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ATOMIC WEAPONS RESEARCH ESTABLISHMENT

AWRE REPORT No. O.- 70/63

The Aldermaston Nuclear Data Library
as at May 1963

K. Parker

AWRE,
Aldermaston, Berks.

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Summary

This report is a guide to the contents and conventions of the Aldermaston Nuclear Data Library which consists principally of cross-sections and related data for neutrons of energies up to 14 MeV. The Library stores conveniently vast amounts of data which can be used to prepare input data for neutronics computer codes.

Approved by

A. H. Armstrong, Senior Superintendent

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Table of Contents

1. The Aldermaston Nuclear Data Library and associated IBM 7030 Computer Programmes for the Preparation of Input Data for Neutronics Calculations

The present report is one of a series which together will give a comprehensive description of the methods adopted at AWRE Aldermaston to handle the vast quantities of data used in multigroup neutronics calculations on high speed digital computers.

In preparing input data for calculations three stages of work can be distinguished.

In the first stage the experimental and theoretical data on neutron cross-sections for a given element or isotope are surveyed and a set of best values tabulated. This type of work has been undertaken in several laboratories. AWRE work in this field is described in reports which appear from time to time. Currently detailed information is only available for Be [1] and C [2] but further reports are in preparation. A comprehensive summary of AWRE data in use at April 1960 is given in AWRE Report O-28/60* [3].

In the second stage the assembled best data on microscopic cross-sections are represented on punched cards or magnetic tape in a form suitable for further processing using a large computer. The present report describes in detail the organisation, the formats used and the present contents of the AWRE Nuclear Data Library and forms a guide to all who need to use this library for further work. The preparation of this library requires a number of IBM 7030 and IBM 1401 programmes. The main features of these programmes are outlined here. It is planned to describe the full details of these programmes in further reports - see sections 8-11 and related appendices.

In the third stage the stored data of stage two are converted into group cross-sections, mean free paths, collision probabilities and other

*Now out of print

quantities which are directly usable as input to neutronics programmes. This conversion is carried out using appropriate machine programmes. The main AWRE programmes of this type are GALAXY, which prepares group cross-sections for use in S_n and other multigroup methods of solving the transport equation or the diffusion equation, and the DICE Mark IV system which produces input data for Monte Carlo calculations*. GALAXY and the DICE Mark IV system will be described in two further reports of this series.

As far as data collection and processing is concerned the output from GALAXY and the DICE Mark IV systems represents the end-product. But for completeness we may note that these processed data are used in a number of versatile AWRE neutronics programmes including STRAINT, an IBM 7030 S_n code [4] and MAGGIE, a Monte Carlo code which computes multiple scatter corrections to experimental data on elastic and inelastic neutron scattering [5]. The general problem of carrying out Monte Carlo calculations on a large computer is considered in reference [6].

The reader should be warned that the nuclear data system described in the present report and other reports of the series replaces the 1957 AWRE system which is described in references [7] [8] and [9]. Much of the actual data remains the same pending revision but the card formats and processing programmes are different. The 1957 system was designed for IBM 704/709/7090 machines.

The present nuclear data system has been developed from the 1957 AWRE system in close collaboration with workers at AEE, Winfrith and has been designed for use with IBM 7030 and 7090 machines. The Winfrith Nuclear Data Library and the associated 7090 machine programmes are described in a series of AEE reports including "The Winfrith Nuclear Data Library" by M. F. James [10] which parallels the present report. Other Winfrith reports will provide

*DICE Mark IV is the whole complex that enables a neutron's fate at a collision, its subsequent mean free path and the position of its next collision to be determined. MOULD, the initial part of DICE, converts the nuclear data into a form suitable for use in the later stages of DICE.

descriptions of the 7090 version of GALAXY and of 7090 (and in some cases 7030) versions of library preparation programmes (see above).

In order to provide complete descriptions for the 7030 and 7090 versions of this nuclear data system a certain amount of duplication is deliberately planned between the AWRE series of reports which generally describe the 7030 version and the AEE series of reports which generally describe the 7090 version. Descriptions of data compilations such as references [1], [2] and [11] are issued by the originating laboratory.

A nuclear data system such as that described in this series of reports does not remain static. At the very least new data are constantly being added and old data revised. New types of data may be included. The reader should therefore bear in mind that at a given time the available reports on the system may not be completely up-to-date and that revision of reports may be necessary from time to time. The present report describes card and tape formats which are designed for future needs such as the accommodation of photon cross-section data in addition to neutron cross-section data.

A similar general introduction will be included in all reports of this series.

2. Data Considered

2.1 General

The ultimate aim is to include in the library information on neutron interaction, photon production and photon interaction cross-sections. Information will then be available to enable a very wide range of neutron and photon transport problems to be solved on high speed computers.

For neutron cross-sections the energy range covered extends from 0.001 eV or less up to 15 MeV although for certain nuclides a smaller range is covered and in some cases the cross-sections are tabulated below 0.001 eV.

For photon cross-sections the range covered is likely to be 0.01 - 20 MeV as was the case with the old (1957) AWRE system [12].

2.2 Classification of Data

Classification of data is by substance (nuclide, natural element, molecule, mixture etc) on the one hand and by reaction on the other.

All reactions occurring for a particular substance are classified by a five digit "reaction type number" (R.T.N.) which is subdivided into a two digit general classification number (G.C.N.) followed by a three digit particular classification number (P.C.N.).

General Classification Numbers (G.C.N.)

These are as follows:

0	Heading information	(plain)
1	Neutron cross-section	(blue)
2	Neutron angular distribution	(mauve)*
3	Neutron energy distribution	(green)
4	Miscellaneous quantities for neutrons ($\bar{\nu}$, η etc)	(yellow)
5	Resolved resonance data for neutrons	(rose)*
6	Statistical data for unresolved neutron resonances	(brown)
7	Thermal neutron scattering law data	(grey)
8	Photon cross-section	(plain)
9	Photon angular distribution	(brown)
10	Photon secondary energy	(green)
11	Photon production angular distribution	(yellow)
12	Photon production secondary energy	(mauve)
13	Photon production multiplicity	(grey)

11, 12 and 13 cover photon production data on processes initiated by neutrons.

Colours in brackets are the colours of the Nuclear Data File Cards used to store the appropriate type of data - see sections 6, 7 and 8.

Further general classification numbers can be allocated if required.

* Mauve = IBM "rose stripe". Rose = IBM "red stripe".

Particular Classification Numbers (P.C.N.)

These are as follows:

1 Total

2 Elastic

3 Non-elastic (= Total - Elastic)

4 Total (n,n') = total inelastic scattering summed over all final states

5 (n,n') to 1st excited state

6 (n,n') to 2nd excited state

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

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

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

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

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

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

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

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

15 (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.

16 (n,2n) or (γ,2γ) - pair production

17 (n,3n)

18 Fission = (n,f) + (n,n'f) + (n,2nf) + -------

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

20 (n,n'f)

21 (n,2nf)

22 (n,n')α

23 (n,n')3α

24 (n,2n)α

25 (n,3n)α

26 (n,2n) isomeric state

27-100 To be allocated

101 Parasitic absorption (or disappearance) - no secondary neutrons produced

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 To be allocated

151-200 Used to classify resolved and statistical resonance information. The detailed meaning of the numbers (which differs in the resolved resonance, G.C.N. = 5, and statistical resonance, G.C.N. = 6, cases) is given in sections 7.5 and 7.6.

201 Total transport cross-section with direct averaging and use of the diagonal transport approximation. $\sigma_{tr} = \sigma_T - \bar{\mu}\,\sigma_n$, where $\bar{\mu}$ is the average laboratory angle cosine in elastic scattering and anisotropy of non-elastic processes is ignored. 201 represents a derived quantity - see reference [8], p24.

202 $\bar{\nu}\sigma_f$ - the product of the fission cross-section and the average number of neutrons per fission.

203 $\eta\sigma_\chi$ - the product of the non-elastic cross-section and the average number of neutrons per non-elastic event. (also known as σ_M)

204 $\sigma_T - \sigma_f$, the cross-section for all processes in which fission does not occur.

205 Total transport cross-section derived from constituent cross-sections using reciprocal averaging, the microscopic total transport cross-section being defined as in the case of P.C.N. 201.

206 The total cross-section in relation to total transfer matrices (summed over all reactions yielding secondaries).

207 The total (n,n') cross-section in relation to total (n,n') transfer matrices (summed over (n,n') reactions 5-15).

208 The removal cross-section in relation to a particular energy group. This gives the cross-section for removing neutrons from the group either by parasitic absorption (disappearance) or by scattering to another energy group.

209-300 To be allocated.

301-450 Energy release rate parameter ($\overline{\sigma E}$) for total and partial cross-sections The cross-section concerned is identified by subtracting 300 from this P.C.N. Thus 301 denotes the total energy release rate parameter whilst 302 denotes that from the elastic scatter (302 = 300 + 2).

451-999 To be allocated.

The following conventions may be noted.

(a) 1-100 denote reactions in which secondaries of the same type as the incident particle appear.

(b) 101-150 denote reactions in which no secondaries of the same type as the incident particle appear.

(c) 151-200 are used to classify resolved and statistical resonance information.

(d) 201-450 denote quantities which are not normally given in the library but which are calculated by user programmes such as GALAXY. These quantities will be discussed in more detail in other reports of the series but we note that the energy release rate parameter is discussed on p30 of reference[8] whilst PCN 204 is used to label the non-fission transfer matrix which occurs when the neutron transport equation is solved by the S_n method using a fission source technique. Similarly PCN 206 labels the total transfer matrix and PCN 207 labels the total (n,n') transfer matrix.

(e) The specification of the reactions is such that the P.C.N. enables the final product nuclei to be uniquely determined. Thus with C^{12} the reaction $C^{12}(n,n')3\alpha$ has PCN 23 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 = 16 implies that U^{237} + 2n are the final products. This enables nuclide counts to be made when transmutations are taking place. The notation and nomenclature largely follows that devised by Goldstein and adapted for use by EANDC and the AEC Nuclear Cross Section Advisory Group [31].

It will be seen that ample P.C.N's remain for allocation should the Nuclear Data Library need extending.

Examples of Reaction Type Number Allocation

Total cross-section for neutrons	=	1001
Elastic cross-section for neutrons	=	1002
Angular distribution of fission neutrons	=	2018
Secondary energy of (n,2n) reaction neutrons	=	3016
Mean number of neutrons per fission, $\bar{\nu}$	=	4018
Ratio of capture to fission cross-section, α	=	4102
(γ,2γ) cross-section	=	6016
Energy spectrum of photons produced in (n,n') continuum reaction	=	12015
Thermal scattering law data	=	7002

Nuclide Identification Number (~~N.I.N.~~ DFN)

Different sets of data within the library - either different sets of data for the same substance or sets of data for different substances - are identified by the "nuclide identification number", a somewhat misleading name as data for a nuclide, for a natural element, for a chemical compound or for a mixture can all be included and the "number" consists of three Hollerith characters.

It is possible that there may be more than one representation of the same data for the same nuclide, for example, they may be given by (a) a mixture of cross-sections and resonance parameters or (b) in cross-section form alone using cross-sections generated from resonance parameters in representation (a) for some temperature(s). In this case the different sets of data are given different nuclide identification numbers. If data

are available in the same form for a given nuclide at different temperatures then the same nuclide identification number is used for each temperature.

The way in which reaction type numbers are constructed means that it is possible, for natural carbon say, for a nuclide identification number to cover a data set containing neutron interaction, photon production and photon interaction data for the same substance. In practice the energy ranges for these three different types of data are given may be different and three different N.I.N's may be used, thus providing a double differentiation (by N.I.N. and R.T.N.) between the three types of data.

Alphanumeric Nuclide Identification Numbers

Although alphanumeric N.I.N's are allowed in theory they are difficult to handle in practice. However the label field of the punched cards used to store the data is limited to three symbols* and here use of alphabetic symbols is essential if N.I.N's above 999 are to be allowed. This restriction does not apply to the data field where larger numerical N.I.N's may be stored. In order to extend the range beyond 999 in the label field the following convention is followed:-

Label Field	Data Field
001 - 999	001 - 999
J00 - J99	1000 - 1099
K00 - K99	1100 - 1199
L00 - L99	1200 - 1299
M00 - M99	1300 - 1399
N00 - N99	1400 - 1499
P00 - P99	1500 - 1599
⋮	⋮
Z00 - Z99	2500 - 2599

* This restriction does not apply to data derived by various processing programmes (see below).

The letter O is omitted to avoid confusion. Further extensions can obviously be made if necessary.

Nuclide Identification Numbers for Mixtures

It is desirable to distinguish data for mixtures, molecules etc which form part of the basic data library and processed data which are derived by using the various processing programmes (GALAXY etc) and then mixing. Mixtures produced by the processing programmes should be given N.I.N's starting at 10001 (arrangements must be made for the processing programme to insert the correct N.I.N. when mixing is done). When the processed data is derived from a single entry in the nuclear data file (e.g. water cross-sections at less than 10 eV) then the N.I.N. will be the same as in the basic library (< 10000).

2.3 Contents of the Library at 1st May 1963

At 1st May 1963 the contents of the Aldermaston Nuclear Data Library can be divided into two sections.

The first section having nuclide identification numbers in the range 101 - 200 consists of data compiled at Aldermaston between 1956 and 1963. Most of this data formed part of the old (1957) system and has been entered into the present library using an IBM 7090 card conversion programme. The contents of this first section are given in Table 1. N.I.N. = 101 - 190 cover neutron interaction cross-sections. N.I.N. = 191 - 200 cover photon interaction cross-sections.

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Table 1 Aldermaston Nuclear Data Library - Data compiled at Aldermaston

N.I.N.	Element Isotope etc	Basic Data Mark Number	CANDY Group Constant Mark Number	Date of compilation, reference, energy range covered and comments	
101	U^{235}	1/U235	6	Spring 1959 [3]	0.025eV-14MeV
102	U^{238}	1/U238	6	Spring 1959 [3]	0.025eV-14MeV
103	Pu^{239}	1/Pu239	8	Spring 1959 [3]	0.025eV-14MeV
104	Pu^{240}	1/Pu240	7	Spring 1959 [3]	0.025eV-14MeV
105	Allocated		6	November 1957	0.025eV-14MeV
106	Fission Product	1/F.P.	6	June 1959	0.025eV-15MeV
107	H	1/H	6	November 1957 [3]	0.025eV-14MeV
108	D	1/D	6	November 1957 [3]	0.025eV-14MeV
109	T(1)	1/T(1)	6	November 1957 [3]	0.025eV-14MeV
110	He^{3}	1/He3	6	November 1957 [3]	0.025eV-14MeV
111	He^{4}	1/He4	6	November 1957 [3]	0.025eV-14MeV
112	Allocated		6	Spring 1959	0.025eV-14MeV
113	Allocated		7	Spring 1959	0.025eV-14MeV
114	Be^{9}	2/Be9	9	October 1959 [1]	0.025eV-15MeV
115	Natural B	1/B	7	April 1957 [3]	0.025eV-14MeV
116	B^{10}	1/B10	6	April 1957 [3]	0.025eV-14MeV
117	Natural C	2/C	7	June 1960 [2]	0.025eV-15MeV
118	Natural N	1/N	6	April 1957 [3]	0.025eV-14MeV
119	Natural O	1/O	6	December 1956 [3]	0.025eV-14MeV
120	Al^{27}	1/Al	6	June 1957 [3]	0.025eV-14MeV
121	Natural Si	1/Si	6	October 1958 [3]	0.025eV-14MeV
122	U^{233}	1/U233	6	Spring 1959 [3]	0.025eV-14MeV
123	U^{234}	1/U234	6	Spring 1959	1keV-14MeV
124	U^{236}	1/U236	6	Spring 1959	1keV-14MeV
125	Allocated		6	Spring 1959	1keV-14MeV
126	Allocated		6	Spring 1959	1keV-14MeV
127	Allocated		6	Spring 1959	1keV-14MeV
128	Pu^{238}	1/Pu238	6	Autumn 1962 Fission cross-section only	0.025eV-14MeV
129	Pu^{241}	1/Pu241	6	Spring 1959 [3]	0.025eV-14MeV
130	Np^{237}	1/Np237	6	1959 Fission cross-section only	100keV-14MeV

Table 1 (continued)

N.I.N.	Element Isotope etc	Basic Data Mark Number	CANDY Group Constant Mark Number	Date of compilation, reference, energy range covered and comments	
131	Th^{232}	1/Th232	6	Spring 1959 [3]	0.025eV-14MeV
132	Natural Cr	1/Cr	6	October 1958 [3]	0.025eV-14MeV
133	Natural Fe	1/Fe	6	February 1959 [3]	0.025eV-15MeV
134	Natural Ni	1/Ni	6	October 1958 [3]	0.025eV-14MeV
135	Natural Pb	1/Pb	6	August 1959 [3]	0.025eV-15MeV
136	Natural Cd	1/Cd	6	November 1958 [3]	0.025eV-14MeV
137	Au^{197}	1/Au197	6	December 1961 (n,γ), $(n,2n)$ Au^{196} and $(n,2n)$ Au^{196m} cross-sections only	1keV-15MeV
138	Natural Ca	1/Ca	6	October 1958 [3]	0.025eV-14MeV
139	Na^{23}	1/Na	6	October 1958 [3]	0.025eV-14MeV
140	F^{19}	1/F	6	November 1957 [3]	0.025eV-14MeV
141	Natural Cl	1/Cl	6	February 1959 [3]	0.025eV-15MeV
142	Allocated		6	1959	0.025eV-15MeV
143	Allocated		6	1959	0.025eV-15MeV
144	Allocated		6	1959	0.025eV-15MeV
145	Allocated		6	1959	0.025eV-15MeV
146	Allocated		6	1959	0.025eV-15MeV
147	Allocated		6	1959	0.025eV-15MeV
148	Allocated		6	1959	0.025eV-15MeV
149	Allocated		6	1959	0.025eV-15MeV
150	Allocated		6	January 1962	0.025eV-15MeV
151	Absorbium	1/ABS	6	1961 Approximates total absorption	0.025eV-15MeV
152	T(2)	1/T(2)	6	November 1957 [3]	0.025eV-14MeV
153	U^{235}	2/U235	1	Winter 1960-61	0.025eV-14MeV
154	U^{238}	2/U238	1	Winter 1960-61	0.025eV-14MeV
155	U^{235}	3/U235	7	December 1961	0.025eV-15MeV
156	U^{238}	3/U238	7	December 1961	0.025eV-15MeV
157	Allocated		7	March 1962	1keV-14MeV
158	Allocated		7	March 1962	1keV-14MeV
159	H_2O		6	1957 No basic data. Group cross-sections only	

Table 1 (continued)

N.I.N.	Element Isotope etc	Basic Data Mark Number	CANDY Group Constant Mark Number	Date of compilation, reference, energy range covered and comments
160	D_2O		6	1957 No basic data. Group cross-sections only
161	Allocated		-	1957 No basic data. Group cross-sections only
162	Allocated		-	1957 No basic data. Group cross-sections only
163	U^{235}	3A/U235	7	June 1962 0.025eV-15MeV) Adjusted
164	U^{238}	3A/U238	7	June 1962 0.025eV-15MeV) sets from
165	U^{238}	3B/U238	7	June 1962 0.025eV-15MeV) 3/U235 and
166	U^{238}	3C/U238	7	June 1962 0.025eV-15MeV) 3/U238
167	Allocated		-	August 1962 1keV-15MeV
168	Allocated		7	April 1962 0.025eV-14MeV
169	Allocated		8	April 1962 0.025eV-14MeV
170	Allocated		-	August 1962 1keV-15MeV
171	Allocated		-	August 1962 1keV-15MeV
172	Thin Air	1/Thin Air	-	September 1962 0.025eV-15MeV Approximates a vacuum
173	U^{236}	2/U236	-	August 1962 1keV-15MeV
174	U^{234}	2/U234	-	August 1962 1keV-15MeV
175	Allocated		-	May 1963 0.001eV-15MeV
176	Allocated		-	May 1963 0.001eV-15MeV
177	Allocated		-	No data. Used only to identify reaction product
178	Pu^{242}		-	No data. Used only to identify reaction product
179	Zr	1/Zr		May 1963* 0.025eV-15MeV
180				
181				
182				
183				
184				
185				
186				
187				

*Data supplied by P. J. Hemmings of the Authority Health and Safety Branch, Risley.

Table 1 (continued)

N.I.N.	Element Isotope etc	Basic Data Mark Number	CANDY Group Constant Mark Number	Date of compilation, reference, energy range covered and comments
188				
189				
190				
191	H	1/H G	1	April 1961 [12] Photon cross-sections 0.01-20MeV
192	Be	1/Be G	1	April 1961 [12] Photon cross-sections 0.01-20MeV
193	C	1/C G	1	April 1961 [12] Photon cross-sections 0.01-20MeV
194	N	1/N G	1	April 1961 [12] Photon cross-sections 0.01-20MeV
195	O	1/O G	1	April 1961 [12] Photon cross-sections 0.01-20MeV
196	Al	1/Al G	1	April 1961 [12] Photon cross-sections 0.01-20MeV
197	Fe	1/Fe G	1	April 1961 [12] Photon cross-sections 0.01-20MeV
198	Pb	1/Pb G	1	April 1961 [12] Photon cross-sections 0.01-20MeV
199	U	1/U G	1	April 1961 [12] Photon cross-sections 0.01-20MeV
200	Pu	1/Pu G	1	April 1961 [12] Photon cross-sections 0.01-20MeV

Notes on Table 1

(a) The basic data mark number is used for administrative purposes only. It does not appear on the cards.

(b) The CANDY group constant mark number appears on cards, tapes and prints containing group cross-sections calculated using CANDY [8]. It is only applicable to data which was available in the old (1957) system [7].

(c) The date of compilation generally means the date of the latest reference referred to in the compilation.

(d) Absorbium has an atomic weight of 8.0, a total cross-section of 1000 barns, an (n,γ) cross-section of 1000 barns and an elastic cross-section of 0.001 barns.

(e) Thin air has an atomic weight of 10,000, a total cross-section of 10^{-10} barns. The total cross-section is derived entirely from elastic scattering for which the angular distribution is strongly biased towards zero scattering angle. In the unlikely event of a collision, incident energy and direction will be virtually unaltered. This "nuclide" is introduced for convenience in certain Monte Carlo calculations.

(f) Whilst N.I.N's 191-200 have been allocated for photon interaction data the relevant information is not yet included in the library. It is however available in the old (1957) system [12].

The second section of the Aldermaston Nuclear Data Library having nuclide identification numbers in the range 1-100 consists of data prepared by workers at AEE Winfrith. In most cases the data has been derived from data given in Table 1 by modifying and extending the data below an energy generally of 1eV but sometimes greater and sometimes less. This modification has been made using a "splicing" programme specially designed for this purpose. In a few cases the data sets do not make use of any data compiled at Aldermaston and where this is the case the fact is noted in Table 2 which gives the contents of this second section.

Table 2. Aldermaston Nuclear Data Library - Data Partly or Wholly Compiled at Other Laboratories

N.I.N.	Element Isotope, etc.	Basic Data Mark Number	Date of compilation, reference, energy covered and comments
1			Not allocated
2	U^{235}	4/U235	Spring 1963 0.005eV-15MeV. As NIN 101 above 6eV
3	Pu^{239}	2/Pu239	Spring 1963 0.002eV-14MeV. As NIN 103 above 6eV
4	Xe^{135}	1/Xe135	Spring 1962 [11] 0.01eV-1keV. Data compiled at AEE Winfrith. Temperature = 293°K
5	U^{238}	4/U238	Spring 1963 0.001eV-15MeV. As NIN 102 above 1.75keV
6	Natural C	3/C	Spring 1963 0.0001eV-15MeV. As NIN 117 above 1keV
7	BeO	1/BeO	Spring 1963 0.001eV-1keV
8	Be^{9}	3/Be9	Spring 1963 0.001eV-15MeV. As NIN 114 above 10keV
9	U^{233}	2/U233	Data not yet available
10	H	2/H	Spring 1963 0.0033eV-14MeV. As NIN 107 above 0.15eV
11	D	2/D	Spring 1963 0.001eV-14MeV. As NIN 108 above 1keV
12	Na^{23}	2/Na	Spring 1963 0.01eV-14MeV. Based on data of Schmidt [13]. Reported in [32]
13	B^{10}	2/B10	Spring 1963 0.001eV-14MeV. As NIN 116 above 1eV
14	Natural N	2/N	Spring 1963 0.0001eV-14MeV. As NIN 118 above 1eV
15	Natural B	2/B	Spring 1963 0.001eV-14MeV. As NIN 115 above 1eV
16	Al^{27}	2/Al	Spring 1963 0.0006eV-14MeV. As NIN 120 above 1eV
17	Natural Cr	2/Cr	Spring 1963 0.0001eV-14MeV. As NIN 132 above 0.05eV
18	Natural Fe	2/Fe	Spring 1963 0.001eV-15MeV. As NIN 133 above 0.03eV
19	Natural Ni	2/Ni	Spring 1963 0.0001eV-14MeV. As NIN 134 above 1eV
20	Natural O	2/O	Spring 1963 0.0001eV-14MeV. As NIN 119 above 1eV. (n,γ) cross-section added below 1eV

Table 2 (continued)

N.I.N.	Element Isotope, etc	Basic Data Mark Number	Date of compilation, reference, energy range covered and comments
21	Au^{197}	2/Au197	Data not yet available
22	Th^{232}	2/Th232	Spring 1963 0.0001eV-14MeV. As NIN 131 above 1eV
23	F^{19}	2/F	Spring 1963 0.0001eV-14MeV. As NIN 140 above 1eV
24	Cd	2/Cd	Spring 1963 0.0001eV-14MeV. As NIN 136 above 1eV
25	Si	2/Si	Spring 1963 0.0001eV-14MeV. As NIN 121 above 0.1eV
26	Pb	2/Pb	Spring 1963 0.0001eV-15MeV. As NIN 135 above 0.1eV
27	H_2O	2/H2O	Spring 1963 0.0006eV-0.5eV
28	D_2O	2/D2O	Spring 1963 0.0005eV-9.0eV
29	Pu^{240}	2/Pu240	Spring 1963 0.001eV-14MeV. As NIN 104 above 1.5keV
30	Pu^{241}	2/Pu241	Data not yet available
31	He^{4}	2/He4	Spring 1963 0.001eV-14MeV. As NIN 111 above 0.025eV
32	He^{3}	2/He3	Spring 1963 0.001eV-14MeV. As NIN 110 above 1keV
33	Cl	2/Cl	Data not yet available
34	Ca	2/Ca	Data not yet available

3. Handling of Neutron Interaction Data

3.1 Cross-sections

Energies and corresponding cross-sections are given in pairs in order of ascending energy. All cross-sections are in barns and energies in MeV. The points are the end points of linear segments of the cross-section graph plotted on a log-log scale (as in BNL 325 [14]). Sufficient points are chosen so that the error on linear interpolation is acceptably small and thus the cross-section can be determined quite accurately at all energies.

The energy region covered for the nuclide may be divided into a number of ranges and a cross-section may only be specified within certain ranges for several reasons including the following:

(a) the cross-section is zero or negligible in certain ranges

(b) the cross-section should be generated directly from resonance parameters in certain ranges.

(c) convenience, as when the energy range covered for a particular nuclide is extended.

There is no restriction on the range of energy considered. The energies at which the cross-section is specified may be as small or as large as one pleases.

For any range in which a cross-section is given the cross-section must be specified and non-zero at the end points of the range. A zero cross-section is not allowed at any point. These two restrictions arise because interpolation is on a log-log scale basis. Where two ranges touch the boundary point must be repeated with the same value of the cross-section.

For a given nuclide the total and all partial cross-sections must be specified at the same points in order to facilitate checking. The ranges do not necessarily coincide (e.g. the total cross-section and a cross-section with a threshold may have different numbers of ranges).

If temperature dependence is important the temperature to which the cross-section is appropriate must be specified.

3.2 Angular Distributions of Secondary Neutrons

Angular distributions of secondary neutrons may be specified either range-wise or point-wise as far as variation with incident neutron energy is concerned.

In the range-wise representation the energy region for which the appropriate cross-section is specified is divided into a number of ranges in each of which a particular normalised probability distribution for scattering as a function of $\cos\theta$ is assumed to hold for each secondary neutron. θ is the scattering angle and may be specified in either centre of mass or laboratory

systems. For each distribution the lower and upper energy limits (in MeV) of the range are given together with pairs of (cos θ, probability) values determined from a linear-linear plot of the probability curve. Sufficient points are chosen so that the error on linear interpolation is acceptably small.

Since the true angular distribution is approximated by linear segments the resulting representation, in general, will be un-normalised. Renormalisation will be necessary within user programmes if the assumption of unit normalisation is made within such programmes. The pairs are specified in order of increasing cosθ i.e. starting with cosθ = i.e. starting with cosθ = -1 and ending with cosθ = +1.

In the point-wise representation normalised probability distributions are specified for each neutron at a number of energies chosen so that linear interpolation in energy and cosθ give an acceptable representation of the probability for any given energy and scattering angle. Each specified distribution is constructed in the same way as for the range-wise representation.

In all cases the total energy range covered by the angular distribution must coincide with that covered by the corresponding cross-section. If, say, an elastic cross-section is specified in the energy range 0.001eV - 14 MeV, then with point-wise representation the first angular distribution must be for energy 0.001 eV and the last for 14 MeV; for 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.

For a given energy range or a given energy point linear combinations of up to six normalised probability distributions are allowed.

For a given reaction for a given nuclide a mixed representation is not allowed. Such a mixed representation can always be forced into point-wise representation by specifying the angular distribution for each range twice (at each end of the range).

The choice between centre of mass and laboratory scattering angles depends on the particular reaction. Generally elastic scattering and inelastic scattering to specified levels in which a fairly simple correlation between initial and final energy exists require the centre of mass angle to be used whilst for other non-elastic processes the laboratory angle is more convenient.

When energy loss is calculated from a dynamical formula it is necessary to specify the atomic weight of the nuclide considered.

The special case of thermal scattering is considered under a separate heading.

3.3 Energy Distributions of Secondary Neutrons

When there is a known correlation between incident and secondary energies and scattering angle the secondary energy will be calculated, by processing programmes. No secondary energy distributions should be specified in such cases.

In other cases secondary energy laws are specified and correlation between scattering angle and secondary energy is generally ignored.

Seven secondary energy laws have been specified to date, namely:-

1. Neutrons emitted with a known discrete energy.
2. Neutrons emitted with an energy k $(E_o - E_B)$, where k is a constant (the reduction factor), E_o is the initial energy and E_d is a discrete energy. This covers the case of exciting a single level in an (n,n') reaction (approximately).

3. Continuous (normalised) spectra independent of initial energy, e.g. fission spectrum (to a good approximation).

4,5,6 Neutrons with secondary energy, E, represented by the normalised probability function

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

where f is some function and E_o is the initial energy. q can take the values 0, $\frac{1}{2}$ and 1 to give laws 4, 5 and 6 respectively. An "evaporation" spectrum falls in class 5.

7. This law gives a more refined representation of the fission spectrum, allowing variation with incident energy and with fissioning nuclide. It is given by the normalised probability function

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

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

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

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

where a,b,c are constants

ν 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 (all energies in MeV)

σ_{nf}, $\sigma_{nn'f}$ and σ_{n2nf} are the cross sections for the (n,f) (n,n'f) and (n,2nf) reactions

It will be seen that law 7 is specified by four parameters a,b,c and E_f (the remaining quantities being available from the nuclear data file).

The continuous functions of laws 3,4,5,6 are specified by pairs of (argument, probability) values such that linear interpolation on a linear-linear scale between specified points gives acceptable accuracy. It should be noted that, although these functions are normalised (to a certain degree of accuracy) within the range of arguments considered, certain arguments may be inaccessible on energy conservation grounds. (e.g. the emergent energy of a secondary neutron may be greater than the incident energy in an (n,n') reaction). Renormalization, either on physical or mathematical grounds, is generally necessary in user programmes.

The energy region for which the appropriate cross section is specified is divided into a number of ranges in each of which the secondary energies (in MeV) are determined by linear combinations of these laws. Different linear combinations of laws are allowed for different neutrons in the case of (n,2n) and (n,3n) reactions.

The special case of thermal scattering is considered under a separate heading.

3.4 Miscellaneous Quantities - $\bar{\nu}$, η, etc.

These include

n, the number of secondaries per collision (elastic and non-elastic)

$$n = (\sigma_n + \sigma_{n'} + 2\sigma_{2n} + 3\sigma_{3n} + \bar{\nu}\,\sigma_f + - - - -)/\sigma_T$$

η, the number of secondaries per non-elastic event

$$\eta = (\sigma_{n'} + 2\sigma_{2n} + 3\sigma_{3n} + \bar{\nu}\,\sigma_f + - - - -)/\sigma_X$$

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

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

The first three of these quantities are computed from the appropriate formula and are specified only at points (a common mesh) at which the cross-sections etc. appearing in the formula are specified and the law for interpolation between energy points is not a simple one.

$\bar{\nu}$ is represented in exactly the same way as cross-sections, the specified points being end points of linear segments of a log-log plot of $\bar{\nu}$ versus energy.

The energy points at which $\bar{\nu}$ is specified are not necessarily the same as those at which the cross-sections are specified but the lowest and highest energy points at which the fission cross-section is specified must be included in the representation of $\bar{\nu}$. This means that when $\bar{\nu}\ \sigma_f$ is formed interpolation in $\bar{\nu}$ will generally be necessary.

It may be useful to specify further miscellaneous quantities at a later date.

It should be noted that, whilst $\bar{\nu}$ is given in the library for all fissile nuclides, specification of n, η and α is optional.

3.5 Resolved Resonance Data

In energy regions where resonances are well resolved the cross sections can be generated by means of various formulae which are approximate and are derived from the R-matrix theory of nuclear reactions (Lane and Thomas - reference [15] - herein referred to as LT). Since it is possible to make many different approximations the format for this part of the library is arranged so as to facilitate easy addition of new formulae (this may well be necessary when subject is investigated further).

Six approximations are considered here.

(a) Breit-Wigner formula for a single isolated level involving $\ell = 0$ neutrons.

N.B. Not used in library.
A resonance parameter library is envisaged (N.E.)
NPL may also be ...

(b) Breit-Wigner formula for $\ell = 0$ neutrons and many levels when elastic scattering and radiative capture are the only important processes.

(c) The Reich-Moore formula - a multilevel formula with few fission channels for $\ell = 0$ neutrons.

(d) The Vogt formula - a few level formula for $\ell = 0$ neutrons

(e) The multilevel formula for neutrons of all ℓ in the case when only elastic scattering need be considered.

(f) Breit-Wigner formula for a single isolated level involving neutrons of any ℓ.

It turns out to be possible to use exactly the same card format for cases (a) and (b).

(a) Breit-Wigner Formula for a Single Isolated Level for $\ell = 0$ Neutrons

This is a rather hypothetical case as one assumes that there is a large energy range in which the cross-section is due to the single resonance and in which there is no interference from other resonances.

Referring to LT p322 the general single level formula (all values of ℓ allowed) can be written in the form, for a reaction proceeding through a single isolated resonance λ of spin J and definite parity

$$\sigma_{aa'} = \frac{\pi}{k_a^2} g_J \frac{(\Sigma' \Gamma_{\lambda c})_{\ell s} (\Sigma' \Gamma_{\lambda c})_{\ell' s'}}{(E_\lambda + \Delta_\lambda - E)^2 + \frac{1}{4}\Gamma_\lambda^2} \qquad (1)$$

where the primed sums ℓs, $\ell' s'$ are such that

$$\underline{\ell} + \underline{s} = \underline{J} = \underline{\ell}' + \underline{s}' \qquad (2)$$

and parity is conserved

$$\sigma_{aa} = \frac{\pi}{k_a^2} \left\{ \sum_{Js\ell} 4g_J \sin^2\phi_c \right.$$

$$-g_J \sum_{s\ell} \Gamma_{\lambda c} \left[\frac{2(E_\lambda + \Delta_\lambda - E) \sin 2\phi_c + \Gamma_\lambda (1-\cos 2\phi_c)}{(E_\lambda + \Delta_\lambda - E)^2 + \frac{1}{4}\Gamma_\lambda^2} \right]$$

$$\left. +g_J \frac{(\Sigma'\Gamma_{\lambda c})\ (\Sigma'_{s\ell\ s'\ell'}\ \Gamma_{\lambda c'})}{(E_\lambda + \Delta_\lambda - E)^2 + \frac{1}{4}\Gamma_\lambda^2} \right\} \qquad (3)$$

In the formulae

α and α' denote ingoing and outgoing channels respectively so that σ_{aa} is the elastic scattering cross-section.

k_a is the wave number for the ingoing channel

$g_J = \frac{2J+1}{2(2I+1)}$, the spin statistical factor.

I is the spin of the target nucleus

J " " " " " compound nucleus level λ

s " " channel spin = $I \pm \frac{1}{2}$

ϕ_c is the hard sphere scattering phase and is independent of s and J

E_λ is an eigenvalue for the internal region

Δ_λ is the shift factor for the level λ

$\Gamma_{\lambda c}$ $\Gamma_{\lambda c'}$ are level widths for the level λ

$\Gamma_\lambda = \Sigma\Gamma_{\lambda c}$

The more familar forms are obtained by a special choice of the boundary conditions for the eigenfunctions corresponding to the E_λ.

This gives $E_\lambda + \Delta_\lambda(E_r) = E_r$ where E_r is the observed resonance energy. We note that, in general Δ_λ is a function of energy as is $\Gamma_{\lambda c}$.

If J is fixed and $\ell = 0$ there is only one value of s whilst if the internal interaction (nuclear potential) is represented by a square well then $\phi_c = k_a a$ for $\ell = 0$, where a is the scattering length (or channel radius).

Expanding $E_\lambda + \Delta_\lambda - E$ about the observed resonance energy E_r and setting $\ell = 0$, $\sin^2\phi_o^2 = k_a^2 a^2$ we obtain the well known formulae for the contribution to the cross-section <u>from a single resonance</u>

$$\sigma_{nn} = \pi \lambda g_J \frac{\lambda\Gamma_n^2 + 4a\Gamma_n(E-E_r) + 4\pi a^2}{(E-E_r)^2 + \Gamma^2/4} \qquad (4)$$

$$\sigma_{n\gamma} = \pi\lambda^2 g_J \frac{\Gamma_n \Gamma_x}{(E-E_r)^2 + \Gamma^2/4} \qquad (5)$$

$$\Gamma = \sum_x \Gamma_x \qquad (6)$$

x covers emission of gamma radiation or particles. λ is the reduced wavelength (<u>centre of mass system</u>).

In (4), (5) and (6) it is assumed that there is no interference from other resonances - the only interference term arises from potential-resonance interference in the elastic scattering formula.

Use of the Breit Wigner formula for $\ell = 0$ neutrons and a single isolated level requires a knowledge of the following parameters

I, J, E_r

a

Γ_n, Γ_x (all x), Γ - all evaluated at E_r

Additionally it is necessary to know how the partial widths vary with energy - the usual assumption is that Γ_γ is independent of energy whilst $\Gamma_n(E) = \Gamma_n^0\sqrt{E}$ where Γ_n^0 is the reduced neutron width (corresponding to the value of Γ_n at E = 1eV) so that $\Gamma(E) = \Gamma_n^0\sqrt{E} + \Gamma_\gamma$ when only elastic scattering and radiative capture are of importance.

All the previous discussion depends on the representation of the nuclear potential by a square well of radius a. Use of a diffuse potential (as in most optical model calculations) will lead to somewhat different formulae and may possibly change the dependence of Γ_n on energy slightly.

(b) Breit Wigner Formula for ℓ = 0 Neutrons and Many Levels when Elastic Scattering and Radiative Capture are the only Allowed Reactions

This situation is found in nearly all medium and heavy non-fissile nuclides in the electron volt region.

Since the spacing between resonances is quite small one expects to find resonance-resonance interference terms. In fact such interference terms enter only into the elastic scattering cross section. The existence of many photon channels ensures (random sign approximation) that the interference terms vanish in the case of radiative capture. For particle emission or fission in which few channels are involved strong level interference effects are likely and the formulae are more complicated.

The elastic and radiative capture cross sections for many levels with the same J are given by

$$\sigma_{el} = 4\pi a^2 + \pi\lambda^2 g_J \left\{ \sum_r \frac{\Gamma_{rn}^2 - 2\Gamma_{rn}\Gamma_r a^2/\lambda^2 + 4(a/\lambda)\Gamma_{rn}(E-E_r)}{(E-E_r)^2 + \Gamma_r^2/4} \right.$$

$$\left. + \sum_r \sum_{s\neq r} \frac{2\Gamma_{rn}\Gamma_{sn}}{[(E-E_r)^2 + \frac{1}{4}\Gamma_r^2]\,[(E-E_s)^2 + \frac{1}{4}\Gamma_s^2]} \left[\tfrac{1}{4}\Gamma_r\Gamma_s + (E-E_r)(E-E_s)\right] \right\} \qquad (7)$$

$$\sigma_{n\gamma} = \pi\lambda^2 g_J \sum_r \frac{\Gamma_{rn}\Gamma_{r\gamma}}{(E-E_r)^2 + \Gamma_r^2/4}$$

The sums are over resonances. In application it must be remembered that, except when I = 0, we have $J = I \pm \frac{1}{2}$ to consider.

The discussion of energy variation of widths and nuclear potentials under (a) is equally applicable here.

In practice allowance must often be made for the contribution to the cross-section from distant levels - this usually has a 1/v energy variation.

(c) The Reich-Moore Formula - a Multilevel Formula with Few Fission Channels for $\ell = 0$ Neutrons

The theory is given by Reich and Moore [16] and has been applied to U233 [17], U235 [18] and Pu241 [19]. It applies principally to the low energy cross sections of thermally fissile nuclides (only $\ell = 0$ resonances are considered) but is valid for any reaction which proceeds essentially through only a few channels. A few fission channels only are allowed (one or two in the practical applications) but interference is allowed between resonances.

The total, elastic and fission cross-sections for fixed J are given, in the two fission channel case, by

$$\sigma_T = 2\pi \lambda^2 g_J \, RF(1-S_{11}). \tag{9}$$

$$\sigma_n = \pi \lambda^2 g_J \, |1-S_{11}|^2 \tag{10}$$

$$\sigma_f = \pi \lambda^2 g_J (|S_{12}|^2 + |S_{13}|^2) \tag{11}$$

The expressions for S_{11}, S_{11}, S_{13} are rather complicated but are given in reference [16]. The following quantities are needed for each resonance to give a complete specification of the cross-section.

E_λ (not necessarily equal to E_r)

J, $\ell(=0)$, I

Γ_λ, the total width

$\Gamma_{\lambda n}$, the neutron width

$\Gamma_{\lambda\gamma}$, the radiation width

$\Gamma_{\lambda f}$, the fission width

$\beta_{\lambda 2}$ and $\beta_{\lambda 3}$

Relative signs of $\beta_{\lambda 1}$ $\beta_{\lambda 2}$ and of $\beta_{\lambda 1}$ $\beta_{\lambda 3}$

$$|\beta_{\lambda 1}| = (\Gamma_{\lambda n}/2)^{\frac{1}{2}} \qquad (12)$$

$$\Gamma_{\lambda f} = 2(\beta_{\lambda 2}^2 + \beta_{\lambda 3}^2) \qquad (13)$$

In the one fission channel case the only additional quantity needed over the single level formula case is the relative sign of $\beta_{\lambda 1}$ and $\beta_{\lambda 2}$.

It may be neither necessary nor desirable to include interference terms for all resonances, (i.e. some levels can be calculated using a single level formula).

It is often desirable to add in 1/v terms to the various cross-sections to account for the effects of distant levels, etc.

(d) <u>The Vogt Many Channel, Few Level Formula for ℓ = 0 Neutrons</u>

The theory is given by Vogt [20] and has been applied to U233, U235 and Pu239 [20] [21]; it was developed to account for the low energy cross-sections of fissile nuclides. Reference [20] gives formulae for elastic, (n,γ) and fission cross-sections.

For each resonance λ the following quantities provide a complete specification of the cross-section

E_λ (not necessarily equal to E_r)

J, I

Γ_λ $\Gamma_{\lambda n}$, $\Gamma_{\lambda\gamma}$, $\Gamma_{\lambda f}$

A c-dimensional vector $\underline{g}_{\lambda f}$ where c is the number of fission channels - alternatively one need only specify the angles between all pairs $g_{\lambda f}\, g_{\lambda' f}$ since $|g_{\lambda f}|^2 = \Gamma_{\lambda f}$.

For simplicity it is probably better to specify the c components of the $\underline{g}_{\lambda f}$ for each λ. As in the case of the Reich-Moore formula 1/v terms may be added to the contribution to the cross-section from the specified resonances.

(e) The Multilevel Formula with Pure Scattering as Used by Hibdon

This is useful in analysing data for certain light nuclides (e.g. Na and Aℓ) in which radiative capture, inelastic scattering etc are all unimportant compared to elastic scattering and so $\Gamma \sim \Gamma_n$. The formula for the scattering cross section then becomes (in the case when level widths are much less than spacings)

$$\sigma_n = 4\pi \lambda^2 \sum_{\ell} \sum_{J} g_J \Big| \sum_{r} \frac{\frac{1}{2}\Gamma_r}{E-E_r + \frac{1}{2} i\Gamma_r} + e^{i\phi_\ell} \sin\phi_\ell \Big|^2 \qquad (14)$$

where r denotes a particular level corresponding to known values of J and ℓ. Γ_r is the (total) width for resonance r whilst ϕ_ℓ is the hard sphere phase for neutrons of angular momentum ℓ on the square well model.

(14) expands into the form (for group of levels having same ℓ and J)

$$\sigma_n = \sum_{\ell} (2\ell+1)\, 4\pi \lambda^2 \sin^2\phi_\ell + \pi \lambda^2 g_J \Big\{ \sum_{r} \frac{\Gamma_r^2 \cos 2\phi_\ell + \Gamma_r (E-E_r) \sin 2\phi_\ell}{(E-E_r)^2 + \frac{1}{4}\Gamma_r^2} + \sum_{r} \sum_{s \neq r} \frac{2\Gamma_r \Gamma_s}{[(E-E_r)^2 + \frac{1}{4}\Gamma_r^2][(E-E_s)^2 + \frac{1}{4}\Gamma_s^2]} [\tfrac{1}{2}\Gamma_r\Gamma_s + (E-E_r)(E-E_s)] \qquad (15)$$

There is a fairly obvious relation between (15) and (7).

This formula requires the specification of the following parameters for each resonance

E_r

I, J, ℓ

Γ_r

ϕ_ℓ for all ℓ values.

In fact ϕ_ℓ may be computed from theoretical formulae based on the square well potential model.

Hibdon has applied (15) to analyse resonances in aluminium [22] and in sodium [23].

(f) Breit-Wigner Formula for a Single Isolated Level Involving Neutrons of any ℓ

This applies in very light nuclei where resonance - resonance interference can be neglected. Generalising (14) and (15) to a single resonance of given J, ℓ and with several reactions but no change in channel spin on elastic scattering gives:

$$\sigma_{nn} = \sum_{\ell} (2\ell+1)\, 4\pi \lambda^2 \sin^2\phi_\ell + \pi\lambda^2 g_J \frac{\Gamma_n^2 - 2\Gamma_n\Gamma \sin^2\phi_\ell + 2\Gamma_n(E-E_r)\sin 2\phi_\ell}{(E-E_r)^2 + \frac{1}{4}\Gamma_r^2} \qquad (16)$$

$$\sigma_{nx} = \pi\lambda^2 g_J \frac{\Gamma_n \Gamma_x}{(E-E_r)^2 + \frac{1}{4}\Gamma_r^2} \qquad (17)$$

$$\text{with} \quad \Gamma = \Gamma_n + \sum_x \Gamma_x \qquad (18)$$

More general formulae are given in reference [24].

This particular case needs further investigation and no card format is given for the parameters involved.

3.6 Statistical Data for Unresolved Resonances

This subject requires careful consideration before card formats are determined. At present (May 1963) this investigation has not been undertaken.

3.7 Thermal Scattering Law Data

Thermal scattering law data is concerned with neutron interactions in (neutron) energy ranges where the relative motion of nucleus and neutron and the possibility of atomic interactions (binding effects) must be taken into account. The energy and angular distributions of neutrons after scattering collisions is determined by the scattering law, a function $S(\alpha,\beta)$ where $\alpha = [E + E' - 2(EE')^{\frac{1}{2}} \cos\theta]/AkT$ and $\beta = (E'-E)/kT$. E is the initial neutron energy, E' is the final energy and θ is the laboratory scattering angle so that α and β are related to the momentum and energy transfers in the collision. kT is the temperature in energy units and A is the ratio of the mass of the nucleus to the mass of the neutron (this definition must be extended in the case of molecules).

In the case of a monatomic gas where there are no binding effects

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

In terms of $S(\alpha, \beta)$ the cross-section for a neutron to be scattered from energy E to energy E' through a laboratory angle θ is given by

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

A [illegible] has worked on this a while, [illegible] of [illegible]

where σ_b is the bound atom cross-section.

$$\sigma_b = \sigma_f (A+1)^2/A^2$$

where σ_f is the free atom cross-section

For a fuller account the reader is referred to the articles by Egelstaff [25] and Egelstaff and Schofield [26] and the references therein.

The thermal scattering law data is specified by giving $S(\alpha, \beta)$ at sufficient values so as to allow linear interpolation in α and β. In addition the lower energy limit of the static nucleus model for scattering is specified. Since $S(\alpha, \beta)$ may not be known for all accessible α, β below this lower energy limit the monatomic gas model form of $S(\alpha, \beta)$ is assumed in the absence of other information - this takes the same (parametric) form for all materials.

In certain cases $S(\alpha, \beta)$ has a δ function at $\beta = 0$ and in this case we write

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

where $S^*(\alpha, \beta)$ and λ are specified in the file.

Two further points require consideration. Firstly in the case of molecules the effective mass (ratio) used to define α is somewhat arbitary and will generally be a function of the particular analysis of the experimental results. Secondly it may be desirable to allow the free atom cross section to vary with energy. A simple case - the only one considered - is when the total scattering cross-section is set equal to the elastic cross section given in the file (R.T.N. = 1002) and the secondary energy distribution is computed using the monatomic gas law of $S(\alpha, \beta)$.

4. Handling of Photon Interaction Data

The general features of photon interaction data are discussed by Buckingham and Pendlebury [12]. Since photon interaction data is currently (May 1963) not included in the library a full discussion of this subject is left over for a later version of the present report.

5. Handling of Photon Production Data

This subject remains to be investigated.

6. Representation of Data on Punched Cards - General Features

All Nuclear Data File information is recorded on IBM symbolic cards having 960 punching positions (12 rows x 80 columns). Figure 1 illustrates the layout of the symbolic card. An actual card is shown in figure 2.

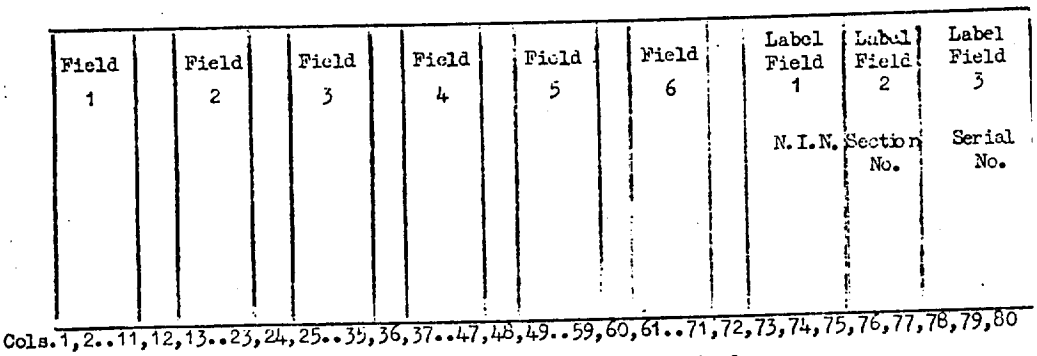

Figure 1. The Symbolic Card

The card has six data fields each eleven columns wide separated by a blank column and three label fields in columns 73-80.

Punching conventions

One piece of information only is recorded in each field and this must be punched so that there are no blank columns at the right-hand end of the field. Punching is facilitated by using the special data punching sheet shown in figure 3.

No cards may have a B in column 1 but numbers are permissible. This requirement ensures compatibility with the IBM 7030 Master Control Programme.

If a particular field is to be left blank it is permissible, and sometimes convenient, to punch a zero in the field.

Number representation

Unless otherwise stated all data is in floating point mode (magnitude limited only by machine capacity). No fixed point number may exceed 32767.

Labelling - Identification and Serial Numbering

Label field 1 (73-75) contains the nuclide identification number (common to all cards for one set of data for one substance). For each set of data there are a number of sections and label field 2 (76-77) gives the section number. A section contains all the nuclear data for a particular reaction type (number) and the same reaction type will have different section numbers for different substances depending on where it is filed in each card deck. Note that 1002 (elastic cross-section) and 2002 (elastic angular distributions) occupy two sections not one. The relation between section number and reaction type number is specified on the nuclide heading cards (see below) occupying section 00. Within each section the cards are numbered serially starting at one in label field 3 (78-80).

It will be seen that the label fields ensure that cards do not get out of order, or mixed with cards for another section or with different vintage data for the same substance.

The label fields are normally occupied by integers but if necessary the range of any label can be extended by using alphabetic characters.

Ordering of Sections

The ordering of sections is according to the order of (a) Neutron data (b) Photon interaction data (c) Photon production data. Within each of (a) (b) (c) the order is by, firstly, particular classification number and, secondly, by general classification number. For instance we might have.

Heading cards	Section	00		
Neutron data		01	1001	Total cross-section
		02	1002	Elastic cross-section
		03	2002	Elastic angular distribution
		04	1003	Non-elastic cross-section
		05	1004	(n,n') total cross-section
		.	.	
		.	.	
		.	.	
Photon interaction data		XY	8001	Total cross-section
		.	.	
		.	.	
		.	.	
Photon production data		VW	11005	Photon production angular distribution from first level

It should be noted that as far as neutron data is concerned all the data for a particular reaction appears together (cross-section, angular distribution secondary energy, number of secondaries).

In practice packs containing all three types of data simultaneously are unlikely to occur, particularly as photon interaction data depends only on Z and not on A.

Description of Card Contents - Nuclear Data File Cards

A description of the data is printed on each card together with an interpretation of the card contents. An additional guide to the contents of a card is provided by using the special Nuclear Data File cards in which case different colours are used for different general classification numbers

(see section 2.2 for details). These Nuclear Data File cards are also designed to allow easy reading of the interpretation of their contents.

Nuclide Heading Cards

The first section of each nuclide (section 00) contains heading cards which list in section number order the reaction types occurring for the nuclide concerned together with their section number and the number of cards in each section. The card format is

Card 1 Field 1 Nuclide identification number * (fixed point). This number identified the isotope, element or mixture referred to by the data and is identical with the number punched in columns 73-75 (label field 1) on every card. (If the data is revised, it is given a new identification number).

2 Total number of cards used to represent this nuclide including the cards in section 00 (fixed point).

3 Number of cards in section 00 (fixed point).

4 The atomic number (Z) (fixed point).

5 The atomic or molecular weight (A) (fixed point - six places following the decimal)

6 Number of different reaction types that occur in the nuclide (fixed point).

Card 2 Field 1 Section number (fixed point)

2 Reaction type number (fixed point)

3 Number of cards in this section (fixed point).

4 Section number (fixed point).

5 Reaction type number (fixed point).

6 Number of cards in this section (fixed point).

The field pattern from Card 2 onwards is repeated for each reaction type in the nuclide. In the case of mixtures, the atomic number (Z) is omitted and molecular weight (A) is that appropriate to the mixture.

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* For further details about nuclide identification numbers see section 2.2

Atomic and Molecular Weights

These are specified as fixed point decimal numbers (F10.6) so that for U^{238} we have A = 238.050760. The physical scale in which C^{12} = 12.000000 is used.* Values of A are given by König et al. [27]. On this scale the neutron mass is 1.008665 and it should be remembered that in elastic and inelastic scattering the ratio of nucleus mass to neutron mass is involved and not A itself. The same tables are used to compute Q-values. In forming macroscopic constants care must be exercised to use the correct value of Avogadros' number. This is a $N_o = 6.02295 \times 10^{23}$ ($= 6.023 \times 10^{23}$ for normal purposes since the accuracy of densities does not justify more figures).

7. Representation of Neutron Interaction Data on Punched Cards

7.1 Neutron Cross Sections (G.C.N.1)

The format for each cross-section reaction type is as follows:-

Card 1 Field 1 Reaction type number (fixed point)

2 Number of energy ranges (fixed point)

3 "Q" value of the reaction in MeV

4,5,6 Additional information if required

Card 2 Field 1 Lower limit of the first energy range

2 Upper limit of the first energy range

3 Material temperature (degrees absolute) to which cross-section is appropriate (left blank if temperature dependence not considered).

4 Number of cards used to represent this temperature for this energy range, including this card (fixed point)

5 Number of cross-section points for this temperature in this energy range (fixed point)

6 Number of temperatures still to be fully considered (i.e. includes this one) for this energy range (fixed point). If the temperature dependence of the cross-sections is not considered this field contains a 1.

*Most of the existing data has atomic and molecular weights referred to $A(O^{16}) = 16.000000$.

All the following cards contain energy values (in MeV) in fields 1,3 and 5 with the corresponding cross-sections in fields 2,4 and 6.

The field pattern from card 2 onwards is repeated for each temperature (for a fixed energy range) and for each energy range so that a new temperature and/or a new energy range mean the start of a new card similar to card 2. When temperature dependence is considered it is convenient to use at least two ranges with an inter-range boundary at or slightly above the highest energy at which temperature dependence occurs. In this way repetition of temperature independent data is avoided.

If punched cards for several cross-sections of a particular material are prepared manually according to the above format some multiplication of work occurs due to the necessity of repeating the energies at which cross-sections for each reaction are tabulated.

The IBM 7030 S1 (Fortran) language programme REFORM removes the need for such repetition. As input it accepts data in which several cross-sections are specified for a range of energy points, each energy point being specified only once and produces labelled cross-section data cards in the above format.

Operating instructions for REFORM are given in Appendix A. An IBM 7090 Fortran II language version of REFORM also exists.

7.2 Angular Distribution of Secondary Neutrons (G.C.N.2)

The card format is as follows:-

Card 1 Field 1 Reaction type number (fixed point).

2 Number of energy ranges - or energy points if the angular distribution is given at energy points (fixed point).

3 Atomic weight (fixed point - six places following the decimal).

Card 1 Field 4 1 - data for centre of mass system
2 - data for laboratory system.

5,6 Additional information if required.

Card 2 Field 1 Lower limit of first energy range.

2 Upper limit of first energy range.

3 Number of cards used to represent this range - including this one (fixed point).

4 Number of different angular distributions for the first neutron for the first energy range (fixed point).

5. Probability of the first angular distribution for the first neutron (or for all neutrons in fission or any other process in which the number is variable).

6 Number of values given for the first angular distribution for the first neutron (fixed point).

The following cards contain cosθ values in fields 1,3 and 5 with the corresponding probabilities in fields 2,4 and 6.

After the values of the first angular distribution for the first neutron have been specified, the field pattern is repeated from card 2 field 1 onwards for the remaining angular distributions of the first neutron (in these repetitions the cards similar to card 2 have identical entries in fields 1-4).

When all the angular distributions for the first neutron have been specified, the field pattern is repeated from card 2 field 1 onwards for all other neutrons in the reaction (field 4 of the card similar to card 2 will, in general, be different from field 4 of corresponding cards for the first neutron). The reaction type number indicates how many neutrons are involved in the reaction (and implies whether laboratory or centre of mass data is involved although this is explicitly given in field 4 of card 1).

After all neutrons have been considered for the first range the first neutron is considered for the second range starting with a card similar to card 2.

It will be seen that a new distribution for a given neutron, a new neutron or a new energy range all begin on a new card similar to card 2.

If the angular distribution is given pointwise rather than rangewise then field 1 on card 2 (and similar cards) is used to record the energy value and field 2 on card 2 (and similar cards) is left blank.

7.3 Energy Distributions of Secondary Neutrons (G.C.H.3)

The card format is as follows:-

Card 1 Field 1 Reaction type number (fixed point).

2 Number of energy ranges (fixed point).

3,4,5,6 Additional information if required.

Card 2 Field 1 Lower limit of the first energy range.

2 Upper limit of the first energy range.

3 Number of cards used to represent this energy range - including this one (fixed point).

4 Number of different laws for the first neutron (fixed point).

5 Probability of the first law for the first neutron

6 Law number (fixed point).

The field pattern on card 3 (and later similar cards) depends on the law number.

Law 1

Card 3 Field 1 Number of discrete energy values to be considered. Then follow in successive fields (discrete energy, corresponding probability) pairs.

Law 2

Card 3 Field 1 Number of pairs (discrete energy loss, reduction factor) to be considered.

2 Discrete energy loss ($\mathcal{E}_d$)

3 Reduction factor (k)

4 Corresponding probability.

5 Discrete energy loss and so on.

Laws 3,4,5 and 6

Card 3 Field 1 Number of spectrum values.

The subsequent fields contain spectrum "energy" arguments followed by the corresponding probabilities.

Law 7

Card 3 Field 1 "a"

2 "b"

3 "c"

4 "E_f"

The card pattern repeats from card 2 field 1 whenever there is (a) a new law for a given neutron (b) a new neutron (the number of neutrons is defined by the reaction type number) and (c) a new energy range. In cases (a) and (b) this means the repetition of a certain amount of information (card 2 fields 1-4 for (a) and card 2 fields 1-3 for (b)) but simplifies programming for users. Information is considered in the order

(a) all laws (in order) for one neutron for one energy range

(b) all neutrons (in order) for one energy range

(c) all energy ranges in ascending order

7.4 Miscelleneous Neutron Interaction Quantities (G.C.N.4)

The format is exactly the same as for cross-sections except that field 3 of card 1 is left blank.

7.5 Resolved Neutron Resonance Data (G.C.N.5)

In order to make the system flexible and to allow for future additions the various approximations to the full R-matrix theory are given different reaction type numbers. The reaction type number is given on the first card and the format of succeeding cards varies with the law number.

The card format is as follows:

Card 1 Field 1 Reaction type number (fixed point) which implies the particular approximation to full R-matrix theory

5151 Single level Breit-Wigner formula, $\ell = 0$ neutrons, isolated resonance

5152 Single level Breit-Wigner formula for $\ell = 0$ neutrons and many levels for elastic scattering and radiative capture.

5153 Reich-Moore multilevel formula

5154 Vogt multilevel formula

5155 Multilevel formula with pure scattering

5156 - 5200 to be allocated.

2 Number of energy ranges (fixed point)

3 Nuclear spin I

4, 5, 6 Additional information if required

Card 2 Field 1 Lower limit of first energy range

2 Upper limit of first energy range

3 Number of cards used to represent this energy range including this one (fixed point)

4 Number of resonances in this energy range (fixed point)

5,6 Additional information if required

The format of the following cards depends on the reaction type number.

RTN = 5151, 5152

Card 3 Field 1 Lower limit of range of validity of cross-sections calculated from resonance parameters in this energy range

2 Upper limit of range of validity of cross-sections calculated from resonance parameters in this energy range

3 a, the scattering length (in units of 10^{-12}cm)

4 A fixed point number indicating how Γ_n, Γ_γ etc are to cary with energy

e.g. 1 means $\Gamma_n = \Gamma_n^{\circ}\sqrt{E}$ and Γ_γ fixed (Γ_n° is the reduced neutron width = value at resonance divided by $\sqrt{E_r}$)

5 A fixed point number indicating the partial widths which are specified and their order on cards 4, 5 etc.

1 = Γ_n, Γ_γ

2 = Γ_n, Γ_γ, Γ_f

3 = Γ_n

etc.

6 Additional information if required

Card 4 Field 1 Energy in MeV

2 Value (barns) of additional 1/v component of elastic cross-section at this energy

3 Energy in MeV

Card 4 Field 4 Value (barns) of additional 1/v component of first partial non-elastic cross-section at this energy.

5) Similar information for same reactions and in
6) same order as implied by order of partial widths in field 5 of card 3 going to cards 5 and 6 if necessary

Card 5 Field 1 E_r, the resonance energy (MeV)

2 J, the angular momentum of the compound nucleus

3 Γ, the total width evaluated at E_r

4 onwards (going on to cards 5, 6 etc. if necessary) Values of the partial widths evaluated at E_r and given in the order determined by the number in field 5 of card 3. All widths are given in eV.

Information on each resonance starts on a new card. In the most frequently occurring cases the information for one resonance will only occupy one card.

RTN = 5153

Card 3 Field 1 Lower limit of range of validity of cross-sections calculated from resonance parameters in this range.

2 Upper limit of range of validity of cross-sections calculated from resonance parameters in this range

3 a, the scattering length (in units of 10^{-12}cm)

4 A fixed point number indicating how $\Gamma_{\lambda n}$, $\Gamma_{\lambda\gamma}$, $\Gamma_{\lambda f}$ etc are to vary with energy

e.g. 1 means $\Gamma_{\lambda n} = \Gamma_{\lambda n}{}^{o} \sqrt{E}$

$\Gamma_{\lambda\gamma}, \beta_{\lambda 2}, \beta_{\lambda 3}$ independent of energy

5 A fixed point number indicating the number of fission channels

6 Additional information if required

Card 4 Field 1 Energy in MeV

2 Value (barns) of additional 1/v component of elastic cross-section at this energy

3 Energy in MeV

4 Value (barns) of additional 1/v component of radiative capture cross-section at this energy

5 Energy in MeV

6 Value (barns) of additional 1/v component of fission cross-section at this energy.

Card 5 Field 1. E_λ (MeV)

2 J, the orbital angular momentum of the compound nucleus

3 Γ_λ, the total width evaluated at E_λ

4 $\Gamma_{\lambda n}$, the neutron width evaluated at E_λ

5 $\Gamma_{\lambda\gamma}$, the radiative width evaluated at E_λ

6 $\Gamma_{\lambda f}$, the total fission width evaluated at E_λ

Card 6 Field 1 $2\beta_{\lambda 2}^2$

2 Relative sign of $\beta_{\lambda 1}$, $\beta_{\lambda 2}$

3 $2\beta_{\lambda 3}^2$

4 Relative sign of $\beta_{\lambda 1}$, $\beta_{\lambda 3}$

and so on within the number given in field 5 of card 3.

Information on each resonance starts on a new card

RTN = 5154

Cards 3, 4, 5 As in the case RTN = 5153

Card 6 Field 1 onwards Components of $g_{\lambda f}$ in units of $(eV)^{1/2}$

The number of fields used is equal to the number given in fields of card 4.

Information on each resonance starts on a new card.

RTN = 5155

Card 3 Field 1 Lower limit of validity of cross-sections calculated from resonance parameters in this energy range

2 Upper limit of validity of cross-sections calculated from resonance parameters in this energy range

3 a, the scattering length (in units of 10^{-12}cm)

4 A fixed point number indicating how Γ_r varies with energy for given J, ℓ

5 A fixed point number indicating how ϕ_ℓ is to be determined

1 - determined from values at resonances with given energy variation

2 - calculated from formulae

Field 6 Additional information if required

Card 4 1 Maximum value of ℓ for which ϕ_ℓ is needed in this energy range

2 Energy below which ϕ_1 is negligible

3 Energy below which ϕ_2 is negligible
and so on, going on to additional cards if necessary

Card 5 Field 1 E_r, the resonance energy (MeV)

2 J

3 ℓ

4 Γ_r

5,6 etc. Values of ϕ_0 ϕ_1 ---- ϕ_ℓ^{max} if Card 3 Field 5 contains a 1

Information on each resonance starts on a new card.

In all cases a new energy range is started by a card similar to Card 2.

7.6 Statistical Data for Unresolved Neutron Resonances (C.C.N.6)

The card format is as follows:

Card 1	Field 1	Reaction type number (fixed point) which implies the way in which the following parameters are to be processed to give cross-sections.
		These go 6151, 6152 etc.
	2	Number of energy ranges (fixed point)
	3	Nuclear Spin, I
	4,5,6	Additional information if required
Card 2	Field 1	Lower limit of first energy range (MeV)
	2	Upper " " " " "
	3	Number of cards used to represent this energy range (fixed point)
	4	Lower limit of range of validity of cross-sections calculated from statistical resonance parameters in this energy range.
	5	Upper limit of range of validity of cross-sections calculated from statistical resonance parameters in this energy range.
	6	Additional information if required.
Card 3	onwards	Information appropriate to the reaction type number. The detailed format is not yet decided.

Each new energy range starts a new card similar to card 2.

7.7 Thermal Neutron Scattering Law Data

The card format is as follows:

Card 1 Field 1 Reaction type number = 7002 (fixed point)

2 Number of energy ranges = 1 (Fixed point)

3 σ_{fr}, the free atom cross-section

4 ε, the value of E/kT above which the static nucleus model of elastic scatter is adequate

5 A', the effective value of the ratio mass of "molecule" to mass of neutron to be used.

6 E_m, the upper energy limit for constant σ_{fr}. Above this energy σ_{cl} (RTN = 1002) must be used in conjunction with the monatomic gas law.

Card 2 Field 1 Material temperature (degrees absolute) to which scattering law data is appropriate (left blank if temperature dependence of $S(\alpha, \beta)$ is not considered)

2 Number of cards used to represent this temperature, including this card (fixed point)

3 Number of β values (fixed point)

4 Number of temperatures still to be fully considered (i.e. including this one). If the temperature dependence of $S(\alpha, \beta)$ is not considered this field contains a 1.

5 λ the parameter in the δ - function contribution $e^{-\lambda\alpha}\,\delta(\beta)$ to $S(\alpha, \beta)$. If there is no contribution from this term then λ is set equal to zero.

6 Additional information if required

Card 3 onwards contains

β_ℓ The ℓ^{th} order β - value, β values being given in ascending

n_ℓ The number of α values corresponding to β_ℓ (fixed point)

$\alpha_{\ell j}$ $j = 1$ ---- n_ℓ, the values of α being in ascending order [i.e. n_ℓ values of α]

$S(\alpha_{\ell j}, \beta_\ell)$ $j = 1$ ---- n_ℓ [i.e. n_ℓ values of $S(\alpha, \beta)$]

Each β value is in field 1 of a new card and the format of card 3 and following cards is repeated.

If $n_t = 0$ for same t then the α values are the same as for the previous value of β and they are not repeated.

The field pattern from card 2 onwards is repeated for each temperature.

8. Representation of Photon Interaction and Production Data on Punched Cards

This remains to be determined but the general form it will take can probably be discerned by a study of section 7 and a comparison of the properties of photon interaction and production data with neutron interaction data.

9. Representation of Data on Magnetic Tape

It is generally more convenient to use magnetic tape rather than punched cards as a storage medium. High density magnetic tape written in BCD mode is used for this purpose and a tape contains exactly the same information as the corresponding symbolic cards.

Each tape starts with an index * listing the order in which the nuclides appear on the tape and the format of this index is as follows:

Card 1 Field 1 Number of nuclides on the tape (fixed point).

2,3,4,5,6 Additional information if required

Card 2 Field 1 Nuclide identification number of first nuclide on tape (fixed point)

2 Total number of cards used to represent this nuclide (fixed point)

3,4,5,6 Additional information if required.

The field pattern from card 2 onwards is repeated for each nuclide on the tape. Columns 73-77 of each list "card" are left blank and columns 78-80 contain a serial number.

* Optionally, the tape can be magnetically labelled in which case the magnetic label occupies a one record file at the beginning of the tape.

Tapes can be prepared and modified using the IBM 1401 programme NDTP which is described in detail in reference [28]. This replaces a previous programme RH 81 which has been found to be too restrictive.

The main facilities of NDTP allow the

(a) Write n nuclides on tape from cards ($1<n<125$)

(b) Copy a tape containing n nuclides.

(c) Modify any specified records (cards) on an existing tape. Heading section cards cannot be modified by NDTP.

(d) Take m ($m>0$) nuclides from cards and n ($n>0$) nuclides from an existing tape containing p ($p>n$) nuclides and write a new tape containing m + n nuclides in a specified order.

(e) Print the output tape (if required) - this gives a straight listing (see section 11).

Facility (c) can be used to correct tapes when punching errors came to light in card decks used to prepare the tapes.

10. Checking of Data

Before library data is put into general use it is absolutely essential that the accuracy of representation be checked. Large numbers of punched cards (or magnetic tape records) are involved and the possibility of random punching errors etc. occurring cannot be ignored. A certain amount of checking must be done by comparing card/tape listings (see section 11) with the lists of data prepared for punching but much of the tedium of checking can be avoided by using the IBM 7030 S1 (Fortran) language programme CHECK [29].* This takes the cards or magnetic tape containing data* for one nuclide and applies a great variety of logical and arithmetical checks. For instance in the case of cross-sections the sum of the partial cross-sections at a given energy is compared with the total cross-section at that energy whilst the energies are checked to see that they monotomically increasing.

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*CHECK currently deals only with neutron interaction cross-sections, angular distributions, secondary energies and miscelleneous quantities but is designed to allow extension to other types of data later.

Further details of the checking programme are given in appendix B and in reference [29].

It should be recognised that certain data errors are not detectable by a programme such as CHECK and users of library data should be constantly alert to detect errors which have hitherto passed unnoticed. Unexpected values of group-averaged cross-sections may arise from some error in representation of the input basic library data to the group-averaging programme.

11. Listing of Data

It is possible to get a direct listing of library data from either cards or magnetic tape using standard IBM 1401 programmes. Such a direct listing gives the contents of one card on each line arranged in nine columns corresponding to the six data fields and three label fields.

Whilst a direct listing is useful for tracing errors, correcting cards etc. it is extremely tiresome to read. Annotated listings of library data can be obtained using the programme NDF PRINT, which is fully described in reference [30]. When such annotated listings are read in conjunction with the present report they provide an easily understood description of the data contained on the cards. Currently NDF PRINT deals only with data within general classification numbers 1-4 (Neutron cross-sections, angular distributions, secondary energies and miscellaneous quantities) but it is designed so as to allow extension to other types of data at a later stage. Appendix C lists the information which is provided in the annotated listing.

12. Modification and Up-Dating of Data

Corrections (rather than revisions) of data can be incorporated in the library as described in section 9. Additionally it is desirable to be able to incorporate new data for a particular nuclide. The best experimental values for a given cross-section may change. Alternatively it may be desirable to have several estimates available of a cross-section which is poorly known. Again it may be necessary to extended existing data to either lower or higher energies. It is desirable then to develop a range of programmes which will make major modifications to existing data sets without the necessity of punching large numbers of cards. It is planned to develop such programmes for use with the library. For instance a programme is envisaged which will change one partial cross-section and make compensatory changes in another specified cross-section whilst keeping a third (total, say) cross-section constant.

The splicing programme (for the IBM 7090) developed at AEE Winfrith and designed to allow the extension of Aldermaston data to lower energies is not likely to be of sufficient generality for contained use; it will be superseded eventually by more versatile programmes.

13. Acknowledgments

Many workers at both AEE Winfrith (W) and AWRE Aldermaston (A) have contributed to the work described in this report.

The card formats are based on original proposals by S. Francescon (W) modified as a result of discussions with L. H. Underhill (A), E. D. Pendlebury (A), I. C. Pull (W) and the author.

The preparation of files of data for the Aldermaston Nuclear Data Library was undertaken by B. A. Brett (A) D. M. Jarman (A) and Miss S. M. Miller (A) using ancillary programme developed by B. A. Brett (A) D. M. Jarman (A), L. W. Elott (W), V. J. Bell (W) and R. Hinves (A).

Potential users of the data made many suggestions which led to improvements in the library.

Thanks are due to J. S. Story (W), M. F. James (W), L. W. Elott (W) and other Winfrith workers who supplied cards and listings for the Winfrith data incorporated in the library.

Our thanks go also to all other Aldermaston and Winfrith workers who have contributed but who are not mentioned by name.

Appendix A

Operating Instructions for the IBM 7030 S1 (Fortran) Language Programme, REFORM

The programme can be used only for cross-sections tabulated over one energy range and for one temperature. There is no limit on the number of cross-sections which may be processed in one run, nor on the number of materials. The number of energy points for any one cross-section must not exceed 20,000.

Input

This consists of the programme pack followed by

(1) 1st card contains NN (format I11)

NN is the number of nuclides (materials) for which data are to be processed

(2) 2nd card contains IN, NR, NEP (format I11, 2I12)

IN = Nuclide identification number of first nuclide

NR = number of reactions for which data are given

NEP= number of energy points at which data are tabulated

(3) 3rd and following cards contain the list of energies at which the data are tabulated punch six values to a card (format E11.6, 5E12.6) - nuclear data file cards may be used conveniently for this purpose.

(4) After the energy point cards follows a card containing ISN, IRN, Q, EL, EU, T (format I11, I12, 4E12.6)

ISN = Section number of following tabulated cross-section

IRN = Reaction type number of following tabulated cross-section

Q = Q value for this reaction

EL = energy of first tabulated point for this reaction

EU = energy of final tabulated point for this reaction

T = material temperature (°K) to which following data are temperature independent

(5) Then follow cards containing the tabulated cross-sections for the appropriate reaction punched six values to a card (format E11.6, 5E12.6) - nuclear data file cards may be used conveniently for this purpose.

(6) For further reactions repeat from (4).

(7) For further nuclides repeat from (2).

The PRELUDE control card contains IDIM (format I11). IDIM must be punched as some integer greater than or equal to the maximum number of energy points for one cross-section for the set of nuclides (materials) in the input. IDIM must not exceed 20,000.

Output

For each reaction in the input a deck of cards is produced ready in all respects for incorporation as one complete section into the Nuclear Data Library.

Appendix B

The IBM 7030 S1 (Fortran) Language Programme, CHECK

CHECK is fully described in reference [29]. The following is a list of checks performed by the current version of the programme.

(1) Labelling of cards.

(2) Consistency of heading section information with following sections.

(3) Ordering of data within sections (e.g. energies at which cross-sections are specified must be monotomic increasing).

(4) Signs of positive quantities (e.g. energy, atomic weight, temperature (^{o}K) etc.)

(5) Correct normalisation of secondary energy spectra and angular distributions.

(6) Arithmetical consistency of cross-sections. For any specified relation between a composite cross-section and its component cross-sections the programme determines the difference between the sum of the component cross-sections and the composite cross-section relative to the composite cross-section and compares with two specified input numbers. These can be chosen in such a way that one comparison detects small (rounding) errors whilst the other detects gross errors due to punching mistakes (for example, factors of ten wrong).

The type of relation used includes -

(a) Total cross-section = sum of all partial cross-sections

(b) Total cross-section = elastic cross-section + non-elastic cross-section

(c) Non-elastic cross-section = sum of all partial cross-sections except the elastic cross-section.

Appendix C

Information Provided by the Data Listing

Programme NDF PRINT

The print out provided by NDF PRINT is arranged as follows:

(1) Heading (e.g."Nuclear Data for 3/U238.N.I.N. = 156).

(2) Atomic number, atomic weight, number of reaction types occuring, total number of cards.

(3) Index to sections giving contents of each section and number of cards in section.

(4) Index of reactions occurring with R.T.N's and Q-values.

(5) Table of cross-sections arranged in order of increasing energy. A column of energies and seven columns of cross-sections are given on each printed page so that different cross-sections can be compared at the same energy.

(6) Angular distribution of secondary neutrons for each appropriate reaction type in turn with details of specification (range wise or point wise; laboratory or centre of mass system).

(7) Energy distributions of secondary neutrons for each appropriate reaction type in turn with details of law numbers (not given where there is a known relation between initial and final energies and masses as for elastic scattering). For each secondary energy law the appropriate parameters are given.

(8) Mean number of secondary neutrons per fission (for fissile nuclides).

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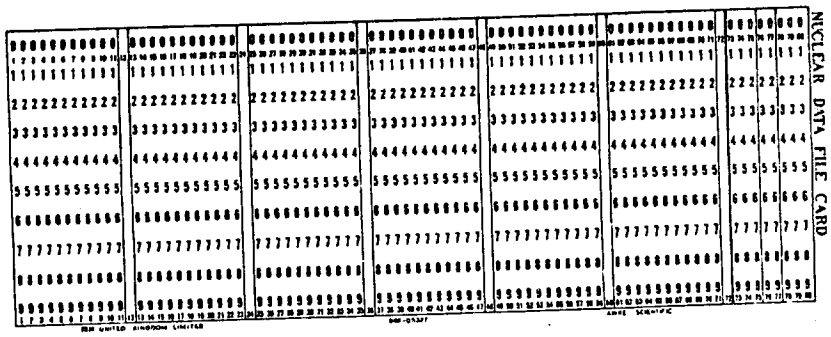

FIGURE 2. A NUCLEAR DATA FILE CARD

SHEET NUMBER OF SHEETS

NUCLEAR DATA FILE
DATA FOR PUNCHING

MATERIAL _____ WRITTEN BY _____ DATE _____ CHECKED BY _____ DATE _____

TYPE OF DATA _____ PUNCHED BY _____ DATE _____ CHECKED BY _____ DATE _____

CARD COLOUR _____ NOTES _____

I = Decimal integer which must be placed at right hand side of field. Numbers in 73-80 are alpha-numeric characters. All other numbers are floating point of form X.XXXXXXE ± X or-X.XXXXXE ± X. If X not specified it is zero.

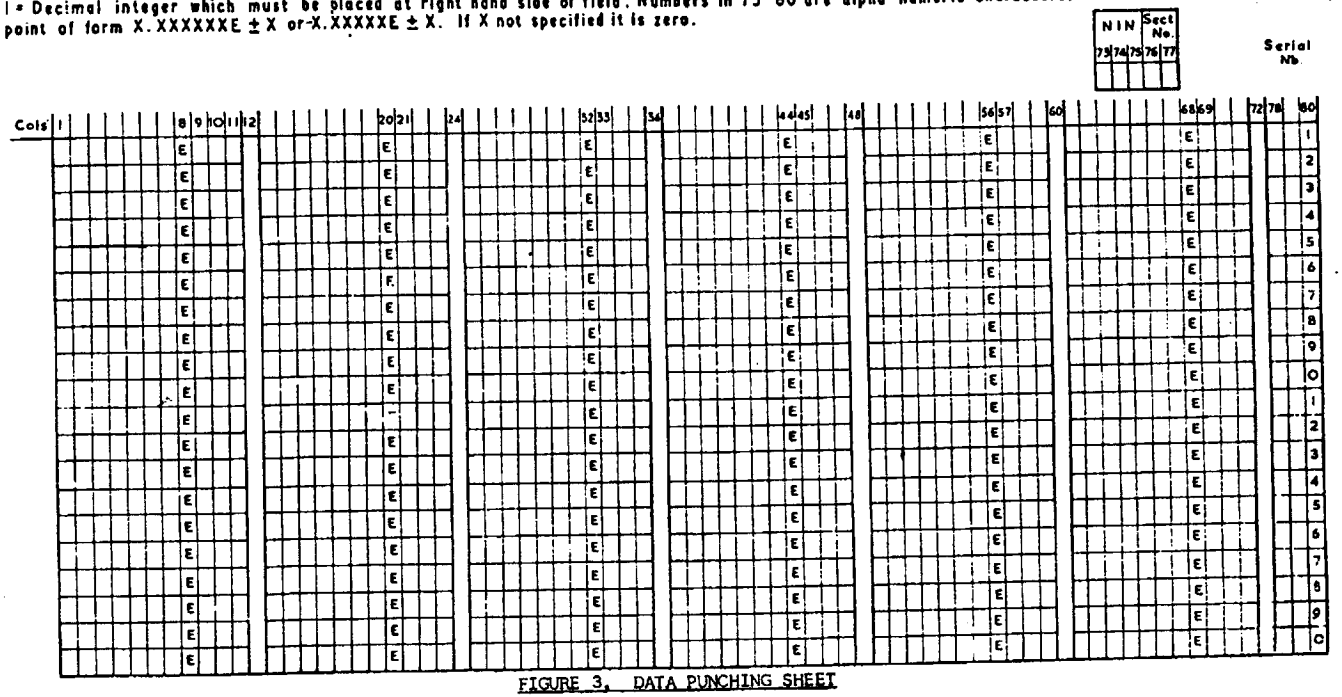

FIGURE 3, DATA PUNCHING SHEET