups. Each such sub-group (n), characterized by its cross-section value σ_n, has its own weight a_n, so that

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

The groupwise representation is a convenient method of representing 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 σ_n for the energy E under consideration. Sub-group representation can also be used for resolved resonances provided it is not necessary to have a detailed energy dependence curve for the data in the energy interval in question.

This format assumes that a total correlation exists between the full and partial sub-group cross-sections, i.e. that neutrons of a given sub-group n have not only a uniform total cross-section σ_n but also uniform partial cross-sections σ_{rn}. If this approximation is not valid, the sub-group method becomes impracticable.

For the angular and energy distributions of secondary particles one can use different modes of representation reflecting one or other mechanism of a given nuclear reaction. In the FTN classification we propose to construct angular and energy distributions in the form of a superposition of these representation modes with an assigned probability for each one of them.

In addition, the FTN makes possible a more flexible arrangement of the data stored in the library. In particular it becomes possible to change as desired the number and order of subordination of the variables (parameters) on which the data in the library are dependent. In other words, the FTN are so designed as to allow not only different modes of data presentation in the library (discrete points, parametric presentation, etc.) but also different hierarchies among the variables which govern the data.

Generally speaking, the structure of the FTN depends on the RTN and is specified by the GCN. Thus, for a given GCN, the FTN can be sufficiently well defined by a three-digit number (FTN = $n_1 n_2 n_3$) whose components assume different meanings dependent on the GCN. Supplementary information to specify the FTN more exactly is provided where deemed necessary. The identification of the FTN components and the supplementary information will be discussed in the section on formats for presentation of GCN data.

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

For the present we are determining only the format for Breit-Wigner resonance parameter data. Formats for recording the parameters used in other formulae will be developed as programmes based on other formulae are compiled and used for calculating cross-sections.

Our format is based on that used by the UK Resonance Parameter Laboratory 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:

$$\sigma_{nn}(E) = \pi\lambda^2 \sum_{J^\pi} g_J \left[\sum_{c=c_1}^{c_2} \left\{ \sin^2\varphi_{cy} + \sum_{r=1}^{N} B_r(E) \left[\Gamma_{rn}\Gamma_{rnc} \cos 2\varphi_{cy} - 2\Gamma_{rx}\Gamma_{rnc} \sin^2\varphi_{cy} + 2(E-E_r')\Gamma_{rnc} \cdot \sin 2\varphi_{cy} \right] \right\} + \sum_{r=1}^{N} B_r(E) \left[\Gamma_{rn} \cdot d_r - 2(E-E_r') B_r \right] \cdot \Gamma_{rn} + \sigma_{nn}^{distant}(E) \qquad (1)$$

Reaction cross-section (n,R)

$$\sigma_{nR}(E) = \pi\lambda^2 \sum_{J^\pi} g_J \sum_{r=1}^{N} \Gamma_{rn}\Gamma_{rR} B_r(E) + \sigma_{nR}^{distant}(E) \qquad (2)$$

Total cross-section

$$\sigma_{nT}(E) = \sigma_{nn}(E) + \sum_{R} \sigma_{nR}(E) \qquad (3)$$

*) Translation note.
In this section the variable y is used to represent the incident neutron total angular. It is more commonly represented by j.

The following notation is used here:

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

$$\alpha_r = \frac{1}{\ell_s} \cdot \sum_{s \neq r} \frac{\Gamma_{sn}(\Gamma_s + \Gamma_r)}{D_{sr}} \tag{5}$$

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

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

$$\Gamma_{rn} \equiv \Gamma_{rn}(E) = \sum_{\ell=\ell_1}^{\ell_2} \Gamma_{rnc}(E)$$

Total neutron width (8)

$$\Gamma_{rx} \equiv \Gamma_{rx}(E) = \sum \Gamma_{rx}(E)$$

Width of inelastic interactions (9)

$$\Gamma_r \equiv \Gamma_r(E) = \Gamma_{rn}(E) + \Gamma_{rx}(E)$$

Total width (10)

Effective resonance energy E_r':

$$E_r' = E_r + \frac{1}{2} \sum_{\ell=\ell_1}^{\ell_2} \left[\delta_\ell(|E_r|) - \delta_\ell(E) \right] \Gamma_{rnc}(|E_r|) / P_\ell(|E_r|) + \\ + \frac{1}{2} \sum_{R} \left[\delta_\ell(|E_r|) - \delta_\ell(E) \right] \cdot \Gamma_{rR}(|E_r|) / P_R(|E_r|) \tag{11}$$

For $\ell = 0$, S_c is independent of E. Usually S_R is taken as constant for other reactions too. If, as was done here, S is specified 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 sum (for γ and π) is taken for all systems of levels which can contribute to the cross-section.

The sum for ℓ is taken for all neutron orbital moments which can form states with given y and π:

$$L_1 = \min\left\{\left|y - \left|I - \tfrac{1}{2}\right|\right|;\ \left|y - I - \tfrac{1}{2}\right|\right\}, \tag{12}$$

if

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

where π_I is the parity of the ground state of the target nucleus. If the parity condition in expression (13) is not fulfilled, L_1 is one unit higher than would follow from expression (12).

$$L_2 = y + I + \tfrac{1}{2}, \tag{14}$$

if

$$(-1)^{L_2} = \pi \pi_I \tag{15}$$

or a unit lower if the condition in expression (15) is not fulfilled.

Because of the parity conservation condition,

$$(-1)^{\ell} = \pi \cdot \pi_I \tag{16}$$

the value of ℓ in the sum changes by 2 from one term to the other.

Since usually

$$\Gamma_{nL_1} \gg \Gamma_{n(L_1+2)} \gg \ldots \gg \Gamma_{nL_2}, \tag{16a}$$

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

The next to the last term in expression (1) allows for interresonance interference within the Breit-Wigner approximation. This is accurate if only one of the following conditions is fulfilled:

(a) The resonances are well separated and interference is insignificant;

(b) Only one neutron channel is significant (only S-neutrons or neutrons with high moments interact, but the target nucleus spin is $I = 0$).

The phase shift $\varphi_{\ell y}$ is determined by the channel radius $a_{\ell y}(E)$: $\varphi_{\ell y} = k a_{\ell y}$. Here

$$k = 2{,}19685 \cdot 10^{-3} \sqrt{E}\ \frac{M}{M + 1{,}03665}\quad (\text{barn})^{-1/2}$$

where M is the mass of the nucleus (taking 12 as the mass of ^{12}C), and

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

is the effective radius of the nucleus for the particular channel. If the energy dependence of $a_{\ell y}$ is substantial, this dependence is entered in the library for $a_{\ell y}$ (and not for $\Delta a_{\ell y}$).

The last terms in equations (1) and (2) describe the contributions of distance resonances and also omitted levels. These cross-sections are either represented pointwise or are calculated from the mean resonance parameters. In formula (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. Otherwise $\sigma_{nn}^{sm}(E)$ will in effect describe the result of interference from many levels.

I.6.2. Approximations to the Breit-Wigner formula

(a) Neglecting the term describing interresonance interference

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

(b) Approximate calculation of interresonance interference with positive solutions

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

$$4 \sin^2 \varphi^{*}_{\ell y}(E) = 4 \sin^2 \varphi_{\ell y} + \sum_{\substack{s \\ s \neq r}}^{r \pm \varepsilon} B_s(E)\left[\Gamma_{sn}\Gamma_{sn\varepsilon} \cos 2\varphi_{\ell y} - 2\Gamma_{sx}\Gamma_{sn\varepsilon} \sin^2 \varphi_{\ell y} + 2(E - E_s')\Gamma_{sn} \sin 2\varphi_{\ell y}\right] \qquad (16b)$$

The calculation is performed according to formula (1) with the interresonance term omitted but with $\varphi^{*}_{\ell y}(E)$ instead of $\varphi_{\ell y}$, which ensures a positive cross-section.

(c) Neglecting the shift factors

Since $S_c(E)$ is a constant, this is important only for $\ell > 0$ and only far from the resonance. Therefore, parameters determined in this approximation can be used directly in an accurate formula.

(d) Approximations for the low-energy region

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

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 formula.

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

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

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

(1) For neutron channels P_ℓ and S_ℓ they are calculated for a square well. In particular,

$$P_0 = 1;$$

$$P_1 = \frac{(kR)^2}{1+(kR)^2};$$

$$P_2 = \frac{(kR)^4}{9+3(kR)^2+(kR)^4};$$

$$P_3 = \frac{(kR)^6}{225+45(kR)^2+6(kR)^4+(kR)^6} \qquad (16c)$$

For other reactions it is assumed that $P_R(E) = 1$ and $S_R(E) = 0$.

(2) P_R, S_R, P_ℓ and S_ℓ can be represented in tabular form as neutron energy functions, since they are determined empirically or calculated from a theoretical model (e.g. for reactions with the emission of charged particles).

(3) Phase shifts and penetrations are calculated by an algorithm, the number of which is indicated in the library data.

II. REPRESENTATION OF DATA ON PUNCHED CARDS

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

The symbolic card is a standard 80-column card. However, the manner in which the information is distributed on the card varies according to the particular computer facility used. Let us therefore make a few general comments regarding the information distribution and the codification of the information on the cards.

In the case where 960 positions (12 rows x 80 col.) are used for the coding of the information, the information distribution can take the form of 6 fields (each 11 columns wide) separated by blank columns, used for the basic information (data fields), and a service field in columns 73 to 80. This information distribution is used in the UK evaluated nuclear data library. If input elements such as those in the M-20 computer facility are used, it is more convenient to adopt a different scheme of codification. In this case the basic information is coded on the six upper rows, and the service information is coded on the following two rows. The remaining four rows of the card are not used.*/

These two types of codification are equivalent in the sense that the information coded on the symbolic card, when printed out by the corresponding service equipment, 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 library1/. The form in which numbers are presented depends on

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1/ 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. Its format has yet to be developed.

*/ Literally, the Russian says: "The top six rows are used for the basic information and the following rows for service information." But we assume the original translator had additional information.

their sense content. All nuclear data are represented in a binary-decimal code with floating decimal.

In the second case it is possible to have a slightly different information distribution on the card. Since the number of significant digits in numerical data is usually not large, one can also store the service information in parallel with the basic information, using for instance the three last decimal locations (third address) in each of the six rows containing basic information. This would allow one standard punched card to accommodate two symbolic cards.

The data for a given substance, defined by a specific NIN, constitute a complete set of information in the sense that this information can henceforth be used independently, without recourse to any other information set which may 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" (using the English word: file). Each file is assigned a Specific Library Number (LFN) which is also entered in the first four places of the NIN.

Each file is sub-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 Reaction Type (RTN). Thus in different files a given reaction type may be assigned to a different section. The correspondence between the section number and the RTN is defined by special "heading cards" located in the zero section of each file. Within each section the cards are numbered consecutively. The numbering of sections within each file is autonomous.

The order of sections for neutron data depends primarily on the PCN (quantity type), and, for similar PCN, on the GCN (reaction type).

Examples of ordering of sections

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

Section number	RTN	Data definition
07	02005	Angular distribution of inelastically-scattered neutrons for excitation of first level
08	03005	Energy distribution of inelastically scattered neutrons for excitation of first level

Both the content, and the location of information on 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 the NIN (LFN), the number of the section, the serial number of the card in the section and also the cyclic sum of information punched in the first eight rows of the punched card.

In line with the type of card punches and input equipment most widely used at present in the USSR, we have adopted coding by rows for our cards.

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

The seventh row carries a nine-digit whole number, the last two places giving the number of the section in which data of the relevant type are located[2/]; the first four places are used to record the first four NIN sub-numbers (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 the form of a number with floating point. The numbering of the cards commences anew in each section from card number 1 (always containing the title information for the section).

The ninth row contains the cyclic sum of the numbers recorded in the first eight rows, but the sign of the check sum is not punched in this row. This makes it possible to feed continuously into the computer a set consisting of many cards. After the data have been inserted the check sum can be used to check for correctness of input on each punched card and reveal any defective cards.

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

III. FORMATS OF NUCLEAR DATA IN THE LIBRARY

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

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

1. In certain energy regions the data will be negligibly low or zero (as at the threshold of a reaction);
2. In some energy intervals the data are not energy dependent, or are represented identically;
3. In some energy intervals the data have different representations or different temperature dependences.

The sub-division of the energy scale into intervals sometimes helps to avoid duplication of results. One should strive to minimize the number of energy intervals. 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 the threshold process will have different numbers of intervals. Wherever possible it is desirable to have a correspondence of energy intervals for total cross-sections and their associated partial cross-sections. This makes it easier to find gross errors by means of special programmes.

Usually, nuclear data are 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 foreseen in the FTN classification.

Where data are quoted as a function of 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 reasonable degree of accuracy by interpolating between neighbouring points available in the file. In some cases interpolation is performed on a log scale. 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 available programmes; this information is then entered into the heading of the FTN.

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

$$INT \equiv i_1'' i_2'' i_3'' i_1' i_2' i_3' i_1 i_2 i_3 \quad *)$$

Using the INT number it is possible to determine the method of interpolation for functions of one, two and three variables.

The last three places, $i_1 i_2 i_3$, determine the interpolation rule for the last 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 first 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 sub-number i_1 governs 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 sub-numbers determine the scale on which interpolation should be performed, i_2 on the ordinate (scale of the interpolated function), i_3 on the abscissa (scale of the argument).

The scale is determined by the following table:

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

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

Examples: 1. One-variable function $\sigma(E)$.

INT = ++ 09 111 000 000

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

2. Two-variable function - a secondary neutron spectrum versus incident neutron energy: $f(E_o, E)$.

INT = ++ 09 100 000 000

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

*) Translation note. In the examples given below the nine integers are preceded by ++09. This quantity is the sign and exponent required by the M220.

3. Three-variable function - superposition of angular distributions: $f(E,\mu) = \sum_{k=1}^{k} a_k(E) f_k(E,\vartheta)$ ($a_k(E)$ can have, for instance, the meaning of energy-dependent sub-group weighting coefficients, and f_k that of sub-group angular distributions).

INT = ++ 09 101 001 003

denotes in the case of precedence of the variables a, E and ϑ, that $a_k(E)$ must be interpolated linearly on graphs of a_k versus $\ell_n E$ ($i''_1=1$, $i''_2=0$, $i''_3=1$), and that f_k must be interpolated similarly for energy ($i'_1=1$, $i'_2=0$, $i'_3=1$) and linearly with respect to the cosine of the angle ϑ($i_1=1$, $i_2=0$, $i_3=3$).

Temperature dependence is indicated when it is considered to be important. If it can be included in analytical calculations, the specification of a single temperature is enough. Otherwise the results are adduced for several different temperatures so that data for any desired temperature can be obtained by interpolation. For example:

INT = ++ 09 102 000 000

denotes that interpolation must be performed linearly on the graph of the cross-section versus $\sqrt{T}$ ($i''_1=1$, $i''_2=0$, $i''_3=?$).

The RTN specification is such that it allows 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, are not always known for every secondary reaction product separately, but are known in some cases only for certain groups of particles of these 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 can contain smaller sets. The assignment of data to specific sets depends on the nature of the data themselves and on features which are common to them: for instance they may be data having the same RTN or FTN, data belonging to the same energy range or characterized by the same temperature, and so on.

All data sets are provided with special headings. Each heading contains a description of the set and information on the amount of information included,

and possibly the configuration of the sub-files within the set. One knows, therefore, the general nature of the file and its internal content without having to "unpack" the whole set.

Each heading begins with a new card. The format of each 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 pertinent to the form (representation) type is defined by the FTN. Energy headings, neutron sub-groups, etc. fall into this category.

In the following we refer to a column (field) or a row (line) as a location. In the description of specific formats the cards are numbered with Roman numerals and the positions of cards within a set containing basic information with Arabic numerals. Zeros are punched in positions not containing information.

III.1. File heading

The file heading occupies the zero section and establishes the correspondence between the section number, the reaction type number and the number of cards in the section. The heading card format is the following:

Type of card

I. 1. MIN

2. Total number of cards in file, including the heading cards

3. Number of cards in the zero section

4. Atomic number Z of element (a zero is used for chemical compounds and mixtures)

5. Atomic or molecular weight A

6. Number of different RTN that occur in 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. The 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 cross-section increase. In the formats adopted here, energy is given in MeV, temperature in degrees K, and cross-section in barns.

The energy and temperature values are chosen in such a way that the cross-sections can be obtained by interpolation. 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.

In the FTN classification scheme it is possible to assign the cross-section for the whole energy interval at once provided it is constant over that interval.

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

III.2.1. FTN classification for GCN = 01

The first FTN sub-number (n_1) defines the manner in which the data are represented in the set, 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 sub-group parameters
3	Parametrically by means of resonance formulae for resolved resonances
4	Parametrically by means of statistical information for unresolved resonances

Subsequent n_1 values (5-9) are reserved for new data presentation forms, if and when they are formulated.

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

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

n_3 - indicates the order of priority of these parameters.

In the case of two parameters (energy E and the number of the sub-group i) the meaning of the low priority FTN sub-numbers 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_2n_3 = 01 case means assigning a cross-section value to the whole energy interval at once.

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

For n_1 = 3 the second FTN sub-number (n_2) determines the type of the resonance formula. In accordance with RPL [7] we assume:

n_2 = 1 for the Breit-Wigner formula

n_2 = 2 for formulae based on the reduced R matrix (Reich-Moore formula)

n_2 = 3 for the R-matrix Brissenden-Durston formula

n_2 = 4 for the S-matrix Adler-Adler formula;

n_3 equal to zero means that the resonance parameters are not cited in the section for a given PCN and that they must be taken from the section for total cross-section (PCN = 001). In the section for total cross-section, n_3 = 0 for the

lowest of the cited temperatures is inadmissible. The remaining values, $n_3 = 1, 2, \ldots 9$, denote the number of the approximation to the general formula which is recommended for use in calculations with given parameters. $n_3 = 1$ always means that the parameters are intended for use with the general formula. 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 identified.

III.2.2. Card format for GCN = 01 with assignment of cross-sections at discrete points as functions of E and T ($n_1 = 1$)

I. 1. RTN

2. Number of energy intervals (ΔE) for this RTN

3. Q - energy of the reaction in MeV

4.) 5.) 6.) Reserved for supplementary information belonging to this RTN

II. 1. E_H - lower energy limit of ΔE

2. E_b - upper energy limit of ΔE

3. Number of cards for the representation of cross-sections in this ΔE, including the present card

4. Number of temperature values considered in this ΔE

5. INT number determining temperature interpolation rule

6. Reserved for additional information in this ΔE

III. 1. Temperature T, at which cross-section is given

2. FTN number for cross-sections at this temperature

3. Number of cards for representing cross-sections at this temperature, including this card

4.) 5.) 6.) Reserved for additional information at this T

The format of subsequent cards depends on the FTN.

Case (1) Cross-section in the given ΔE is not energy dependent (one sub-group)

IV. 1. FTN = 101

2. Cross-section value σ

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

IV. 1. FTN = 111

2. Number of energy values

3. Number of cards for this FTN

4. INT number determining the law for energy interpolation of the cross-section

5. E

6. $\sigma(E)$

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

Case (3) Sub-group representation of the cross-section structure for the whole ΔE

IV. 1. FTN = 112

2. Number of sub-groups

3. a_1

4. σ_1

5. a_2

6. σ_2

If necessary the information is continued on subsequent cards in the format of locations 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-section by this FTN (including this card)

4. Number of sub-groups (if it does not depend on E)

5. INT number determining the energy interpolation law

6. Number determining which quantity must be averaged

(a) If direct averaging of a_i and σ_i is possible for certain intervals ΔE or ΔU falling within the interval $\lceil E_H, E_b \rceil$, we enter in this position either the maximum lethargy 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:

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

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

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

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

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

$$T_n(t) = \sum_{k=1}^{p} a_k \sigma_{kn} e^{-\sigma_{kt} t}$$

(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 $\langle \sigma_t \rangle$, $\langle \sigma_R \rangle$, $\langle 1/\sigma_t \rangle$, $\langle 1/\sigma_t^2 \rangle$, $\langle \sigma_R/\sigma_t \rangle$ (if the number of sub-groups = 2) or $\langle \sigma_t^2 \rangle$, $\langle 1/\sigma_t^3 \rangle$ and $\langle \sigma_R \sigma_t \rangle$ (if the number of sub-groups = 3) or, finally, also $\langle \sigma_t^3 \rangle$, $\langle 1/\sigma_t^4 \rangle$ and $\langle \sigma_R \sigma_t^2 \rangle$ (if the number of sub-groups = 4) and subsequently to determine the sub-group parameters for the interval by solving the system of algebraic equations

$$\langle \sigma_t^n \rangle = \sum_{k=1}^{p} a_k \sigma_k^n \qquad (p = 2,3 \; ; \; n = \pm 1, \pm 2, \pm 3 - 4),$$

$$\langle \sigma_R \sigma_t^n \rangle = \sum_{k=1}^{p} a_k \sigma_{Rk} \sigma_k^n \qquad (p = 2,3 \; ; \; n = 0, +1, 2)$$

(d) Integral positive numbers 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. σ_1

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

Generally speaking, this format allows representation of a different number of sub-groups for different Es. In practice, however, the number of sub-groups for all Es within a given ΔE will usually be the same.

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

IV. 1. FTN = 122

2. Number of sub-groups

3. Number of cards for this FTN

4. Reserved

5. INT number determining the energy interpolation rule

6. Conventional number determining the method of obtaining 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. (Reserved)

4. E_1

5. a_{il}

6. σ_{il}

If necessary the information is continued on subsequent cards in the format of locations 3 and 4 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. Reserved

3. Number of cards for this FTN

4-6. Reserved

II. 1. E_H

2. E_b

3. Number of isotopes

4-6. Reserved

(b) Information on the isotope

III. 1. Atomic weight of first isotope

2. Its percentage concentration

3. Number of cards for this isotope (including this one)

4. $\pm$ radius of neutron channel (in Fermi) (with minus sign if the energy dependence of the radius is given or its dependence on ℓ and y)

5. $\pm$ I parity and spin of the target nucleus

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 radiation capture reaction = 102

4. PCN of fission reaction (if there is one) = 019. If no fission, then zero

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. Flag for presence of non-resonance scattering cross-section, nrr:

nrr = 0 if there is no such contribution

nrr = 1 if it is given in a series of energy points

nrr = 2 if it has to be calculated with formulae on the basis of the mean resonance parameters

nrr > 2 if it has to be calculated on some other basis.

2. Flag for the method of calculating penetrabilities and displacement 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 by certain specific formulae.

3. Flag for the presence of a non-resonance radiation capture cross-section (analogous to the corresponding flag for scattering), nrz.

4. Flag for the method of calculating penetrabilities and displacement factors for radiation 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 ℓ

khupz = + 1, if they are given at fixed energies for different values of ℓ

khupz $\geqslant$ 2, if they have to be calculated with formulae.

5. Flag for the presence of a non-resonance fission cross-section (analogous to the corresponding flag for scattering), nrd.

6. Flag for the method of calculating penetrabilities and displacement factors for fission (analogous to the corresponding sign 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 displacement factors is recorded on subsequent cards in the format of position 3-4 of card V.

(c) Representation of neutron channel radii

VI. 1. Maximum value of ℓ for which $a_{\ell y}$ are given

2. Zero, if the radii of the neutron channels are given below for fixed energies

Unity, if the quantities $a_{\ell y}(E)$ have to be calculated from the mean resonance parameters of the omitted levels.

VII. 1. First value of ℓ

2. Number of energies at which values of $a_{\ell y}$ are specified for given ℓ

3. Number of values of y for which values of $a_{\ell y}$ are specified for given ℓ

4. First value of y for given ℓ

5. Second value of y for given ℓ

6. Third value of y for given ℓ, etc.

If the number of values of y for given ℓ is more than 3, the information is put on subsequent cards in the format of positions 4-6 of card VII.

VIII.1. E is energy (= E_H if the radii are specified at one energy)

2. $a_{\ell y}(E)$ for given ℓ and first value of y

3. $a_{\ell y}(E)$ for given ℓ and second value of y etc. (proceeding to subsequent cards if number of values of y is more than 5).

Cards of type VII, VIII and IX are repeated for $\ell = 1, 2, \ldots, \ell_M$

(d) Representation of non-resonance cross-sections

(If at least one of these is represented in the form of a table of cross-sections for fixed energies)

IX. 1. PCN for the first reaction for which a non-resonance cross-section is given

2. Number of energy points

3. Number of cards with data for this non-resonance cross-section (including this card)

4-6. Reserved

X. 1. E_1

2. σ_1, etc.

If necessary, information is carried on to subsequent cards in the format of card XI. Type X and XI cards are repeated for each reaction for which a non-resonance cross-section is specified.

(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 = 02

2. The number of ℓ for which penetrability energy relationships, etc. are given

3. Number of cards with data on penetrabilities and shift factors for the reaction of interest

4. Flag for dependence of data on ℓ(= 1)

5-6. Reserved

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. Reserved

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. $S_{\ell_1}(E_2)$

The information is carried on to the following cards in the format of card XIII. Type XIII and XIV cards are repeated for all necessary values of ℓ.

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 penetrations and shift factors for the reaction

4. Flag for independence of data from $\ell(=-1)$

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 level 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 ℓ' is punched instead of ℓ.

(f) Resonance parameters proper

XVI. 1. E_r - resonance energy of the first resonance

2. $\pm y$ - parity and spin of the compound state

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 higher orbital momentum

4. $\Gamma_{rn1}(|E_r|)$ - neutron width

5. $\Gamma_{r\gamma}$ - radiation width[3/]

6. Γ_{rf} - fission width[4/]

If $\ell < 0$ the next card takes the following form:

XVII.1. $\pm\ell_2$ - next angular momentum of neutrons which can form the given state (with minus sign if it is not the maximum possible)

3/ If the penetrability for any reaction is energy dependent, the width is specified for the energy $|E_r|$.

4/ The format does not envisage more than four ℓ input values.

2. $\Gamma_{rn\ell_2}(|E_r|)$ - the corresponding neutron width

3. $\pm\ \ell_3$ (if $\ell_2 < 0$). Otherwise zeros are printed in positions 3-6

4. $\Gamma_{rn\ell_3}(|E_r|)$

5. ℓ_4**) (if $\ell_3 < 0$). Otherwise zeros are printed in positions 5-6

6. $\Gamma_{rn\ell_4}(|E_r|)$

If there are reactions differing from (n,n), (n,γ) and (n,f), we have:

XVIII.1. PCN for the first of these reactions

2. $\Gamma_{rR_1}(|E_r|)$ - 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. $\Gamma_{rR_2}(|E_r|)$ - 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-XVII are repeated for each isotope.

III.2.4. Card format for data on statistical parameters of unresolved resonances (GCN = 01, n_1 = 4)

(a) General information

I. 1. FTN

2. Reserve

3. Number of cards for this FTN

4-6. Reserve

II. 1. E_H is the lower boundary of the region in which it is recommended that calculations of parameters of unresolved resonances should be performed.

2. E_B - the upper limit of this region

3. Reserve

4. Number of isotopes

5. Numerical flag, khr, defining the nature of the variation of the mean resonance parameters:

khr = 1, if these parameters are constant in the interval

khr = 2, if they vary linearly from one energy point to another

khr = 3, if they are considered constant within the sub-intervals into which the interval is divided

6. The number of energy points (if khr = 2) or sub-intervals (if khr = 3) or zero (if khr = 1)

(b) Information on the isotope

III. 1. Atomic weight of the first isotope

2. Its percentage concentration

3. Number of cards with data on this isotope

4. Neutron channel radius in Fermi (punched with minus sign if its energy dependence and/or dependence on ℓ and y is given)

5. $\pm$ 1 - the parity and spin of the target nucleus

6. Reserve

IV. 1. Number of reactions for which parameters are given

2. PCN of elastic scattering reaction = 002

3. PCN of total radiation capture reaction = 102

4. PCN of fission reaction = 019 (if one takes place) or 0

5. PCN of fourth reaction (if it takes place) or 0

6. PCN of fifth reaction (if it takes place) or 0

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

V. 1. Flag 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 or in sub-intervals together with the mean resonance parameters
nrr > 1, if it has to be calculated by some particular formula

2. Flag for the method of calculating penetrability and shift factors for the neutron channel, khupn

khupn $\pm$ 0, if these penetrabilities are calculated by the usual method
khupn = 1, if they are specified for discrete energies or in sub-intervals together with the mean resonance parameters
khupn > 1, if they have to be calculated by some particular formula

3. Flags for the presence of a non-resonance radiation capture cross-section, nrz (analogous to the corresponding sign for scattering)

4. Flag for the method of calculating the penetrability and shift factors for radiation capture, khupz

   khupz = 0, if these quantities are not energy dependent (which is usually the case)
   khupz = -1, if they are given together with the mean resonance parameters at fixed energies or in sub-intervals with no relation to ℓ
   khupz = +1, if they are given together with the mean resonance parameters for different values of ℓ
   khupz > 1, if they have to be calculated by some particular formula

5. Flag for the presence of a non-resonance fission cross-section (analogous to the corresponding symbol for scattering), npd

6. Flag for the method of calculating the penetrability and shift factors for fission (analogous to the corresponding symbol 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 penetrability and shift factors is recorded on succeeding cards in the format of positions 3-4 of card V

(c) Information for the energy point or interval

VI. 1. E: if khr = 1, E = E_B;
   if khr = 2, E is the energy point at which the mean resonance parameters are specified (the first point should coincide with E_H and the last with E_B)
   if khr = 3, E is the upper energy limit of the sub-interval (for the last sub-interval it should coincide with E_B)

2. The parity of the compound nucleus which is considered first (+ 1 or - 1).
   If there is a 0 here, the data are independent of the parity of the state of the compound nucleus

3. The number of cards for a given energy point (sub-interval), including this card

4. The number of values of y considered (spin of the compound nucleus)

5-6. Reserve

(d) Specification of neutron channel radii

(If radius a in position 4 of card III is negative)

VII. 1. ℓ_M is the maximum value of ℓ for which $a_{\ell y}$ are specified

2. Reserve

3. Number of cards with information on the radius, including this card

4-6. Reserve

VIII. 1. First value of $\ell = \ell_m$ (minimum)

2. Number of values of y for which values of $a_{\ell y}$ are specified for a given ℓ

3. First (minimum) value of y

4. Next value of y and so on

If necessary information on the values of y continues on the next card in the format of positions 3-6 of card VIII.

IX. 1. $a_{\ell y}$ for a given ℓ and first value of y

2. $a_{\ell y}$ for a given ℓ and next value of y and so on, continuing on the following cards if the number of values of y exceeds six

Type VIII and IX cards are repeated for $\ell = \ell_m + 1, \ell_m + 2 \ldots, \ell_M$

(e) Representation of non-resonance cross-sections of reactions

(If there is such a contribution for at least one reaction in accordance with the data of card V (positions 1, 3, 5) and other cards of the same type)

X. 1. Number of reactions for which there are non-resonance contributions

2. Reserve

3. Number of cards with information on non-resonance contributions to the cross-sections

4-6. Reserve

XI. 1. PCN of the first reaction for which there is a non-resonance contribution

2. The corresponding contribution to the cross-section

3. PCN of the second reaction with non-resonance contribution to the cross-section

4. The corresponding contribution

and so on, continuing on subsequent cards in the same format.

(f) Representation of penetrability and shift factors

(If penetrability and shift factors are specified for at least one reaction in accordance with data of card V (positions 2, 4, 6) and other cards of the same type)

XII. 1. The number of reactions, for which penetrability and shift factors are given

2. Reserve

3. Number of cards with information on penetrabilities and shift factors

4-6. Reserve

XIII.1. PCN of the first reaction for which penetrability and shift factors are given

2. Penetrability for the first reaction

3. First reaction level shift factor

4. PCN of the second reaction for which penetrability and shift factors are given

5. Penetrability for second reaction

6. Shift factor for second reaction

If necessary the information is continued on subsequent cards in the format of card XIII.

(g) Information for a specific spin state

IX. 1. y - the spin of the compound nucleus (starting with the lowest value)

2. N - the number of possible values of ℓ for given y, π, and E[5/]

3. Number of cards with information for given set of y, π, E

4. ℓ_{min} - the minimum value of ℓ for given y, π, E

5. ℓ_{max} - maximum value of ℓ for given y, π, E

6. $D_{y\pi}$ - the mean distribution between levels for given y, π, E

5/ The step of the change in ℓ is $\delta_\ell = (\ell_{max} - \ell_{min})/(N-1)$. If only elastic scattering is possible, $\delta_\ell = 2$. If there is inelastic scattering, $\delta_\ell = 1$ is also possible.

X. 1. Mean radiation width, $\bar{\Gamma}_{\gamma,y,\pi}$

2. Number of degrees of freedom for $\bar{\Gamma}_{\gamma,y,\pi}$

3. Mean fission width $\bar{\Gamma}_{f,y,\pi}$

4. Number of degrees of freedom for $\bar{\Gamma}_{f,y,\pi}$

5. Mean reduced neutron width for $\ell = \ell_{min}$, $\bar{\Gamma}_n^{(o)},y,\ell_{min}$

6. Number of degrees of freedom for $\bar{\Gamma}_n^{(o)},y,\ell_{min}$

If $\ell_{max} \neq \ell_{min}$, the data on $\bar{\Gamma}_n^{(o)}{}_{y,\ell}$ and the corresponding numbers of the degrees of freedom are printed on subsequent cards in the format of positions 5 and 6 of card XI.

XI. Data for reactions differing from elastic scattering, total radiation capture and fission (if such reactions are included in the list given on card IV or subsequent type IV cards)

1. PCN of reaction

2. Number of values of ℓ' possible with this reaction (= 1, if reaction not characterized by orbital momentum of secondary neutrons)

3. The first value of ℓ' (if the figure 1 is in position 2, this information is not used)

4. The mean reduced width for the given reaction and the value of ℓ' under consideration

5. Number of degrees of freedom for this reaction with the value of ℓ' under consideration. If the reduced channel width for the reaction is assumed to be non-fluctuating, the number of degrees of freedom is arbitrarily set at zero.

6. Reserve

If the number of permissible values of ℓ' is more than 1, the information is continued on subsequent cards in the format of positions 3, 4 and 5 of card XI.

Cards IX-XI are repeated for each value of y and π for a given energy (or energy interval).

Cards VI-XI are repeated for each energy (or energy interval).

Cards III-XI are repeated for each isotope.

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

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

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

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

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

We envisage the specification of angular distributions at discrete points as a function of μ, where $\mu = \cos\vartheta$, ϑ being the scattering angle. We shall call this the μ representation. The second possible representation is parametrical in the form of ω_ℓ coefficients of the $f(\vartheta)$ expansion in Legendre polynominals $P_\ell(\cos\vartheta)$, such that

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

We shall call this the ω representation. The data are stored in order of increasing μ, from - 1 to + 1. The scattering angle ϑ can be either in the centre-of-mass system, or in the laboratory system; indication as to which of the two co-ordinate systems is used for a particular data set is given as additional information contained in the FTN identifier in the form of a numerical flag, 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 different levels, where a simple relationship exists between the energies of the primary and secondary particles, it is probably sensible to keep the data in the CM system. For other inelastic processes data are usually given in the laboratory system. In this connection, the following must be kept in mind. Where a simple analytical

expression relating the angular and energy dependences in these two systems of co-ordinates 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 co-ordinate 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 μ representation of the data, the choice of E and μ values must be such that the values at intermediate points can be obtained by interpolation of the stored data with adequate accuracy. In the case of an ω representation, the necessary accuracy is guaranteed by specifying a sufficiently large number of expansion coefficients (i.e. n number).

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 μ representation is roughly approximated, say, by linear intervals, that the resulting representation will be normalized. It may therefore be necessary in some cases to perform additional normalization of the angular distributions obtained from the data files.

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

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

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

The current formats require that all related partial distribution functions $f_i(\vartheta)$ be given in the same representation (either in the μ or ω form) and in the same co-ordinate system. Should it become necessary, however, the FTN structure is such that this restrictive condition can be relaxed.

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 pointwise energy dependent representation, the first angular distribution must be for energy 0.001 eV and the last for 14 MeV: in the case of a rangewise representation, the lower energy boundary of the first range must be 0.001 eV and the upper energy boundary of the last range must be 14 MeV. This general rule should also be useful for spotting 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 sub-number according to the following table:

n_1	Type of angular distribution representation
1	At discrete points as a function of μ (μ representation)
2	Parametrically in the form of Legendre coefficients (ω representation)

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

The low-priority FTN sub-numbers 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 order of priority of these parameters with regard to each other.

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

n_2n_3	High priority variable	Low priority variable
01	-	-
02	-	-
11	E	-
12	a_i	-
21	E	a_i
22	a_i	E

III.3.2. Card format for GCN = 02

I. 1. RTN

2. Number of energy intervals ΔE for this RTN

3. A - atomic weight

4.) 5.) 6.) Reserved for supplementary information

II. 1. E_H - lower energy limit of ΔE

2. E_B - upper energy limit of ΔE

3. Number of cards for this ΔE, including the present card

4. Number of groups of secondary particles for which angular distributions are specified in this ΔE

5-6. Reserve

III. 1. Flag identifying the group of secondary particles

2. Number of FTNs assigned to angular distributions for this group of particles

3. Number of cards to represent angular distributions of this group, including this card

4.) 5.) 6.) Reserved for additional information on this group of secondary particles

The format of subsequent cards depends on the FTN.

Case (1) Isotropic angular distribution in ΔE

In this case card IV specifies only the Form Type Number (FTN = 101 for the μ representation, FTN = 201 for the ω representation) and the flag identifying the co-ordinate system.

IV.	1.	FTN = 101	IV.	1.	FTN = 201
	2.	Co-ordinate system flag, co		2.	Co-ordinate system flag, co

Case (2) Angular distribution for the whole ΔE

IV.	1.	FTN = 102	IV.	1.	FTN = 202
	2.	Co-ordinate system flag, co		2.	Co-ordinate system flag, co
	3.	Number of μ values		3.	Number of ω values
	4.	INT number determining the method of interpolating $f(\mu)$ with respect to μ		4.	ω_1
				5.	ω_2
				6.	ω_3
	5.	μ_1			
	6.	$f(\mu_1)$			

Case (3) Angular distributions with fixed E

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.	Co-ordinate system flag, co		4.	Co-ordinate system flag, co
	5.	INT number determining the method of interpolating for E and μ		5.	INT number determining the method of interpolating ω_e with respect to E
	6.	Number of values of ϑ, μ, if it is common for the whole ΔE, or zero		6.	Number of values of ω, if it is common for the whole ΔE, or zero
V.	1.	E	V.	1.	E
	2.	Number of μ values		2.	Number of ω values
	3.	μ_1		3.	ω_1
	4.	$f(\mu_1)$ etc.		4.	ω_2 etc.

Case (4) Superposition of angular distributions for the whole ΔE

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.	Co-ordinate system flag, co		4.	Co-ordinate system flag, co
	5.	INT number determining the method of interpolating $f(\mu)$ with respect to μ		5-6.	Reserve
	6.	Reserve			
V.	1.	a	V.	1.	a
	2.	Number of μ values		2.	Number of ω values
	3.	μ_1		3.	ω_1
	4.	$f(\mu_1)$ etc.		4.	ω_2 etc.

Case (5) Superposition of angular distributions for fixed E

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.	Co-ordinate system flag, co		4.	Co-ordinate system flag, co
	5.	INT number determining methods of interpolating $a(E)$ with respect to E, $f(E,\mu)$ with respect to E and $f(E,\mu)$ with respect to μ		5.	INT number determining methods of interpolating $a(E)$ with respect to E and $\omega_\ell(E)$ with respect to E
	6.	Number of values of μ, if it is common for the whole ΔE, or zero		6.	Number of values of ω, if it is common for the whole ΔE, or zero
V.	1.	E	V.	1.	E
	2.	Number of a values		2.	Number of a values
	3.	Number of cards for this E		3.	Number of cards for this E
	4-5.	Reserve		4-5.	Reserve
	6.	Number of μ values, if it is common for all a values, or zero		6.	Number of ω values, if it is common for all a values, or zero

VI.	1.	a	VI.	1.	a
	2.	Number of μ values for this a		2.	Number of ω values for this a
	3.	μ_1		3.	ω_1
	4.	$f(\mu_1)$ etc.		4.	ω_2 etc.

Case (6) Angular distributions for given a at different E values

IV.	1.	FTN = 122	IV.	1.	FTN = 222
	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.	Co-ordinate system flag, co		4.	Co-ordinate system flag, co
	5.	INT number determining the methods of interpolating a(E) with respect to E, $f(E,\mu)$ with respect to E and $f(E,\mu)$ with respect to μ		5.	INT number determining the methods of interpolating a(E) with respect to E and $\omega_\ell(E)$ with respect to E
	6.	Number of values of E, if it is common for all values of a, or zero		6.	Number of values of E, if it is common for all a values, or zero
V.	1.	a	V.	1.	a
	2.	Number of E values		2.	Number of E values
	3.	Number of cards for this a		3.	Number of cards for this a
	4-5.	Reserve		4-5.	Reserve
	6.	Number of μ values, if common for all E, or zero		6.	Number of ω values if common for all E, or zero
VI.	1.	E	VI.	1.	E
	2.	Number of μ values		2.	Number of ω values
	3.	μ_1		3.	ω_1
	4.	$f(\mu_1)$ etc.		4.	ω_2 etc.

In all the above formats for angular distribution FTNs we have specified, for illustrative purposes, a minimum amount of information, i.e. one pair of $\lceil \mu, f(\mu) \rfloor$ and one value of ω. It is presupposed that, wherever necessary, this information will be continued on subsequent field locations of the same card or on subsequent cards.

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

When the analytical relationship between the energies of the primary and secondary particles is known, it is not necessary to specify the energy dependence of secondary particles; it can easily be calculated by means of special data processing (computer) programmes. In other cases it is necessary to specify secondary particle energy distribution laws.

The following energy distribution laws have been formulated to date.

Law (1) Particles emitted with a known discrete energy (e.g. emission of delayed fission neutrons).

Law (2) Particles emitted with an energy $E = k\,(E_o - E_d)$, where E_o is the initial energy, E_d is a discrete energy, and k is a constant (the attenuation factor). Inelastic scattering of neutrons with separate level excitation is a particular case covered by this law: here, k reflects the mean energy transfer to the recoil nucleus.

Law (3) Continuous, normalized fission neutron spectrum independent of initial energy, in the form of

$$S(E) = A\, e^{-BE} \sinh \sqrt{CE}$$

where A, B and C are constants.

Law (4) Fission neutron spectrum, taking into account dependence on initial neutron energy and the nature of the fissioning nucleus. This is given as a normalized probability function,

$$N(E) = \alpha \frac{E}{T^2} \exp\left(-\frac{E}{T}\right) + (1-\alpha)\left(\frac{2}{\pi^{1/2}} B^{3/2}\right) E^{1/2} \exp\left(-\frac{E}{B}\right)$$

with

$$B = a + b\,(\bar{\nu}+1)^{1/2}$$

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

$$T = c\,(E_o - E_f)/(14 - E_f)$$

where a, b and c are constants, $\bar{\nu}$ is the mean number of neutrons per fission, E_f is the threshold for the (n,n'f) reaction, E_o is the initial energy, and σ_{nf}, $\sigma_{nn'f}$ and σ_{n2nf} are the cross-sections

for the (n,f), (n,n'f) and (n,2nf) reactions. This law is specified by four parameters, a, b, c and E_f (the remaining quantities being available from the nuclear data file).

Laws (5, 6, 7) The spectrum of emitted particles is represented by the following normalized probability function:

$$f(E_o, E) = p(E/E_o^q),$$

where E_o is the initial energy, and E is the energy of the emitted particles. Parameter q takes the values

0 for Law (5)
$\frac{1}{2}$ for Law (6)
1 for Law (7)

Law (6) includes the evaporation spectrum.

Law (8) The spectrum of emitted particles is given as an arbitrary function of the initial energy E_o and the final energy E in the form of discrete points. (If there is no dependence on E_o, this law is equivalent to Law (5).)

In the case of Laws (5-7), energy distribution data are specified as pairs of quantities (argument $x = E/E_o^q$, corresponding probability p(x)) such that any intermediate values of these quantities can be obtained in good approximation by interpolation between neighbouring values stored in the data file. It should be noted that, although the probability functions in the case of Laws (5-7) are normalized (to a certain degree of accuracy) within the range for which the arguments are specified, certain arguments may be inaccessible in practice on energy conservation grounds (e.g. the emergent energy of a secondary neutron may be greater than the incident energy). In such cases it will be necessary to renormalize the probability distribution function.

As in the case of angular distributions, the formats for the energy distributions of secondary particles provide for the possibility of specifying final distributions in the form of superpositions of the various laws together with their probabilities. Each law in this case corresponds to one of the possible nuclear process mechanisms. This possibility can also be interpreted as a sub-group representation of secondary particle energy distributions; here, the probabilities of each of the laws are in effect the weights assigned to the sub-groups, and the laws themselves will characterize the energy distributions of the corresponding neutron sub-groups.

The special case of thermal scattering is considered separately.

III.4.1. FTN classification for GCN = 03

The manner in which the data on secondary particle energy distributions are stored is determined by the high-priority FTN sub-number, according to the following table:

n_1	Method of energy distribution presentation
1	In the format of the laws, when the initial energy is not given explicitly */
2	In the form of the laws, when the initial energy is given explicitly

*/ There may be an error or omission here.

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

The two low-priority FTN sub-numbers have the following meaning:

n_2n_3 = 01-49 are reserved for specifying the type of distribution and the number of the corresponding case

$n_2n_3 \geqslant 50$ are reserved for specifying the distribution in the form of superpositions in the following cases:

n_2n_3 = 50: E_o is not given explicitly

n_2n_3 = 51: in all cases at given E_o

n_2n_3 = 52: all E_o for a given case.

III.4.2. Card format for GCN = 03

I. 1. RTN

2. The number of energy ranges ΔE for this RTN

3-6. Reserve

II. 1. E_H lower limit of first energy range

2. E_B upper limit of first energy range

3. The number of cards for this ΔE, including this card

4. The number of secondary particle groups for which energy distributions are given in this ΔE.

5-6. Reserve

III. 1. Flag 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.

Case (1)

IV. 1. FTN = 101

2. The number of discrete energy values E_n for emitted particles

3. E_n value

4. The corresponding probability $p(E_n)$

Case (2)

IV. 1. FTN = 102

2. The number of pairs (E_d, k) being considered

3. Reserve

4. E_d

5. k

6. The corresponding value of the probability p

Cases (3) and (4)

IV. 1. FTN = 103

2. A

3. B

4. C

5.) zero

6.)

VI. 1. FTN = 104

2. a

3. b

4. c

5. E_f

6. zero

Cases (5), (6) and (7)

IV. 1. FTN = 105 (106 or 107)

2. The number of spectrum values

3. Reserve

4. INT number determining the law for interpolating p(x) with respect to x

5. The first value $x = E/E_o^q$

6. The corresponding probability p(x)

Linear combination of cases (E_o is not given explicitly)

IV. 1. FTN = 150

2. The number of different laws in the linear combination

3. The number of cards for this FTN

4-6. Reserve

The format of card V depends on the case number and has the following form:

(a) For cases (1) and (2)

V.	1.	The case number = 01	1.	The case number = 02
	2.	The probability of this case	2.	The probability of this case
	3.	The number of discrete E_n	3.	The number of pairs (E_d, k)
	4.)		4.	E_d
	5.)	Reserve	5.	k
	6.)		6.	The p value

(b) For cases (3) and (4)

V.	1.	The case number = 03	1.	The case number = 04
	2.	The probability of this case	2.	The probability of this case
	3.	A	3.	a
	4.	B	4.	b
	5.	C	5.	c
	6.	zero	6.	E_f

(c) For cases (5), (6) and (7)

V. 1. The case number = 05 (06 or 07)

2. The probability of this case

3. The number of spectrum values

4. INT number determining the law for interpolation of p(x) with respect to x

5. x

6. p(x)

Case (8)

IV. 1. FTN = 208

2. The number of E_o values

3. The number of cards for this FTN

4. INT number determining the laws for interpolating $p(E_o,E)$ with respect to E_o and $p(E_o,E)$ with respect to E

5-6. Reserve

V. 1. E_o

2. The number of E values at this E_o

3. E

4. p(E)

Linear combination of cases (all cases at a given E_o)

IV. 1. FTN = 251

2. The number of E_o values

3. The number of cards for this FTN

4. INT number determining the law for interpolating the probability of the case from the initial energy E_o

5-6. Reserve

V. 1. E_o

2. The number of cases at this E_o

3. The number of cards for this E_o

4-6. Reserve

The format of subsequent cards depends on the case number and has the following form:

(a) For case (8)

VI. 1. The case number = 08

2. The probability of this case

3. The number of E values

4. INT number determining the law for interpolating p(E) with respect to E

5. E

6. p(E)

(b) For cases (1-7) the format of card VI FTN = 251 coincides with the format of card V FTN = 150

Linear_combination_of_cases (all E_o for a given case)

IV. 1. FTN = 252

2. The number of different cases

3. The number of cards for this FTN

4-6. Reserve

V. 1. The case number

2. The number of E_o values

3. The number of cards for this case

4. The probability of this case

5. INT number determining the law for interpolating the probability of the case from the initial energy E_o and, if necessary, the law for interpolating $p(E_o,E)$ with respect to E_o and $p(E_o,E)$ with respect to E

6. Reserve

The format of subsequent cards depends on the case number and has the following form:

(a) For case (1)

VI. 1. E_o

2. The number of discrete E_n

3. E_1

4. $p(E_1)$

5. E_2

6. $p(E_2)$ etc.

(b) For case (2)

VI. 1. E_o

2. The number of (E_d, k) pairs

3. Reserve

4. E_d

5. k

6. p

(c) For case (3)

VI.	1.	E_o
	2.	A
	3.	B
	4.	C
	5-6.	zeros

(d) For case (4)

VI.	1.	E_o
	2.	a
	3.	b
	4.	c
	5.	E_f
	6.	zero

(e) For cases (5), (6) and (7)

VI.	1.	E_o
	2.	The number of spectrum values
	3.	x_1
	4.	$p(x_1)$
	5.	x_2
	6.	$p(x_2)$ etc.

(f) For case (8)

VI.	1.	E_o
	2.	The number of E values at this E_o
	3.	E_1
	4.	$p(E_1)$
	5.	E_2
	6.	$p(E_2)$ etc.

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

The data on energy angular distributions of thermal-neutron scattering characterize the interaction of neutrons with atomic nuclei in the energy region where the relative motion of neutron and nucleus, as well as atomic interactions (e.g. effects of chemical bonding, etc.) are 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 double differential cross-sections and in the form of the scattering law.

In the first case, the matrix of numerical values is preassigned for the function $\sigma(E_o \rightarrow E, \vartheta)$, representing the probability of a neutron with initial energy E_o being scattered at an angle ϑ and having an energy E after scattering. The discrete values of the variables (E_o, E, ϑ) on which the probability function of thermal neutron scattering depends are chosen so that any required values of the function can be obtained with sufficient accuracy by interpolating the values contained in the matrix.

When the energy angular distribution of thermal neutrons is determined by the scattering law, the matrix of $S(\alpha,\beta)$ values for discrete values of the variables is represented by

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

and

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

Here E_0 is the initial neutron energy, E the final energy, ϑ 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 α and β are related to the momentum and energy transfer resulting from collision. The choice of values for the variables α and β must ensure the possibility of obtaining any $S(\alpha,\beta)$ value by interpolation with a sufficient degree of accuracy.

The expression for the cross-section of a process as a result of which a neutron with initial energy E_0 will scatter at an angle ϑ in the laboratory co-ordinate system and will have the energy E, takes the form

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

Here σ_b is the cross-section for a bound atom:

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

σ_{fr} - is the cross-section for a free atom.

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

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

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

When $S(\alpha,\beta)$ has a singularity at $\beta = 0$ in the form of a δ function it may be represented as follows:

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

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

σ_{fr} - the cross-section for a free atom (if it is constant);

$\mathcal{E} = E_{bo}/kT$ - a value corresponding to the lower limit of validity of the elastic scattering static model

E_m - the upper boundary of σ_{fr} as a constant: above this value the energy dependence of σ_{fr} must be taken into account (one can take it to be equal, for instance, to the elastic scattering cross-section σ_{el} (RTN = 01002) which is available in the library, neglecting the contribution of inelastic scattering because of its small value); and

A' - the effective atom (molecule) - neutron mass ratio: for molecules this value is arbitrary to a certain degree and is usually chosen on the basis of 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 sub-number according to 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 sub-numbers define 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 temperatures considered

3. Reserve

4. INT number determining the law for interpolating $\sigma(E_o,E,\vartheta,T)$ or $S(\alpha,\beta,T)$ with respect to temperature T

II. 1. The temperature for which the data are given

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_o values

3. The number of cards for this FTN

4. INT number determining the laws for interpolating $\sigma(E_o, E, \vartheta)$ with respect to E_o, with respect to E and with respect to ϑ

5-6. Reserve

IV. 1. E_o

2. The number of E values at this E_o

3. The number of cards for this E_o

4-6. Reserve

V. 1. E

2. The number of ϑ values at this E

3. ϑ

4. $\sigma(\vartheta)$

Case (2): FTN = 200

III. 1. FTN = 200

2. The number of ß values

3. The number of cards for this FTN

4. λ

5. σ_{fr}

6. ε

IV. 1. E_m

2. A'

3. Reserve

4. INT number determining the laws for interpolating $S(\alpha,\beta)$ with respect to β and with respect to α

5-6. Reserve

V. 1. β

2. The number of α values at this β

3. α_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),

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

η - the number of secondary neutrons per inelastic scattering event,

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

α - capture to fission cross-section ratio,

$$\alpha = \sigma_\gamma / \sigma_f$$

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

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

The first three values are derived and can therefore be calculated from the appropriate formulae; their specification in the library is not necessary in this case. On the other hand, $\bar{\nu}$ is measured directly from experiments 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. But $\bar{\nu}$ values may be defined at points which do not coincide with points specified for other cross-sections, in particular σ_f. Therefore, it is essential that the extreme energy points (the smallest and the largest) at which $\bar{\nu}$ and σ_f are given should coincide. We can then find by interpolation the values of $\bar{\nu}$ and σ_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 coincides with the format for neutron cross-section representation (GCN = 01), with the exception that nothing is punched in location 3 of card I for GCN = 05.

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