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FORMAT OF THE RECOMMENDED NUCLEAR DATA LIBRARY FOR REACTOR CALCULATIONS

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Foreword

This is a translation of a Soviet report on a proposed USSR Evaluated Data file format. The original Russian report was submitted by Dr. M.N. Nikolaev at the Dutch-Belgian-Soviet Seminar held at Melekess in February 1970. This report is to be considered in context of the current development of a Soviet format for evaluated data by Dr. Nikolaev's group at Obninsk.

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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 situation will prevail for a sufficiently long time. Until recently the preparation of multigroup constants required such considerable expenditures of effort and time that the only practical possibility was to use systems of constants with fixed neutron energy ranges dependent on the type of reactors 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 in this manner as well as in the technical difficulties to correct these data.

The development of calculational techniques allows a considerable degree of automatic processing of recommended point-wise nuclear data sets into group constants with arbitrary energy divisions, and to link this process directly with multigroup codes for reactor calculation. The basis for such a system of information processing is a library of recommended nuclear data (1). The library formats of recommended nuclear data (2,3,4), now existing, 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 interaction 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 point-wise, describing a detailed energy behaviour, in the form of resonance parameters, or in the form of subgroup, with different number of subgroups. The differential cross-sections for elastically scattered neutrons may also be specified by different methods: in the form of angular dependence or in the form of Legendre polynomials. Here the subgroup representation of data is also possible.

The choice of one or another type of data representation depends in practice on various considerations: on the nature of a problem, on considerations of convenience, on the codes available, etc. Therefore, it is desirable to provide in the library the possibility to store information in different representations. For this purpose it is convenient to introduce into this storage system a special characteristic - namely, a representation type number.

This report discusses the formats for reactor calculations. They are based on generalizations, and on a further development of the English format described in ref. (2) which is used in a number of foreign laboratories. The essential 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 fuller capabilities of modern computers to be implemented.

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

I. CLASSIFICATION OF NUCLEAR DATA

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

First, all data entered into the library are classified by the isotopic composition of the substance to which they refer. Each data set for a given substance of specific composition is characterized by a "nuclear identification number," (NIN) and represents a more or less indenpendent body of information. Data having a particular NIN are further classified by possible reaction types, which can be induced in the considered substance, and are assigned specific "reaction type numbers" (RTN). Finally, nuclear data with any given RTN are classified by the form in which they are represented in the library, characterized by "form type numbers" (FTN).

1. Nuclear Identification Number (NIN)

Each NIN comprises data of a given isotope, element, chemical compound, mixture, etc.

Classification by NIN permits one to include into the library various data sets for same substance. These can be, for instance, data from different compilations, or data from basic data libraries which have been processed by different (computer) codes. When entering such data into the library, they are assigned new NIN's. In this manner, the NIN characterizes various systems of library data for different substances as well as for the same substance.

The possibility exists to assign NIN's according to the manner in which data were obtained or according to any other criterion. This assignment could be useful in the systematizations existing in nuclear data libraries. However, since consideration of concrete data details is outside the scope of this report, such assignment (possibilities) will not be discussed.

2. Reaction Type Number (RTN)

All data which have the same NIN, are classified according to the reaction induced in the given substance. The Reaction Type Number (RTN)

consists of a five-digit number which is subdivided into two parts: a two-digit "general classification number" (GCN) and a three-digit "particular classification number" (PCN).

The construction of the RTN from the GCN's and PCN's give this nuclear reaction data classification system considerable flexibility. With the use of the RTN, it is possible to combine into one set, for a given NIN, neutron data as well as data on photon production and their interaction with the matter. In practice, however, it is more practical to store these three types of data under three diferent NIN's, especially since their energy ranges do not usually correspond.

This gives rise to the possibility of re-arranging data in the library by means of the NIN and the RTN. This possibility will be further broadened by introducing the form type number (FTN).

3. General Classification Number (GCN)

Classification by GCN subdivides data of a given NIN into groups dependent on the data type. The following GCN's 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 ($\bar{\nu}, \alpha, \eta$, etc.)

The remaining GCN assignments have not been made. Partly, those GCN's which define photon interactions constants have been omitted because they fall outside the scope of data for which we are responsible.

4. Particular Classification Number (PCN)

The Particular Classification Numbers specify nuclear reactions. Each PCN identifies a single process which occurs as a result of neutron or photon interaction with matter. The table that follows lists the PCN assignments for neutrons, based on the UK classification system.

Particular Classification Numbers (P.C.N.)

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 caters for that part of the (n,n') reaction not covered by P.C.N's 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 obsorption (all reactions which do not lead to emission of incident particle)

102 (n,γ) or (γ,e-)

103 (n,p)

104 (n,d)

105 (n,t)

106 (n,He^3)

107 (n,α)

108 (n,2α)

109 - 150 reserved for other possible reactions which do not lead to the production of secondary particles of the same type as the primary (particle)

151 - 200 in the UK library these PCN's are used for the classification of information on resolved and statistical resonance information. The detailed meaning of the PCN's are closely related to the form of the data.

201 - 999 reserved for a variety of other data, which may be introduced in the future.

As can be seen, a large number of PCN's have been left unassigned so as to provide for the future needs of the library of recommended nuclear data.

In the UK classification PCN = 201 - 208 are used for the identification of such reactions as transport and removal cross-sections, $\widetilde{\nu}\sigma_f$ and a number of other deduced quantities. PCN's 301 to 450 are reserved for the parameter ($\overline{\sigma_K E}$) which defines the energy release rate, where $\bar{E}$ is the average energy released in reaction K. These quantities are related to the quantities defined by PCN's 001 to 150; the corresponding reaction is identified by subtracting 300 from this 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 recommended nuclear data, but can be easily obtained with the help of special (computer) programmes. It is therefore reasonable not to assign PCN's to these quantities (at least for the time being). It is probably more convenient to include such quantities in a group-constant library, formulated on the basis of 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, with C^{12} the $C^{12}(n,n')3\alpha$ has PCN = 023 whilst the reaction $C^{12}(n,n')C^{12*}(\gamma)C^{12}$ has PCN = 5 if the 4.43 MeV first excited state is considered. Similarly with U^{238}, PCN = 016 implies that U^{237} + 2n are the final product. In this manner, for any given nuclear transmutation it is possible to determine the state of the residual nucleus as well as the state of the emitted particles from the PCN.

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 $\bar{\nu}$

5. Form Type Number (FTN)

Since data can be represented in the library in a number of ways, they are classified according to a form type number (FTN). The introduction of the FTN permits input of data having the same RTN in various representations, broadening at the same time the potential of the stored recommended nuclear data.

The following modes of data representation are indicated:

- Representation of data in the form of 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.
- Group-wise data representation [5] with optional number of neutron sub-groups.

In the case of a sub-group representation, the neutrons, at a given energy, are shared out amongst N subgroups. Each such subgroup (n), characterized by its cross-section value σ_n, has its own weight a_n, so that

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

A group-wise representation is a convenient method to represent data in the region of unresolved resonances. It can as well be applied to the resolved resonances, if it is not absolutely necessary to have a detailed energy dependence of the data in this energy range.

In the case of angular and energy distributions of secondary particles, one can use different modes of representations, reflecting one or another mechanism of the given nuclear reaction. In the FTN classification it is proposed to construct angular and energy distributions in the form of superpositions of such representation with an assigned probability for each one of them.

In addition, the introduction of the FTN makes it possible to have a more flexible way to rearrange the data stored in the library.

In particular it becomes possible to change at will the number and order of priorities of the variables (parameters) on which the data in the library are dependent upon.

The FTN is designed in such way as to be able to assign different orders of priority to the variables on which the data depend as well as to identyfy the form in which the data are given in the library (at discreet points, parametrically, etc.....)

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 describing the representation of corresponding GCN formats.

II. REPRESENTATION OF DATA ON PUNCHED CARDS

The nuclear data information contained in the library is assumed 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 numeric tabulations and of auxiliary information coded in numerical form, which serve as headings to the data tables. The service information consists of different types of flags (indices), which distinguishes one card from another. The presence of these flags also simplifies computer processing of the stored data.

The symbolic card consists of 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 commehts 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 a blank column, used for the basic information (data fields), and a service field in col. 73 to 80. This information distribution is used in the UK evaluated nuclear

data library. In the case of the M-20 computer facility, it is more convenient to use 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.

Both of these types of codification are equivalent in the sense that the information coded on a symbolic card, when printed out by means of corresponding service equipment, is the same. Either the column field or the row is the basic information unit. Each field (row) contains a single machine word (one number). Alphabetic characters are not coded. The representation of numbers depends on what they represent. All nuclear data are represented in a binary form with floating decimal. The auxiliary information is represented by non-normalized binary numbers recorded on the right hand side of the corresponding rows (fields).

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

The question as to which method is more rational is still open. This is, however, immaterial to the following exposition which deals with the formulation of specific formats for the storage of nuclear data.

The data for a given substance, defined by a specific NIN, constitutes a complete set of information, in the sense that this information can be used from this point on independently, without recourse to any other information set which may contain analoguous data for that same substance. Such a body of information consisting of a closed set of data shall be referred to below as a "file" (using the English word: file). Each file is defined by its own NIN, which can now be called the library file number (LFN).

Each file is subdivided into sections according to the number of reaction types associated with each (NIN). Each section contains cards containing data of a given reaction type (RTN). Thus, a given reaction type in different files may correspond 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 numeration 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).

Example 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 elastic scattered neutrons.
04	01003	Non-elastic cross-section
05	01004	Inelastic cross-section
06	01005	Inelastic cross-section for first level excitation
07	02005	Angular distribution of inelastically scattered neutrons with first level excitation
08	03005	Energy distribution of inelastically scattered neutrons with first level excitation

The content, as well as the location of information on cards depends on the RTN (primarily on the GCN) as well as on the RTN. This will be considered in more detail below. The service information (field) contains the NIN (=LFN), the section number, the card number as well as other information necessary for the handling of the information by means of specialized computer programs. Inasmuch as this service information is closely related to the actual programming, it is not further described here.

III. FORMATS OF NUCLEAR DATA IN THE LIBRARY

Just as the character of nuclear data is determined by the type of the reaction, the format of these data in the library depends on the FTN, primarily on the GCN.

The energy range of a given RTN, is in some cases subdivided into a number of intervals. The following considerations must be taken into account:

1. Absence of data in given energy regions, or cases where data are extremely low in value (as at the threshold of a reaction).
2. In some energy ranges the corresponding data are not energy dependent or are represented in a similar manner.
3. In different energy ranges data have different representations or different temperature dependences.

The subdivision of the energy scale into intervals allows one to avoid duplication of results. One should strive to minimize the number of energy intervals. For different RTN's within a single NIN it is possible to have different numbers of intervals. Wherever possible it is desirable to have a correspondence of energy intervals for total σ's and their associated partial σ's. This is helpful in that one can find gross errors by means of special programs.

Usually, nuclear data are given at discreet energy points. If the data are constant in some energy interval, they could be represented by a (single) value for that E interval. Such a treatment is possible with the help of special formats foreseen in the FTN classification.

In those cases where the data are given as a function of discrete values of those variables, on which the data depend, the choice of the corresponding values and dependent variables must satisfy specific conditions. That is, the values of the variables must be chosen such that the value of the function itself at any given point can be obtained to a

reasonable degree of accurary 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 polynominal are determined by evaluators, taking into account the capabilities of available programs; this information is then entered into the heading of the FTN. Since this type of information is closely related to the programs, its classification has not been included here.

Temperature dependence is indicated when it is considered to be important. If T dependence can be included in analytical calculations, the specification of a single temperature is enough. On the other hand, results are compiled at different temperatures so as to obtain data at any desired temperature by interpolation.

The FTN specification is such that it allows identification of the residual nucleus as well as the reaction products of any given nuclear reaction. In most cases, the number of secondary particles, resulting from a given reaction is uniquely determined.

Inasmuch as some data, as experimental data on angular and energy distributions, are not always known for every secondary reaction product separately, but probably in some cases for definite groups of particles of these products, the corresponding formats provide a special conditional number identifying the groups of particles for which data are specified.

The library formats allow information to be stored in the form of 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 can be data of the same RTN or FTN, data of the same energy range, temperature, etc.....

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 subgroups, and others fall into this category.

In the following we refer to a column (field) or a row (line) as a location. When describing concrete formats, the cards are numbered with roman numerals, and the positions of cards within the set containing basic information are numbered with arabic numerals.

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 each section. The heading card format is the following:

I. 1. LFN (Library file number)
2. Total number of cards in this 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 this section.

If necessary, the information is continued on subsequent cards in the same format as location 1 - 3 of card II.

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. A variable can be the energy , the temperature, the subgoup, number, etc..... Cross-section data are stored in an order determined by the variable; for the case of energy and temperature, this implies a monotonically increasing order. The numeration of subgroups depends on the order of cross-section growth (increase). In the formats adopted here, energy is given in MeV, temperature in degree 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. For cross-sections, one often uses interpolation on a logarithmic scale. In this case it is necessary that the cross-section is non-zero at all points, including the end-points of the interval.

In the FTN classification scheme, it is possible to assign (a single value for) the cross-section for the full energy range at once, if it is constant in that energy range.

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

2.1. FTN Classification for GCN = 01

The high priority FTN sub-number (n_1) defines the manner in which the data are represented in the set, according to the following table:

n_1	Representation form of the cross-section
1	At discrete points as a function of E and T in a sub-group representation.
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 formulas for resolved resonances.
4	Parametrically by means of statistical information for unresolved resonances.

Subsequent n_1 values (5-9) are reserved for new data representation 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 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 corresponds to assigning a cross-section value to the full energy interval.

For the remaining values of n_2, the meaning of n_2n_3 have not yet been determined, nor have the representational formats of these data.

2.2. Card Format for GCN = 01

I. 1. RTN
2. Number of energy intervals (ΔE) for this RTN
3. A value of the reaction in MeV
4. }
5. } Reserved for supplementary information
6. }

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-section in this ΔE, including the present card
4. Number temperature values considered in this ΔE
5. } Reserved for additional information in this ΔE
6. }

III. 1. Temperature T, at which cross-section is given
2. FTN number for the cross-section at this temperature
3. Number of cards to represent the cross-section at this temperature, including this card
4. }
5. } Reserved for additional information at this T.
6. }

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 values σ

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

IV. 1. FTN = 111
2. Number of energy values
3. 4. } Reserved for supplementary information for this FTN*
5. E
6. σ(E)

If necessary, the information is continued onto subsequent location of this and the following card 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 onto subsequent cards in the formats of location 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-paragraphs (if it does not depend on E)
5. 6. } Reserved for supplementary information of this FTN

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* It is presupposed that the method of interpolation is going to be given at this point.

V. 1. E
2. Number of subgroups
3. a_1
4. σ_1

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

Generally speaking, this format allows representation of different number of sub-groups for different E's. In practice, however, the number of sub-groups for all E's 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-paragraphs
3. Number of cards for this FTN
4. } (Reserved)
5. }
6. }

V. 1. Sub-group number (i)
2. Number of energy values
3. (Reserved)
4. E
5. a_{i1}
6. σ_{i1}

If necessary the information is continued onto subsequent cards in the format of locations 3 and 4 of card V.

The formats of cards for FTN's with $n_1 = 2$, $n_1 = 3$ and $n_1 = 4$ have not been determined yet.

3. Angular Distribution of Secondary Particles (GCN=02)

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

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

can be given for a full energy range as well as at individual energy points. The following normalization condition is assumed

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

It is intended to provide the facility to enter angular distributions as discrete points as a function of μ, where $\mu = \cos\theta$, θ being the scattering angle. We shall call this the μ-representation. The second possible representation is parametrical in the form of ω_ℓ coefficient of the $f(\theta)$ expansion in Legendre polynominals $P_l(\cos\theta)$, such that

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

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 systems is used for a given data set is given as additional information contained in the FTN identifier in the form of a numerical flag, which is 1 if the data are in the CM system, and 2 if the data are in the laboratory system.

The use of either one of the systems 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. In those cases when a simple analytical expression to relate the angular and energy dependences in these two systems of coordinates exists, it is actually unimportant in which of the two systems the data is stored. If, however, no such analytical expression exists, the choice of the coordinate system cannot be arbitrary. The decisive factors in this case are the availability of these data in either of the two systems, the users' demand 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 a ω-representation, the necessary accuracy is guaranteed by the availability of a high enough number of expansion coefficients (i.e. n number).

Even though an angular distribution is given as a normalized probability function, it so happens that in those cases where the actual angular distribution in the form of a μ-representation is a rough approximation, as in the form of linear intervals, one cannot say that the resulting representation will be normalized. It may therefore be necessary in some cases to perform additional normalization of angular distribution obtained from the data files.

The foreseen formats would allow storage of total angular distributions $f(\theta)$ in the form of linear combinations of a number of partial distribution functions $f_i(\theta)$, each of which with a given weight a_i, such that

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

Individual $f_i(\theta)$ could describe, for instance, the angular distribution of the product of some nuclear process, which proceeds along different channels, and is therefore described by means of different mechanisms. This gives the possibility to describe the resonance structure of angular distributions in the form of a sub-group representation. In this case a_i

represents the sub-group weighting factor, and $f_i(\theta)$ characterizes the angular distribution of the given neutron sub-group.

The presently considered formats require that all related partial distribution functions $f_i(\theta)$ be given in one and the same representation (either in the μ or ω form), and be in one and the same coordinate system. Should it become necessary, however, the FTN structure is such that this restrictive condition can be suppressed.

In all cases the total energy range covered by the angular distribution must coincide with that covered by the corresponding integral cross-sections. If, for instance, an elastic cross-section is specified in the energy range 0.001 eV to 14 MeV, then in a point-wise 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 range-wise 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 to recognize gross errors in the stored data.

3.1. FTN Classification for GCN = 02

Angular distribution data representation 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 new data representation forms, if and when they are formulated.

The low-priority FTN sub-numbers for $n_1 = 1$ and $n_1 = 2$ have the following meaning:

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 or 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

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.) Reserved for supplementary information
6.)

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. Reserved

III. 1. Flag identifying the group of secondary particles
2. Number of FTN's for the angular distributions for this group of particles
3. Number of cards to represent angular distributions of this group, including this card.
4.)
5.) Reserved for additional information on this group of secondary particles.
6.)

The format of subsequent cards depends on the FTN.

Case (1) Isotropic angular distribution in ΔE

In this case card IV specifies the number of the representation type (FTN = 101 for the μ-representation, FTN = 201 for the ω-representation), and the flag specifying the coordinate system.

IV.	1.	FTN = 101	IV.	1.	FTN = 201
	2.	Coordinate system flag		2.	Coordinate system flag

Case (2) Angular distribution for the whole ΔE

IV.	1.	FTN = 102	IV.	1.	FTN = 202
	2.	Coordinate system flag		2.	Coordinate system flag
	3.	Number of μ values		3.	Number of ω values
	4.	Reserved		4.	ω_1
	5.	μ_1			
	6.	$f(\mu_1)$			

Case (3) Angular distribution at 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.	Coordinate system flag		4.	Coordinate system flag
	5,6.	Reserve		5,6.	Reserve
V.	1.	E	V.	1.	E
	2.	Number of μ values		2.	Number of ω values
	3.	μ_1		3.	ω_1
	4.	$f(\mu_1)$			

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.	Coordinate system flag		4.	Coordinate system flag
	5,6.	Reserve		5,6.	Reserve

V.	1. a	V. 1. a
	2. Number of μ values	2. Number of ω values
	3. μ_1	3. ω_1
	4. $f(\mu_1)$	

Case (5) Superposition of angular distributions for fixed E

IV.	1. FTN = 121	V. 1. FTN = 221
	2. Number of E values	2. Number of E values
	3. Number of cards for this FTN	3. Number of cards for this FTN
	4. Coordinate system flag	4. Coordinate system flag
	5,6. Reserve	5,6. Reserve
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
	4-6. Reserve	4-6. Reserve
VI.	1. a	VI. 1. a
	2. Number of μ values	2. Number of ω values
	3. μ_1	3. ω_1
	4. $f(\mu_1)$	

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. Coordinate system flag	4. Coordinate system flag
	5,6. Reserve	5,6. Reserve
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
	4-6. Reserve	4-6. Reserve
VI.	1. E	VI. 1. E
	2. Number of μ values	2. Number of ω values
	3. μ_1	3. ω_1
	4. $f(\mu_1)$	

In all of the above illustrated formats, related to angular distribution FTN's, the specification is for a minimum amount of information, i.e. one pair of $[\mu, f(\mu)]$ and one value of ω. It is presupposed that, wherever necessary, this information is continued on subsequent field locations of the same card or on subsequent cards.

4. Energy Distribution of Secondary Particles (GCN = 03)

When the analytical dependence 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 be easily 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) Particle 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 covered by this law; in this case k reflects the energy transfer to the recoil nucleus.

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

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

where A, B and C are constants.

Law (4) Neutron fission spectrum, taking into account the dependence on the incident neutron energy and the nature of the fissioning nuclide, given by the normalized probability function,

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

with

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

$$\alpha = \left(\sigma_{nn'f} + \sigma_{n2nf}\right) / \bar{\nu}\left(\sigma_{nf} + \sigma_{nn'f} + \sigma_{n2nf}\right)$$

$$T = c\left(E_0 - E_f\right) / \left(14 - E_f\right)$$

where a, b, 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, 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

$$P\left(E/E_0^q\right) = f\left(E_0, E\right)$$

where f is some function, E_0 the initial energy, and E is the energy of the emitted particle. 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 by any function dependent on the initial energy E_o and the final energy E in the form of discrete points. (If there is no dependence on E_o, then this law is equivalent to Law (5).)

In the case Laws (5-7) energy distribution data are specified by pairs of values (argument $x = E/E_o$, corresponding probability P(x)) such that interpolation between neighbouring values stored in the data file would yield an acceptable accuracy. 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 of considered arguments, certain arguments may be inaccessible in practice on energy conservation grounds (e.g. the emergent energy of secondary neutron may be greater than the incident energy). In such cases, it will be necessary to re-normalize the distribution probability function.

As in the case of angular distributions, the formats for the energy distributions of secondary particles provide for the possibility to specify 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 applied to 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 actual laws will characterize the energy distribution of the corresponding neutron sub-group.

The special case of thermal scattering is considered separately.

4.1. FTN Classification for GCN = 03

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

n_1	The method of energy distribution presentation
1	In those cases when the initial energy is not given explicitly.
2	In those cases when the initial energy is given explicitly.

Subsequent values of n_1 (3-9) are reserved for other representations, if such would appear.

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.

$n_2n_3 \geq 50$ 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.

4.2 Card Format for GCN=03

I. 1. RTN
2. The number of energy ranges 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 FTN's for the energy distributions for this group of particles.
3. The number of cards 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 points (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

VI. 1. FTN = 104
2. a
3. b
4. c
5. E_f

Cases (5)(6) and (7)

IV. 1. FTN = 105 (106 or 107)
2. The number of spectrum values
3. The value $X = E / E_o$
4. The probability p(X) corresponding to it

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. Reserve

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

a) For cases (1) and (2)

V. 1. The case number=01
2. The probability of this case
3. The number of discrete E_n
4. Reserve
5. E_n
6. $p(E_n)$

V. 1. The case number= 02
2. The probability of this case
3. The number of pairs (E_d, K)
4. E_d
5. K
6. The p -value

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

V. 1. The case number = 03
2. The probability of this case
3. A
4. B
5. C

V. 1. The case number = 04
2. The probability of this case
3. a
4. b
5. c
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. Reserve
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
4-6. 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
4-6. 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. Reserve

5. E

6. p(E)

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

5-6. 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_o

3. E_n

4. $p(E_n)$

b) For case (2)

VI. 1. E_o

2. The number of (E_d, K)

3. Reserve

4. E_d

5. K

6. p

c) For case (3)

VI. 1. E_o
2. A
3. B
4. C

d) For case (4)

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

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

VI. 1. E_o
2. The number of spectrum values
3. X
4. p(X)

f) For case (8)

VI. 1. E_o
2. The number of E-values at this E_o:
3. E
4. p(E)

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 pre-assigned for the function $\sigma(E_o \rightarrow E, \theta)$, representing the probability for a neutron of the initial energy E_o to be scattered at angle θ, and to have the 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 could be obtained with sufficient accuracy by interpolating the values contained in the matrix.

In the case when the energy-angular distribution of thermal neutrons is determined by the scattering law, the matrix of $S(\alpha,\beta)$values at discrete

values of the variables is represented by:

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

and $$\beta = (E - E_o) / kT$$

Here E_o 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 as a result of collision. The choice of values for the variables α and β must ensure the possibility to obtain any $S(\alpha,\beta)$ value by interpolation to a sufficient degree of accuracy.

The expression for the cross section of a process, as a result of which a neutron with the initial energy E_o will scatter at angle θ in the laboratory coordinate system and will have the energy E, has the form:

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

Here σ_b is the cross section for a bound atom

$$\sigma_b = \sigma_{fr} (A+1)^2 / A^2$$

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

For a monoatomic gas where the chemical bonding effects play no part 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 the definition of the function $S(\alpha,\beta)$ in those cases when there is no other information on the thermal neutron scattering law.

When $S(\alpha,\beta)$ has a peculiarity 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 card 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,

$\mathcal{E} = E_{th}/kT$ - the value corresponding to the lower boundary of the elastic scattering statistical model,

E_m - the upper boundary of σ_{fr}, above which value it is necessary to take into account the energy dependence of the cross section σ_{fr} assuming it to be equal, for instance, to the elastic scattering cross section σ_{el} (RTN = 01002) which is available in the library, and neglecting the contribution of inelastic scattering because of its small value,

A' - the effective atom (molecule)- neutron mass ratio; for molecules this value is conditional to a certain degree and is usually chosen on the basis of analysis of experimental results.

5.1. FTN Classification for GCN=04.

The method of specifying the data on energy- angular distributions of thermal neutrons is determined by the high priority FTN Sub-numbers according to the following table:

n_1	The method of representing the 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 ordinal number of the format at the given n_1 value.

5.2. Card Format for GCN=04.

I. 1. RTN

2. The number of temperatures considered

3-6. Reserve

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

2. The number of FTN's 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

4-6. 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. $\sigma(\theta)$

Case (2): FTN = 100

III. 1. FTN = 200

2. The number of β -values

3. The number of cards for this FTN

4. λ

5. σ_{fr}

6. ξ

IV. 1. E_m

2. A'

3-6. Reserve.

V. 1. β

2. The number of α values at this β

3. α

4. S(α)

6. Particular Values for Neutrons - $\bar{\nu}, \alpha, \eta$, etc...(GCN=05)

The following quantities fall into this category:

n - the number of secondary neutrons per collision (elastic and inelastic).

$$m = \left(\sigma_m + \sigma_{m'} + 2\sigma_{2m} + 3\sigma_{3m} + \bar{\nu}\sigma_f + \cdots \right) / \sigma_t$$

η - the number of secondary neutrons per inelastic scattering

$$\eta = \left(\sigma_{m'} + 2\sigma_{2m} + 3\sigma_{3m} + \bar{\nu}\sigma_f + \cdots \right) / \sigma_x$$

α - capture to fission cross-section ratio

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

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

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

The first values are derived and can therefore be calculated from the appropriate formulas; 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 method 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. With regard to $\bar{\nu}$ values, they may be defined at points which do not coincide with points specified for other cross sections, in particular, σ_f. Therefore, it is required that the extreme energy points (the smallest and the largest) at which $\bar{\nu}$ and σ_f are given should coincide. In this case we may find by interpolation of the $\bar{\nu}$ and σ_f those values necessary for calculating the $\bar{\nu}\sigma_f$ values.

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).

6.2. Card Format for GCN = 05.

The card format to represent special neutron quantities coincides with the format of neutron cross-section representation (GCN = 01), with the exception that nothing is punched in the location 3 of the card 1 for GCN = 05.

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