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From: H.D. Lemmel

Subject: ENDF/B

Please find attached the paper

D. Hermsdorf, Technical University, Dresden, GDR:
Recommendations for the use of formatting rules in ENDF/B.

This paper had been submitted to the 7th IAEA Consultants' Meeting of Nuclear Reaction Data Center, Obninsk/Moscow, USSR, 17-21 October 1983.

It is meant as an introduction to ENDF/B for newcomers who usually encounter difficulties with the voluminious manual ENDF-102 of ENDF/B Formats and Procedures.

The paper is submitted also to the IAEA Specialists' Meeting on the Format for the Exchange of Evaluated Nuclear Data.

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RECOMMENDATIONS FOR THE USE OF FORMATTING RULES IN ENDF/B

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Contents

Introductary remarks

This paper presents some rules important for planning the formatting procedure of fast neutron nuclear data into the structure ENDF/B-V. All these rules are based on experiences in application of the general description of the format. So, this paper is aimed to be a guide or inverse manual for use of the very voluminous report ENDF 102 /1/ and the brief summary documentation issued by the IAEA /2/.

1. General relations

1.1. Quantities

The format ENDF/B is designed for the storage of as well as the energy and angular dependences of data for neutron induced nuclear reactions. Generally, the dependence of values Y on the variable X is given in tabular form keeping some other parameters (if any) fixed.

The quantity

Y may be a { cross section σ / probability p / Legendre coefficient f_l

whereas

X may be the { neutron incidence energy E / particle/photon emission energy E' / cosine of scattering angle μ / angular momentum l

some other quantities will be used for parametrization of cross sections (decay data, resonance data...).

1.2. Dimensions

Energies: $E, E', Q, U, E_{th}, E'_{max}$ ... eV

Cross sections: $\sigma(E)$ ... barns

$\frac{d\sigma(\Omega,E)}{d\Omega}$	...	barns/sterad
$\frac{d\sigma(E\rightarrow E')}{dE'}$	...	barns/eV
$\frac{d^2\sigma(E\rightarrow E',\mu)}{d\Omega dE'}$	...	barns/eV/sterad
Nuclear temperature: Θ	...	eV
Nuclear radius: a	...	fm
Nuclear masses: m, A	...	amu
AWRI	...	dimensionless
Temperatur: T	...	Kelvin
Cosine of angle: μ	...	dimensionless
Probability distributions:		
$p(\mu)$	...	1/unit cosine
$p(\mu,E)$	...	1/eV/unit cosine
$p(E\rightarrow E')$	...	1/eV
$p(E\rightarrow E',\mu)$	...	1/eV/unit cosine
Legendre' coefficient:		
(order 1) $f_1(E)$	...	dimensionless
$f_1(E\rightarrow E')$	...	1/eV

1.3. Definition of some quantities

1.3.1. Energies

- Q-value for a reaction A(a,b)B:

$$Q = \left\{(m_A+m_a) - (m_B+m_b + \frac{E_B}{9.315016\cdot10^8})\right\} \cdot 9.315016\cdot10^8$$

Attention:

If isotopic mixtures (natural elements) are considered, that Q-value should be choosen which give the lowest energy threshold E_{th}:

$$Q = \min (|Q_1| , \ldots , |Q_i|)$$

- Binding energies

E_B = excitation energy of final state of a residual nucleus (usual the ground state)

- Threshold energy

$$E_{th} = \frac{AWRI+1}{AWRI} \; |Q|$$

Attention:

This definition is not true for fission.

- Maximum emission energy

$$E'_{max} = E - U$$

with E = neutron incidence energy

$$U = \begin{cases} |Q^c| \; \ldots \text{ Q-value for excitation of the level continuum usually} \\ -20 \cdot 10^6 \ldots 30 \cdot 10^6 \text{ for fission} \end{cases}$$

- Averaged energy for an energy distribution

$$\bar{E} = \int_0^{E'_{max}} dE' \; E' \; p(E \rightarrow E')$$

$$\bar{E} < E + E_{th} > \text{ multiplicity} \times E$$

Attention:

The integral can be solved analytically only by using parameterized probability distributions.

1.3.2. Nuclear constants

- Nuclear masses

$$AWRI = A/m_n = A/1.00865$$

- Nuclear radius

$$a = 0.123 \sqrt[3]{AWRI} + 0.08$$

- Wave number

$$k = 2.196771 \cdot 10^{-3} \frac{AWRI}{AWRI+1} \sqrt{E}$$

Attention:

E should be inserted in the lab system.

2. Principal structure and scope of a data massive defined in ENDF/B

2.1. Structure of a MAT

A massive of data for an isotope (or a natural isotopic composition) will be identified unambiguously by a MAT-code assigned by that data centre responsible for the maintenance of the library.

The data are grouped into "Files" according to their physics background and/or the type of dependence on free or fixed parameters. Such a group is identified by a number MF.

Every MF is subdivided into their constituents related to data for different reaction types (reaction channels) by a number MT.

All MF and MT values defined up to now are compiled in /1/ and /2/.

A data massive will be correctly formatted if all subsets are ordered by
- increasing MF's

and

- increasing MT's.

Of course, any MAT must not have data for all MF's and MT's (see 2.2.).

Within a MT the data

$$\text{Y corresponding to} \begin{cases} \sigma & \text{MF} = 3 \\ p \text{ in} & \text{MF} = 4, 5, 6 \\ f_1 & \text{MF} = 4, 6 \end{cases}$$

have to be ordered by an increasing variable X which is equivalent to

$$\text{X means} \begin{cases} E & \text{MF} = 2, 3, 4, 5, 6 \\ E' \text{ in} & \text{MF} = 5, 6 \\ \mu & \text{MF} = 4, 6 \\ 1 & \text{MF} = 2, 4, 6 \end{cases}$$

2.2. Mandatory data in a MAT

ENDF/B is a library format devoted to neutron data mainly. Therefore, all data for reaction channels involving neutron elastic and nonelastic processes are mandatory, i.e.

MF = 3

- elastic scattering cross sections; MT = 2
- neutron inelastic scattering to discrete levels and level continuum; MT's = 51 to 91
- excitation functions for neutron producing reaction; several MT's
- fission; MT = 18
- neutron capture; MT = 102

MF = 4

- angular distributions of neutron elastic scattering; MT = 2
- angular distributions of neutron producing reactions; several MT's

MF = 5

- energy spectra of all neutron producing reactions proceeding via level continuum; several MT's (excluding MT = 2 and MT = 51 to 90)

Also some related quantities are mandatory:

MF = 2

- the effective scattering radius

MF = 3

- ν_1; MT = 251
- $\int$; MT = 252
- ϕ ; MT = 253

MF = 4

- transformation matrix $U_{l,m}$; MT = 2

If data are given in MF = 4, 5, and 6 data for the same MT have to be included also in MF = 3 consequently for normalization (see 5.)

Some cumulative cross sections defined for MF = 3 are redundant but nevertheless of important relevance for practical applications (MT = 1, 3, 101, 203 to 207).

3. Representation of data Y in dependence on variables X

3.1. Independent variables X

3.1.1. Energy E

- Maximum number of energy points at which data Y can be given are:

NRS	$\leq$ 500	for	MF = 2
NP	$\leq$ 5000	for	MF = 3
NE	$\leq$ 500	for	MF = 4
NE	$\leq$ 200	for	MF = 5

- Rules for choice of the energy mesh:
  as much as necessary to store fine structures properly (cross section's maxima and minima); as low as possible to ensure a proper interpolation of data (see 4.);

- Mandatory energy values:

  - energy range 10^{-5} to $2 \cdot 10^{7}$ eV for non-threshold reaction
    E_{th} to $2 \cdot 10^{7}$ eV for threshold reaction
  - 0.0253 eV
  - all E_{th} of MT's for threshold reactions included in a MAT ($\pm$ 10 %)
  - double-valued energy points at the boundaries of energy rangs
  - no other energy point should be used in partial reactions than defined in cumulative cross sections (MT's = 1, 3, 4).

3.1.2. Energy E'

- Maximum number of energy points

  $NF \leq 1000$ for MF = 5

- Maximum energy E'_{max} according to 1.3.1. may not exceeded
- Emission energy E' = 0.0 must be given

3.1.3. Cosine of scattering angle μ

- Maximum number of points

  $NP \leq 101$ in MF = 4

- $\mu = -1$ and $\mu = +1$ must be included
- used in MF = 4 and 6 (LTT = 2) for all nonelastic processes going via the level continuum

3.1.4. Angular momentum l

- mandatory, if LTT = 1 in MF = 2
- mandatory in MF = 4 for discrete levels excitation (MT's = 2, 51...90)
- maximum number of angular momenta

  $NLS \leq 3$ for MF = 2

  $NL \leq 20$ for MF = 4, 6

- NL should be an even number
- NL should be great enough to ensure positive cross sections at all angles

3.2. Dependent variable Y

- zero value at E_{th} in MF = 3;
- zero value at $E' = 0.$ and $E' = E'_{max}$ in MF = 5;
- double-valued at boundaries of energy rangs (discontinuities);
- not more than two cross sections of the same value in the same energy range;
- the sum of all partial cross sections must coincide with the correspondent cumulative quantitie within a 1 % limit of accuracy;
- if MF = 2 is used to represent resonances, then the complete cross section must be obtained from the sum of data calculated by MF = 2 and "residuals" given in MF = 3 (valid for MT = 1, 2, 18, and 102 only).

3.3. Choice of reference system

3.3.1. Laboratory system (LCT = 1)

Data should be given in the Lab-system mandatory for all MT's involving excitation of level continuum, i.e.
- energies in MF = 3
- angular distributions of reactions exciting the level continuum in MF = 4
- energy distributions in MF = 5, 6

3.3.2. Center-of-mass system (LCT = 2)

Data for particle transition to discrete levels have to be transformed mandatory to the c-m-system, i.e.
- angular distributions for elastic and inelastic scattering (MT = 2, 51 to 90) in MF = 4
- angular distributions for neutron-induced charged particle emission (MT = 700 to 717, 720 to 737, 740 to 757, 760 to 777, and 780 to 797) in MF = 4

4. Interpolation of data Y(X)

4.1. Interpolation laws

According to main functional dependences of Y(X) five interpolation laws defined by a number INT can be used

$$\text{INT} = \begin{cases} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{cases} \quad \text{for} \quad \begin{cases} Y = \text{constant} \\ Y \sim X \\ Y \sim \ln X \\ \ln Y \sim X \\ \ln Y \sim \ln X \end{cases}$$

4.2. Recommended choice of INT

MF = 3

- for threshold reactions: INT = 2 or 3
- for (n,γ) reaction (MT = 102): INT = 5
- for (n,n) reaction (MT = 2): INT = 1

MF = 4

for elastic scattering angular distribution in f_1-representation: INT = 2

- for angular distributions in μ-representation for
  $p(\mu,E)$ vs. μ: INT = 4
  $p(\mu,E)$ vs. E : INT = 2

MF = 5

- for $p(E \rightarrow E')$ vs. E: INT = 2 or 3
- for $p(E \rightarrow E')$ vs. E': INT = 2

MF = 6

Analogous to the choice in MF = 4 and 5.

Attention:

Generally, problems arise in using INT = 4, and 5 if zero valued cross sections are involved (see 3.2.).

5. Normalization procedures

By using differential cross sections normalized to the integral one the data massive can easily be corrected for changes in either integral values or angular and energy distributions.

5.1. Normalized angular distributions (MF = 4)

f_l-representation (LTT = 1)

$$\frac{d\sigma(\mu,E)}{d\Omega} = \frac{\sigma(E)}{2\pi} \sum_{l=0}^{NL} \frac{2l+1}{2} f_l(E) P_l(\mu)$$

$$f_0 = 1.0$$

μ-representation (LTT = 2)

$$\frac{d\sigma(\mu,E)}{d\Omega} = \frac{\sigma(E)}{2\pi} p(\mu,E)$$

$$\int_{-1}^{1} p(\mu,E)\, d\mu = 1 \qquad \text{within 0.1 \%}$$

5.2. Normalized energy distributions (MF = 5)

$$\frac{d\sigma(E\rightarrow E')}{dE'} = m\sigma(E)\, p(E\rightarrow E')$$

$$\int_{0}^{E'_{max}} p(E\rightarrow E')\, dE' = 1 \qquad \text{within 0.1 \%}$$

(m = multiplicity)

The distribution p(E→E') can be choosen as a functional (analytic) or a tabulated dependence.

Analytical representation (spectral laws LF)

LF = { 5 general evaporation; 7 Maxwellian spectrum; 9 evaporation spectrum; 11 Watt spectrum

Tabular representation (LF = 1)

Only if data cannot be represented by LF = 7 or 9.

Attention:

Choose the simplest law that will accuratly represent the data.

5.3. Normalized double differential cross sections (MF = 6)

$$\frac{d^2\sigma(E\to E',\mu)}{d\Omega\, dE'} = \frac{\sigma(E)}{2\pi} \sum_{l=0}^{NL} \frac{2l+1}{2} f_l(E\to E') P_l(\mu)$$

$$\int_0^{E'_{max}} f_0(E\to E')\, dE' = 1$$

Final remarks

If the formatting of any data massive is planned a three-step-cycle can be recommended:

(i) preparation of data in a computer-readable format;
(ii) processing the data according formatting rules (normalization, determination of parameters for special representations, sum up partial cross sections);
(iii) check the data by codes CHECKR and FIZCON in parallel /3,4,5,6/.

This sequence should be repeated for all MT's to be prepared for a MAT number.

References

/1/ R. Kinsey ed., ENDF 102, 1979
/2/ M.A. Khalil, H.D. Lemmel, Summary documentation IAEA-NDS-10, Rev. 1, 1981
/3/ anon., BNL-MEMO, May 1980
/4/ O. Ozer, BNL-50300, ENDF 110
/5/ D.E. Cullen, IAEA-NDS-39, 1981
/6/ N. Day Day, IAEA-NDS-29, 1980