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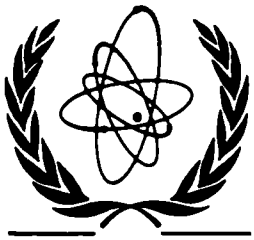

International Atomic Energy Agency

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

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

M.N. Nikolaev

(Extract translation from
Nuclear Constants No. 16,
INDC(CCP)-58/G)

October 1975

IAEA NUCLEAR DATA SECTION, KÄRNTNER RING 11, A-1010 VIENNA

Reproduced by the IAEA in Austria
October 1975
75-8364

INDC(CCP)-69/L

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M.N. Nikolaev

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

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

(a) General information

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

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

(b) Information about isotope

III. 1. Atomic weight of the n^{th} isotope (on ^{12}C scale)

2. Its fractional concentration

3. Number of cards with general information on the isotope; i.e. number of cards of types III-XV

4. $\pm a$ - radius of the neutron channel (Fermi); the minus sign denotes that the radius is dependent on energy or on ℓ and j; in this case, the value of the radius is given for E = 0, for the n^{th} value of ℓ and for the value of j corresponding to the given value of ℓ.

5. ± 1 - parity and spin of the target nucleus; for computers which do not distinguish between +0 and -0, the negative parity for l=0 is duplicated by punching the number sign.

6. Number of resonances given for a given isotope

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

XVI. 1. nu - number of the level system ($1 \leq nu \leq num$)

2. A - atomic number of the isotope

3. $\pm \ell_1$ - lowest orbital angular momentum of the neutrons which can form the state indicated. A minus sign is used if the state can also be formed by neutrons having a higher angular momentum. For computers which do not distinguish between +0 and -0, for $\ell_1 = 0$ the minus sign is duplicated by punching the number sign.

4. $\pm j$ - parity and spin of the compound nucleus. For computers which do not distinguish between +0 and -0, for j = 0 the minus sign is duplicated by punching the number sign.

5-6. Reserve.

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

XVII. 1. E_r - resonance energy

2. mu - number of the level system

3. Number of cards for a given resonance

4. $\Gamma_{rne}(|E_r|)$ - neutron width (eV) for $\ell = \ell_1(mu)$

5. $\Gamma_{r\gamma}$ - radiation width (eV)

6. Γ_{rf} - fission width (eV)

Cards of type XVIII (giving Γ_n for orbital momenta $\ell > |\ell_1(mu)|$ when $\ell_1(mu) < 0$) and type XIX (giving the widths of reactions other than scattering, capture and fission - if such reactions occur) agree in format with the corresponding cards described in Ref. [1] (cards XVII and XVIII).

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

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

(a) Law No. 10

$$Y(E, E_0) = \sum_{n=1}^{N} P_n \, \delta[E - \varepsilon(E_0, \theta, \vec{\alpha})], \qquad (1)$$

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

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

$$\varepsilon(E_o, \theta, Q, M_o, M, m_o, m, m_1) =$$

$$= E_o \frac{m_o}{m} \cdot \frac{m_1}{M} \left[1 - \alpha\left(1 - \frac{M^2}{(m_o M^2 + M_o m^2)\beta\mu} \cdot \frac{Q}{E_o}\right) - \frac{\mu_o}{\beta}\sqrt{1 + \frac{(m_o + M_o)^2}{(m M_o^2 + M m_o^2)} \cdot \frac{Q}{E_o}}\right];$$

$$\alpha = \frac{(2 m_o M_o + M_o^2)(m_o M^2 + M_o m^2) - (m M_o^2 + M m_o^2) M^2}{(m_o + M_o)^2 \cdot (m_o M^2 + M_o m^2)}; \qquad (2)$$

$$\beta = \frac{\alpha (m_o + M_o)^2}{2 M m_o^2}\sqrt{\frac{M^2 m_o + M_o m^2}{m M_o^2 + M m_o^2}}.$$

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

$$\mu_c = \frac{1}{2K^2}\left[y\mu_c^2 - \frac{2 m_o K}{m_o + M_o} \pm \mu_c\sqrt{\mu_c^2 y^2 + 1 - K^2 x - \frac{4 K y m_o}{m_o + M_o}}\right];$$

$$\mu_c = \cos\theta;$$

$$K = \frac{M}{m_o + M_o}\sqrt{\frac{m_o M_o^2 + M m_o^2}{M^2 m_o + M_o m^2}}\sqrt{1 + \frac{(m_o + M_o)^2 m_o}{m M_o^2 + M m_o^2}\frac{Q}{E_o}};$$

$$x = 1 - \alpha\left(1 - \frac{M^2}{(m_o M^2 + M_o m^2)\beta\mu} \cdot \frac{Q}{E_o}\right); \qquad (3)$$

$$y = \frac{\alpha}{\beta}\sqrt{1 + \frac{(m_o + M_o)^2}{(m M_o^2 + M m_o^2)} \cdot \frac{Q}{E_o}}.$$

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

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

IV. 1. FTN = 110

2. m

3-6. Reserve

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

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

$$Y(E_o,\theta,Q,E) = C(E_o,Q)\sqrt{E}\,[E_{max}(E_o,\theta,Q)-E]^{(3n-8)} ;$$

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

$$C(E_o,Q) = \frac{1}{2\pi\int_0^{\pi}\sin\theta\,d\theta\int_0^{E_{max}(E_o,\theta,Q)}\sqrt{E}\,[E(E_o,\theta,Q)-E)^{(3n-5)}\,dE} .$$

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

$$C(E_o) = \frac{2(M+1)^4}{E_o^2\pi^2[a^2(1-\mu_m)+\frac{8}{3}a(1-\mu_m^3)+\frac{8}{5}(1-\mu_m^5)]} ;$$

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

$$C(E_o) = \frac{2(M+1)^4}{E_o^2\pi^2[a^2+\frac{8}{3}a+\frac{8}{5}]} ;$$

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

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

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

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

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

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

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

IV. 1. FTN

2. Number of energies at which the linear combination coefficients are specified. The first energy must coincide with the lowest and the last with the highest energy in the range ΔE for which data are presented.

3. Number of cards with information for this FTN

4. Number of laws used

5. INT determining the law for energy interpolation of the linear combination coefficients (for probability conservation, it is recommended that INT = 111000000 be used in the interpolation process).

6. Reserve

V. 1. E_1

2. $a_1(E)$

3. $a_2(E)$ etc. until the probabilities of all the laws at the first energy have been given

Cards of type V are repeated for each energy.

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

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

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

3. NEW WAYS OF PRESENTING DATA ON ANGULAR DISTRIBUTIONS

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

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

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

When cross-sections are specified by means of resolved resonance parameters, there are greater possibilities of taking into account the contribution of unresolved levels. In the description of the format [1], this contribution was taken into account only as a non-resonance contribution, it being possible to specify the value of the contribution of unresolved levels with the help of mean resonance parameters (see Ref. [1], p. 31 - "Specifying non-resonance cross-sections by representing cross-section data with the help of resolved resonance parameters"; a card of type X is the heading card of the FTN with the help of which the non-resonance cross-section is specified). If this FTN = 411 or 412, one punches 0 in position 2 of this card (see Ref. [1], p. 34; card type 1) if the contribution of the unresolved levels can be taken into account as a non-resonance contribution or 1 if the resonance structure of the unresolved levels has to be taken into account.

To allow for the fact that some levels of one or another system of resonances are resolved and taken into account in the resolved resonance parameters, after a card of type XIV (see Ref. [1], p. 37) a card of type XIV-A with the following format must be introduced:

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

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

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

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

(a) In a complete data file, each cross-section must be specified within the entire range of energies covered by the file. This also applies to threshold reactions: below the threshold, the equality of the threshold to zero must be stated explicitly with the help of FTN = 101.

(b) In the zones for the different reaction cross-sections, the boundaries of energy regions which differ in their type of representation must correspond exactly to the boundaries of the corresponding regions in the zone for the total cross-section, except where the low-energy boundary of the region coincides with the reaction threshold.

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

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

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

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

- A point-by-point representation can only be general for specifying cross-sections of all types. The energies at which the values of the partial cross-sections are specified can be chosen only from the set of energy values at which the total cross-section is specified;
- The sub-group representation can only be general for reactions of all types (non-resonance cross-sections are specified by means of equal values of sub-group cross-sections).

(d) The laws of cross-section interpolation by energy can, generally speaking, be different for different cross-sections. It is recommended, however, that one use a linear-linear or a linear-logarithmic interpolation guaranteeing that the sum of the partial cross-sections will remain equal to the total cross-section.

(e) When one uses FTNs which enable one to describe the energy dependences of the cross-sections for all reactions in the zone for the total cross-section, an external temperature cycle is not permitted; the temperature dependence of the cross-sections must be specified as envisaged by the format of the corresponding FTN. When the energy dependence of cross-sections is specified by means of resonance parameters, the data are presented for only one temperature - 0°K.

An external temperature cycle is retained for specifying cross-sections in FTN = 111, 112, 121, 122.

There is no provision for specifying the temperature dependence of energy and angular distributions.

(f) Angular distributions cannot be specified by means of resonance parameters. Even if cross-sections are specified by means of resonance parameters which also define the angular distributions, the latter must nevertheless be specified in explicit form.

(g) There is no provision for taking into account the resonance structure of the parameters of energy distributions (temperature in laws Nos 9, 11 and 12; transition probabilities in law No. 8) by

means of a sub-group representation.

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

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

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

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

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

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

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

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

6. ERROR IN THE DESCRIPTION OF LAW No. 9

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

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

REFERENCES

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