UNITED KINGDOM ATOMIC ENERGY AUTHORITY

ATOMIC WEAPONS RESEARCH ESTABLISHMENT

AWRE REPORT No. O. - 70/63

The Aldermaston Nuclear Data Library
as at May 1963

K. Parker

AWRE
Aldermaston, Berks.
United Kingdom Atomic Energy Authority

ATOMIC WEAPONS RESEARCH ESTABLISHMENT

ANAE REPORT NO. G-70/63

The Aldermaston Nuclear Data Library
as at May 1963
K. Parker

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 keV. 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
Table of Contents

   - Page 4

2. Data considered
   2.1 General  
   2.2 Classification of Data  
   2.3 Contents of the Library at 1st May 1963  
   - Page 7

3. Handling of Neutron Interaction Data
   3.1 Cross-Sections  
   3.2 Angular Distributions of Secondary Neutrons  
   3.3 Energy Distributions of Secondary Neutrons  
   3.4 Miscellaneous Quantities - $\bar{v}$, $\sigma$, etc.  
   3.5 Resolved Resonance Data  
   3.6 Statistical Data for Unresolved Resonances  
   3.7 Thermal Scattering Law Data  
   - Page 20

4. Handling of Photon Interaction Data  
   - Page 21

5. Handling of Photon Production Data  
   - Page 23

6. Representation of Data on Punched Cards - General Features  
   - Page 25

7. Representation of Neutron Interaction Data on Punched Cards
   7.1 Neutron Cross-Sections  
   7.2 Angular Distributions of Secondary Neutrons  
   7.3 Energy Distributions of Secondary Neutrons  
   7.4 Miscellaneous Neutron Interaction Quantities $\bar{v}$, $\sigma$, etc.  
   7.5 Resolved Neutron Resonance Data  
   7.6 Statistical Data for Unresolved Neutron Resonances  
   7.7 Thermal Neutron Scattering Law Data  
   - Page 35

---
8. Representation of Photon Interaction and Production Data on Punched Cards 53
9. Representation of Data on Magnetic Tape 53
10. Checking of Data 54
11. Listing of Data 55
12. Modification and Up-Dating of Data 56
13. Acknowledgments 56

Appendix A: Operating Instructions for the IBM 7030 SI (Fortran) Language Programme, REFORM 58
Appendix B: The IBM 7030 SI (Fortran) Language Programme, CHECK 60
Appendix C: Information Provided by the Data Listing Programme NBF PRINT 61

References 62

Figure 1: The Symbolic Card 37
Figure 2: A Nuclear Data File Card 63
Figure 3: Data Punching Sheet 64
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 AEGR Aldermaston to handle the vast quantities of data used in multi-group 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. AEGR 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 AEGR data in use at April 1960 is given in AEGR Report 0-28/60* [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 organization, the formats used and the present contents of the AEGR 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 programs. The main features of these programs are outlined here. It is planned to describe the full details of these programs 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 ANL 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 AERE neutronics programmes including STRATOM, an IBM 7030 $S_n$ code
[4] and MAGNE, 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 AERE
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 AERE
system in close collaboration with workers at AERE, Harwell and has been
designed for use with IBM 7030 and 7090 machines. The "Uninfrith Nuclear Data
Library and the associated 7090 machine programmes are described in a series
of AERE reports including "The "Uninfrith Nuclear Data Library" by H. F. James
[10] which parallels the present report. Other "Uninfrith reports will provide
DICE Mark IV is the whole complex that enables a neutron's fate at a collision,
it's subsequent mean free path and the position of its next collision to be
determined. COULD, 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 programs (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 ANRE series of reports which generally describe the 7030 version and the AERB series of reports which generally describe the 7090 version. Descriptions of data compilations such as references [1], [2] and [3] 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 (1:57) N.T.B. 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
1  Neutron cross-section
2  Neutron angular distribution
3  Neutron energy distribution
4  Miscellaneous quantities for neutrons ($\bar{\nu}$, $\eta$ etc)
5  Resolved resonance data for neutrons
6  Statistical data for unresolved neutron resonances
7  Thermal neutron scattering law data
8  Photon cross-section
9  Photon angular distribution
10  Photon secondary energy
11  Photon production angular distribution
12  Photon production secondary energy
13  Photon production multiplicity

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".  Roso = IBM "red stripe".
Particular Classification Numbers (P.C.N.)

Those are as follows:

1. Total
2. Elastic
3. Non-elastic (n 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 enters 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 \((y,2y)\) - pair production
17. \((n,3n)\)
18. Fission = \((n,\gamma)\) + \((n,n')\) + \((n,2n')\) + ------
19. \((n,\gamma)\) - no pro-fission evaporation or direct interaction neutrons
20. \((n,n')\) 2
21. \((n,2n')\)
22. \((n,n')\) 3
23. \((n,n')\) 3
24. \((n,2n)\) a
25. \((n,3n)\) a
26. \((n,2n)\) isomeric state
27-100 To be allocated
101. Parasitic absorption (or disappearance) - no secondary neutrons produced
102. \((n,\gamma)\) or \((\gamma,\alpha^-)\)
103. \((n,p)\)
104. \((n,4)\)
105. \((n,t)\)
106. \((n,He^3)\)
107. \((n,\alpha)\)
108. \((n,2\alpha)\)
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. \( \sigma_T = \sigma_T - \mu \sigma' \) where \( \mu \) 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], p.24.

202 \( \sigma_T \) - the product of the fission cross-section and the average number of neutrons per fission.

203 \( \sigma' \) - the product of the non-elastic cross-section and the average number of neutrons per non-elastic event. (also known as \( \sigma'_f \))

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 \((\Phi_o)\) 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 programs 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 FCN 201 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 FCN 206 labels the total transfer matrix and FCN 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 $^8\text{Be}^{12}$ the reaction $^8\text{Be}^{12}(n,n')$ has FCN 23 whilst the reaction $^8\text{Be}^{12}(n,n')$ $^8\text{Be}^{12} (\gamma)$ has FCN = 5 if the 4.43 MeV first excited state is considered. Similarly with $^{238}\text{U}$, FCN = 16 implies that $^{237}\text{U} + 2n$ 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 NANDC and the AEC Nuclear Cross Section Advisory Group [31].
It will be seen that ample P.D.N.'s remain for allocation should the Nuclear Data Library need extending.

**Examples of Reaction Type Number Allocation**

<table>
<thead>
<tr>
<th>Reaction Type</th>
<th>Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total cross-section for neutrons</td>
<td>1001</td>
</tr>
<tr>
<td>Elastic cross-section for neutrons</td>
<td>1002</td>
</tr>
<tr>
<td>Angular distribution of fission neutrons</td>
<td>2018</td>
</tr>
<tr>
<td>Secondary energy of ((n,2n)) reaction neutrons</td>
<td>3016</td>
</tr>
<tr>
<td>Mean number of neutrons per fission, (J)</td>
<td>4018</td>
</tr>
<tr>
<td>Ratio of capture to fission cross-section, (a)</td>
<td>4102</td>
</tr>
<tr>
<td>((y,2y)) cross-section</td>
<td>5016</td>
</tr>
<tr>
<td>Energy spectrum of photons produced in ((n,n')) continuum reaction</td>
<td>12015</td>
</tr>
<tr>
<td>Thermal scattering law data</td>
<td>7002</td>
</tr>
</tbody>
</table>

**Nuclide Identification Number (P.D.N.)**

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:-

<table>
<thead>
<tr>
<th>Label Field</th>
<th>Data Field</th>
</tr>
</thead>
<tbody>
<tr>
<td>001 - 999</td>
<td>001 - 999</td>
</tr>
<tr>
<td>100 - 999</td>
<td>1000 - 1099</td>
</tr>
<tr>
<td>1000 - 1999</td>
<td>1000 - 1199</td>
</tr>
<tr>
<td>200 - 999</td>
<td>1200 - 1299</td>
</tr>
<tr>
<td>2000 - 299</td>
<td>1300 - 1399</td>
</tr>
<tr>
<td>3000 - 399</td>
<td>1400 - 1499</td>
</tr>
<tr>
<td>4000 - 499</td>
<td>1500 - 1599</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>2000 - 299</td>
<td>2500 - 2599</td>
</tr>
</tbody>
</table>

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

-12-
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). Then 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 Nov. 1963

At 1st Nov. 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.
<table>
<thead>
<tr>
<th>N.I.N.</th>
<th>Element Isotope</th>
<th>Basic Data (Isotopes) Number</th>
<th>CHADY Group Constant (Isotopes) Number</th>
<th>Date of compilation, reference, energy range covered and comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>101</td>
<td>$^{235}$U</td>
<td>1/235</td>
<td>6</td>
<td>Spring 1959 [3] 0.025eV-114keV</td>
</tr>
<tr>
<td>102</td>
<td>$^{238}$U</td>
<td>1/238</td>
<td>6</td>
<td>Spring 1959 [3] 0.025eV-114keV</td>
</tr>
<tr>
<td>103</td>
<td>$^{239}$Pu</td>
<td>1/Pu239</td>
<td>8</td>
<td>Spring 1959 [3] 0.025eV-114keV</td>
</tr>
<tr>
<td>104</td>
<td>$^{240}$Pu</td>
<td>1/Pu240</td>
<td>7</td>
<td>Spring 1959 [3] 0.025eV-114keV</td>
</tr>
<tr>
<td>105</td>
<td>Allocated</td>
<td></td>
<td>6</td>
<td>November 1957 0.025eV-114keV</td>
</tr>
<tr>
<td>106</td>
<td>Fission Product</td>
<td>1/F.P.</td>
<td>6</td>
<td>June 1959 0.025eV-114keV</td>
</tr>
<tr>
<td>107</td>
<td>$^1$H</td>
<td>1/H</td>
<td>6</td>
<td>November 1957 [3] 0.025eV-114keV</td>
</tr>
<tr>
<td>108</td>
<td>$^1$D</td>
<td>1/D</td>
<td>6</td>
<td>November 1957 [3] 0.025eV-114keV</td>
</tr>
<tr>
<td>109</td>
<td>$^1$T(1)</td>
<td>1/T(1)</td>
<td>6</td>
<td>November 1957 [3] 0.025eV-114keV</td>
</tr>
<tr>
<td>110</td>
<td>$^2$He</td>
<td>1/He2</td>
<td>6</td>
<td>November 1957 [3] 0.025eV-114keV</td>
</tr>
<tr>
<td>111</td>
<td>$^4$He</td>
<td>1/He4</td>
<td>6</td>
<td>November 1957 [3] 0.025eV-114keV</td>
</tr>
<tr>
<td>112</td>
<td>Allocated</td>
<td></td>
<td>6</td>
<td>Spring 1959 0.025eV-114keV</td>
</tr>
<tr>
<td>113</td>
<td>Allocated</td>
<td></td>
<td>7</td>
<td>Spring 1959 0.025eV-114keV</td>
</tr>
<tr>
<td>114</td>
<td>$^9$Be</td>
<td>2/Be9</td>
<td>9</td>
<td>October 1959 [1] 0.025eV-114keV</td>
</tr>
<tr>
<td>115</td>
<td>Natural B</td>
<td>1/B</td>
<td>7</td>
<td>April 1957 [3] 0.025eV-114keV</td>
</tr>
<tr>
<td>116</td>
<td>$^{10}$B</td>
<td>1/B10</td>
<td>6</td>
<td>April 1957 [3] 0.025eV-114keV</td>
</tr>
<tr>
<td>117</td>
<td>Natural C</td>
<td>2/C</td>
<td>7</td>
<td>June 1960 [2] 0.025eV-114keV</td>
</tr>
<tr>
<td>118</td>
<td>Natural N</td>
<td>1/N</td>
<td>6</td>
<td>April 1957 [3] 0.025eV-114keV</td>
</tr>
<tr>
<td>119</td>
<td>Natural O</td>
<td>1/O</td>
<td>6</td>
<td>December 1956 [3] 0.025eV-114keV</td>
</tr>
<tr>
<td>120</td>
<td>$^{17}$Al</td>
<td>1/Al2</td>
<td>6</td>
<td>June 1957 [3] 0.025eV-114keV</td>
</tr>
<tr>
<td>121</td>
<td>Natural Si</td>
<td>1/Si</td>
<td>6</td>
<td>October 1958 [3] 0.025eV-114keV</td>
</tr>
<tr>
<td>122</td>
<td>$^{23}$Mg</td>
<td>1/Mg23</td>
<td>6</td>
<td>Spring 1959 [3] 0.025eV-114keV</td>
</tr>
<tr>
<td>123</td>
<td>$^{24}$Mg</td>
<td>1/Mg24</td>
<td>6</td>
<td>Spring 1959 1keV-114keV</td>
</tr>
<tr>
<td>124</td>
<td>$^{25}$Mg</td>
<td>1/Mg25</td>
<td>6</td>
<td>Spring 1959 1keV-114keV</td>
</tr>
<tr>
<td>125</td>
<td>Allocated</td>
<td></td>
<td>6</td>
<td>Spring 1959 1keV-114keV</td>
</tr>
<tr>
<td>126</td>
<td>Allocated</td>
<td></td>
<td>6</td>
<td>Spring 1959 1keV-114keV</td>
</tr>
<tr>
<td>127</td>
<td>Allocated</td>
<td></td>
<td>6</td>
<td>Spring 1959 1keV-114keV</td>
</tr>
<tr>
<td>128</td>
<td>$^{23}$Pu</td>
<td>1/Pu238</td>
<td>6</td>
<td>Autumn 1962 0.025eV-114keV</td>
</tr>
<tr>
<td>129</td>
<td>$^{24}$Pu</td>
<td>1/Pu241</td>
<td>6</td>
<td>Spring 1959 [2] 0.025eV-114keV</td>
</tr>
<tr>
<td>130</td>
<td>$^{237}$Np</td>
<td>1/Np237</td>
<td>6</td>
<td>1959 1000keV-114keV</td>
</tr>
</tbody>
</table>

-14-
<table>
<thead>
<tr>
<th>N.I.N.</th>
<th>Element Isotope and</th>
<th>Basic Data Mark Number</th>
<th>CANDY Group Constant Mark Number</th>
<th>Date of compilation, reference, energy range covered and comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>131</td>
<td>Ti$^{232}$</td>
<td>1/Ti232</td>
<td>6</td>
<td>Spring 1959 [3] 0.025eV-145eV</td>
</tr>
<tr>
<td>132</td>
<td>Natural Cr</td>
<td>1/Cr</td>
<td>6</td>
<td>October 1958 [3] 0.025eV-145eV</td>
</tr>
<tr>
<td>133</td>
<td>Natural Fe</td>
<td>1/Fe</td>
<td>6</td>
<td>February 1959 [3] 0.025eV-150eV</td>
</tr>
<tr>
<td>134</td>
<td>Natural Na</td>
<td>1/Na</td>
<td>6</td>
<td>October 1958 [3] 0.025eV-150eV</td>
</tr>
<tr>
<td>135</td>
<td>Natural Pb</td>
<td>1/Pb</td>
<td>6</td>
<td>August 1959 [3] 0.025eV-150eV</td>
</tr>
<tr>
<td>136</td>
<td>Natural Cl</td>
<td>1/Cl</td>
<td>6</td>
<td>November 1958 [3] 0.025eV-145eV</td>
</tr>
<tr>
<td>137</td>
<td>Au$^{197}$</td>
<td>1/Au197</td>
<td>6</td>
<td>December 1959 1keV-150eV (n,$\gamma$), (n,2n) Au$^{196}$ and (n,2n) Au$^{198}$ cross-sections only</td>
</tr>
<tr>
<td>138</td>
<td>Natural Ca</td>
<td>1/Ca</td>
<td>6</td>
<td>October 1959 [3] 0.025eV-145eV</td>
</tr>
<tr>
<td>139</td>
<td>Na$^{23}$</td>
<td>1/Na</td>
<td>6</td>
<td>October 1958 [3] 0.025eV-145eV</td>
</tr>
<tr>
<td>140</td>
<td>F$^{19}$</td>
<td>1/F</td>
<td>6</td>
<td>November 1957 [3] 0.025eV-145eV</td>
</tr>
<tr>
<td>141</td>
<td>Natural Cl</td>
<td>1/Cl</td>
<td>6</td>
<td>February 1959 [3] 0.025eV-150eV</td>
</tr>
<tr>
<td>142</td>
<td>Allocated</td>
<td></td>
<td>6</td>
<td>1959 0.025eV-150eV</td>
</tr>
<tr>
<td>143</td>
<td>Allocated</td>
<td></td>
<td>6</td>
<td>1959 0.025eV-150eV</td>
</tr>
<tr>
<td>144</td>
<td>Allocated</td>
<td></td>
<td>6</td>
<td>1959 0.025eV-150eV</td>
</tr>
<tr>
<td>145</td>
<td>Allocated</td>
<td></td>
<td>6</td>
<td>1959 0.025eV-150eV</td>
</tr>
<tr>
<td>146</td>
<td>Allocated</td>
<td></td>
<td>6</td>
<td>1959 0.025eV-150eV</td>
</tr>
<tr>
<td>147</td>
<td>Allocated</td>
<td></td>
<td>6</td>
<td>1959 0.025eV-150eV</td>
</tr>
<tr>
<td>148</td>
<td>Allocated</td>
<td></td>
<td>6</td>
<td>1959 0.025eV-150eV</td>
</tr>
<tr>
<td>149</td>
<td>Allocated</td>
<td></td>
<td>6</td>
<td>1959 0.025eV-150eV</td>
</tr>
<tr>
<td>150</td>
<td>Allocated</td>
<td></td>
<td>6</td>
<td>January 1962 0.025eV-150eV</td>
</tr>
<tr>
<td>151</td>
<td>Absorbutium</td>
<td>1/Abs</td>
<td>6</td>
<td>1961 0.025eV-150eV</td>
</tr>
<tr>
<td>152</td>
<td>T(2)</td>
<td>1/T(2)</td>
<td>6</td>
<td>November 1957 [3] 0.025eV-145eV</td>
</tr>
<tr>
<td>153</td>
<td>U$^{235}$</td>
<td>2/U235</td>
<td>1</td>
<td>CITON 1960-61 0.025eV-145eV</td>
</tr>
<tr>
<td>154</td>
<td>U$^{238}$</td>
<td>2/U238</td>
<td>1</td>
<td>CITON 1960-61 0.025eV-145eV</td>
</tr>
<tr>
<td>155</td>
<td>U$^{235}$</td>
<td>3/U235</td>
<td>7</td>
<td>December 1961 0.025eV-150eV</td>
</tr>
<tr>
<td>156</td>
<td>U$^{238}$</td>
<td>3/U238</td>
<td>7</td>
<td>December 1961 0.025eV-150eV</td>
</tr>
<tr>
<td>157</td>
<td>Allocated</td>
<td></td>
<td>7</td>
<td>March 1962 1keV-145eV</td>
</tr>
<tr>
<td>158</td>
<td>Allocated</td>
<td></td>
<td>7</td>
<td>March 1962 1keV-145eV</td>
</tr>
<tr>
<td>159</td>
<td>N$_2$O</td>
<td></td>
<td>6</td>
<td>1957 No basic data. Group cross-sections only</td>
</tr>
<tr>
<td>N.I.N.</td>
<td>Isotopes etc</td>
<td>Basic Data</td>
<td>CANDY Group Constant Lark Number</td>
<td>Date of compilation, references, energy range covered and comments</td>
</tr>
<tr>
<td>-------</td>
<td>--------------</td>
<td>------------</td>
<td>---------------------------------</td>
<td>------------------------------------------------------------------</td>
</tr>
<tr>
<td>160</td>
<td>$D_2O$</td>
<td>6</td>
<td>1957 No basic data. Group cross-sections only</td>
<td></td>
</tr>
<tr>
<td>161</td>
<td>Allocated</td>
<td>-</td>
<td>1957 No basic data. Group cross-sections only</td>
<td></td>
</tr>
<tr>
<td>162</td>
<td>Allocated</td>
<td>-</td>
<td>1957 No basic data. Group cross-sections only</td>
<td></td>
</tr>
<tr>
<td>163</td>
<td>U$^{235}$</td>
<td>3A/0235</td>
<td>7 June 1962 0.025MeV-15MeV Adjusted</td>
<td></td>
</tr>
<tr>
<td>164</td>
<td>U$^{235}$</td>
<td>3A/0238</td>
<td>7 June 1962 0.025MeV-15MeV Acts from</td>
<td></td>
</tr>
<tr>
<td>165</td>
<td>U$^{235}$</td>
<td>3B/0238</td>
<td>7 June 1962 0.025MeV-15MeV 3/0238 and</td>
<td></td>
</tr>
<tr>
<td>166</td>
<td>U$^{238}$</td>
<td>3C/0238</td>
<td>7 June 1962 0.025MeV-15MeV 3/0238 and</td>
<td></td>
</tr>
<tr>
<td>167</td>
<td>Allocated</td>
<td>-</td>
<td>August 1962 1keV-15keV</td>
<td></td>
</tr>
<tr>
<td>168</td>
<td>Allocated</td>
<td>-</td>
<td>7 April 1962 0.025keV-112keV</td>
<td></td>
</tr>
<tr>
<td>169</td>
<td>Allocated</td>
<td>-</td>
<td>8 April 1962 0.025keV-112keV</td>
<td></td>
</tr>
<tr>
<td>170</td>
<td>Allocated</td>
<td>-</td>
<td>August 1962 1keV-15keV</td>
<td></td>
</tr>
<tr>
<td>171</td>
<td>Allocated</td>
<td>-</td>
<td>August 1962 1keV-15keV</td>
<td></td>
</tr>
<tr>
<td>172</td>
<td>Thin Air</td>
<td>1/Thin Air</td>
<td>- September 1962 0.025MeV-15MeV</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Approximates a vacuum</td>
<td></td>
</tr>
<tr>
<td>173</td>
<td>U$^{238}$</td>
<td>2/0236</td>
<td>- August 1962 1keV-15keV</td>
<td></td>
</tr>
<tr>
<td>174</td>
<td>U$^{238}$</td>
<td>2/0234</td>
<td>- August 1962 1keV-15keV</td>
<td></td>
</tr>
<tr>
<td>175</td>
<td>Allocated</td>
<td>-</td>
<td>May 1963 0.001keV-15keV</td>
<td></td>
</tr>
<tr>
<td>176</td>
<td>Allocated</td>
<td>-</td>
<td>May 1963 0.001keV-15keV</td>
<td></td>
</tr>
<tr>
<td>177</td>
<td>Allocated</td>
<td>-</td>
<td>No data, used only to identify reaction product</td>
<td></td>
</tr>
<tr>
<td>178</td>
<td>Pa$^{212}$</td>
<td>-</td>
<td>No data, used only to identify reaction product</td>
<td></td>
</tr>
<tr>
<td>179</td>
<td>Zr</td>
<td>1/Zr</td>
<td>May 1963* 0.025MeV-15MeV</td>
<td></td>
</tr>
<tr>
<td>180</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>181</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>182</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>183</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>184</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>185</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>186</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>187</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Data supplied by P. J. Hurnings of the Authority Health and Safety Branch, Risley.
Table 1 (continued)

<table>
<thead>
<tr>
<th>N.I.N.</th>
<th>Element</th>
<th>Isotope etc.</th>
<th>Basic Data Mark Number</th>
<th>CANDY Group Constant Mark Number</th>
<th>Date of compilation, reference, energy range covered and comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>188</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>189</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>190</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>191</td>
<td>H</td>
<td>1/2 H G</td>
<td>1</td>
<td>April 1964 [12] Photon cross-sections 0.01-20 MeV</td>
<td></td>
</tr>
<tr>
<td>192</td>
<td>Be</td>
<td>1/Be G</td>
<td>1</td>
<td>April 1964 [12] Photon cross-sections 0.01-20 MeV</td>
<td></td>
</tr>
<tr>
<td>193</td>
<td>C</td>
<td>1/C G</td>
<td>1</td>
<td>April 1964 [12] Photon cross-sections 0.01-20 MeV</td>
<td></td>
</tr>
<tr>
<td>194</td>
<td>N</td>
<td>1/N G</td>
<td>1</td>
<td>April 1964 [12] Photon cross-sections 0.01-20 MeV</td>
<td></td>
</tr>
<tr>
<td>195</td>
<td>O</td>
<td>1/O G</td>
<td>1</td>
<td>April 1964 [12] Photon cross-sections 0.01-20 MeV</td>
<td></td>
</tr>
<tr>
<td>196</td>
<td>Al</td>
<td>1/Al G</td>
<td>1</td>
<td>April 1964 [12] Photon cross-sections 0.01-20 MeV</td>
<td></td>
</tr>
<tr>
<td>197</td>
<td>Fe</td>
<td>1/Fe G</td>
<td>1</td>
<td>April 1964 [12] Photon cross-sections 0.01-20 MeV</td>
<td></td>
</tr>
<tr>
<td>198</td>
<td>Pb</td>
<td>1/Pb G</td>
<td>1</td>
<td>April 1964 [12] Photon cross-sections 0.01-20 MeV</td>
<td></td>
</tr>
<tr>
<td>199</td>
<td>U</td>
<td>1/U G</td>
<td>1</td>
<td>April 1964 [12] Photon cross-sections 0.01-20 MeV</td>
<td></td>
</tr>
<tr>
<td>200</td>
<td>Pu</td>
<td>1/Pu G</td>
<td>1</td>
<td>April 1964 [12] Photon cross-sections 0.01-20 MeV</td>
<td></td>
</tr>
</tbody>
</table>

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.

-17-
(d) Absorptium has an atomic weight of 8.0, a total cross-section of 1000 barns, an $(n,\gamma)$ 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.L.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 AECL Chilton. 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" program 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>
<thead>
<tr>
<th>N.I.N.</th>
<th>Element Isotope, etc.</th>
<th>Basic Data Mark Number</th>
<th>Date of compilation, reference, energy covered and comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>U²³⁵</td>
<td>4/0235</td>
<td>Not allocated</td>
</tr>
<tr>
<td>2</td>
<td>Pu²³⁹</td>
<td>2/0239</td>
<td>Spring 1963 0.005eV-15MeV. As NIN 101 above 6eV</td>
</tr>
<tr>
<td>3</td>
<td>Xe¹³⁵</td>
<td>1/Xe135</td>
<td>Spring 1962 [11] 0.01eV-1keV. Data compiled at AEE Winfrith. Temperature = 293°K</td>
</tr>
<tr>
<td>4</td>
<td>U²³⁸</td>
<td>4/0238</td>
<td>Spring 1963 0.0001eV-15MeV. As NIN 102 above 1.75keV</td>
</tr>
<tr>
<td>5</td>
<td>Natural C</td>
<td>5/C</td>
<td>Spring 1963 0.0001eV-15MeV. As NIN 117 above 1keV</td>
</tr>
<tr>
<td>6</td>
<td>Be⁰</td>
<td>1/Be⁰</td>
<td>Spring 1963 0.001eV-1keV</td>
</tr>
<tr>
<td>7</td>
<td>Be⁹</td>
<td>3/Be⁹</td>
<td>Spring 1963 0.001eV-15MeV. As NIN 114 above 10keV</td>
</tr>
<tr>
<td>8</td>
<td>U²³³</td>
<td>2/U233</td>
<td>Data not yet available</td>
</tr>
<tr>
<td>9</td>
<td>Natural H</td>
<td>2/H</td>
<td>Spring 1963 0.003eV-14MeV. As NIN 107 above 0.15eV</td>
</tr>
<tr>
<td>10</td>
<td>D</td>
<td>2/D</td>
<td>Spring 1963 0.001eV-14MeV. As NIN 108 above 1keV</td>
</tr>
<tr>
<td>11</td>
<td>Na²³</td>
<td>2/Na</td>
<td>Spring 1963 0.01eV-14MeV. Based on data of Schmidt [13]. Reported in [32]</td>
</tr>
<tr>
<td>12</td>
<td>B¹⁰</td>
<td>2/B10</td>
<td>Spring 1963 0.001eV-14MeV. As NIN 116 above 1eV</td>
</tr>
<tr>
<td>13</td>
<td>Natural N</td>
<td>2/N</td>
<td>Spring 1963 0.001eV-14MeV. As NIN 116 above 1eV</td>
</tr>
<tr>
<td>14</td>
<td>Natural B</td>
<td>2/B</td>
<td>Spring 1963 0.001eV-14MeV. As NIN 115 above 1eV</td>
</tr>
<tr>
<td>15</td>
<td>Al²⁷</td>
<td>2/Al</td>
<td>Spring 1963 0.0005eV-14MeV. As NIN 120 above 1eV</td>
</tr>
<tr>
<td>16</td>
<td>Natural Cr</td>
<td>2/Cr</td>
<td>Spring 1963 0.0001eV-14MeV. As NIN 132 above 0.05eV</td>
</tr>
<tr>
<td>17</td>
<td>Natural Fe</td>
<td>2/Fe</td>
<td>Spring 1963 0.001eV-15MeV. As NIN 133 above 0.05eV</td>
</tr>
<tr>
<td>18</td>
<td>Natural Ni</td>
<td>2/Ni</td>
<td>Spring 1963 0.001eV-14MeV. As NIN 134 above 1eV</td>
</tr>
<tr>
<td>19</td>
<td>Natural O</td>
<td>2/O</td>
<td>Spring 1963 0.0001eV-14MeV. As NIN 119 above 1eV. (n,γ) cross-section added below 1eV.</td>
</tr>
<tr>
<td>20</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N.I.N.</td>
<td>Isotope, etc</td>
<td>Basic Data Mark Number</td>
<td>Date of compilation, reference, energy range and comments</td>
</tr>
<tr>
<td>-------</td>
<td>-------------</td>
<td>------------------------</td>
<td>--------------------------------------------------------</td>
</tr>
<tr>
<td>21</td>
<td>Au¹⁹⁷</td>
<td>2/au197</td>
<td>Data not yet available</td>
</tr>
<tr>
<td>22</td>
<td>C²³²</td>
<td>2/th232</td>
<td>Spring 1963 0.00001eV-1412eV, As NIN 131 above 1eV</td>
</tr>
<tr>
<td>23</td>
<td>P⁹¹</td>
<td>2/P</td>
<td>Spring 1963 0.0001eV-142eV, As NIN 140 above 1eV</td>
</tr>
<tr>
<td>24</td>
<td>C¹³</td>
<td>2/C</td>
<td>Spring 1963 0.0001eV-142eV, As NIN 136 above 1eV</td>
</tr>
<tr>
<td>25</td>
<td>Si</td>
<td>2/Si</td>
<td>Spring 1963 0.0001eV-142eV, As NIN 121 above 0.4eV</td>
</tr>
<tr>
<td>26</td>
<td>Pb</td>
<td>2/Pb</td>
<td>Spring 1963 0.00001eV-1512eV, As NIN 155 above 0.1eV</td>
</tr>
<tr>
<td>27</td>
<td>H₂O</td>
<td>2/H2O</td>
<td>Spring 1963 0.00006eV-0.5eV</td>
</tr>
<tr>
<td>28</td>
<td>D₂O</td>
<td>2/D2O</td>
<td>Spring 1963 0.00005eV-9.0eV</td>
</tr>
<tr>
<td>29</td>
<td>Pu₂₄¹</td>
<td>2/Pu241</td>
<td>Spring 1963 0.0001eV-142eV, As NIN 104 above 1.2eV</td>
</tr>
<tr>
<td>30</td>
<td>Pu²₄¹</td>
<td>2/Pu241</td>
<td>Data not yet available</td>
</tr>
<tr>
<td>31</td>
<td>H²⁺</td>
<td>2/H4</td>
<td>Spring 1963 0.0001eV-142eV, As NIN 111 above 0.005eV</td>
</tr>
<tr>
<td>32</td>
<td>H²⁺</td>
<td>2/H2⁺</td>
<td>Spring 1963 0.0001eV-142eV, As NIN 110 above 1eV</td>
</tr>
<tr>
<td>33</td>
<td>Cl</td>
<td>2/Cl</td>
<td>Data not yet available</td>
</tr>
<tr>
<td>34</td>
<td>Ca</td>
<td>2/Ca</td>
<td>Data not yet available</td>
</tr>
</tbody>
</table>

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 NUL 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:

-29-
(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. These 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 normalized probability distribution for scattering
as a function of cosθ 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 keV) 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 in 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 = 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 0.001 keV - 14 keV, then with point-wise representation the first angular distribution must be for energy 0.001 keV and the last for 14 keV; for range-wise representation the lower energy boundary of the first range must be 0.001 keV and the upper energy boundary of the last range must be 14 keV.

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 \( k (E_0 - E_q) \), where \( k \) is a constant (the reduction factor), \( E_0 \) is the initial energy and \( E_q \) 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

\[
p \left( \frac{\nu}{E_0} \right) = f \left( \frac{\nu}{E_0} \right) \left( \frac{\nu}{E_0} \right)^q
\]

where \( f \) is some function and \( E_0 \) 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 nuclides. It is given by the normalised probability function

\[
N(\nu) = a \left( \frac{\nu}{E} \right)^2 \exp \left( -\frac{\nu}{E} \right) + (1-a) \left( \frac{2}{\pi} \right)^{\frac{1}{2} E^{\frac{3}{2}}} \left[ \frac{\nu}{E} \right]^\frac{1}{2} \exp \left( -\frac{\nu}{E} \right)
\]

with \( B = a + b \left( \frac{\nu}{E_0} + 1 \right)^\frac{1}{2} \)

\[
\alpha = \frac{\sigma_{nn'} + \sigma_{n2n'}}{\nu (\sigma_{nn'} + \sigma_{nn'} + \sigma_{n2n'})}
\]

\[
T = c \frac{\nu}{E_0} \left( 1 - \frac{E_0}{E} \right)
\]

where \( a, b, c \) are constants

\( \nu \) is the mean number of neutrons per fission

\( \Sigma_f \) is the threshold for the \((n,n')\) reaction

\( E_0 \) is the initial energy (all energies in MeV)

\( \sigma_{nn'}, \sigma_{nn'} \) and \( \sigma_{n2n} \) are the cross sections for the \((n,f)\) \((n,n')\) and \((n,2n)\) reactions

It will be seen that law 7 is specified by four parameters \( a, b, c \) and \( \Sigma_f \) (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 - \(\bar{n}, n, \sigma\), etc.

These include

- \(n\), the number of secondaries per collision (elastic and non-elastic)
  \[
  n = (\sigma_n + \sigma_n' + 2\sigma_{2n} + 3\sigma_{3n} + \bar{\nu} \sigma_\ell + \ldots) / \sigma_T
  \]

- \(\eta\), the number of secondaries per non-elastic event
  \[
  \eta = (\sigma_n' + 2\sigma_{2n} + 3\sigma_{3n} + \bar{\nu} \sigma_\ell + \ldots) / \sigma_X
  \]

- \(\alpha = \sigma_0 / \sigma_T\)

- \(\bar{\nu}\), 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.

\( \tilde{\nu} \) 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 \( \tilde{\nu} \) versus energy.

The energy points at which \( \tilde{\nu} \) 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 \( \tilde{\nu} \). This means that when \( \tilde{\nu} \) of is formed interpolation in \( \tilde{\nu} \) will generally be necessary.

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

It should be noted that, whilst \( \tilde{\nu} \) is given in the library for all fissile nuclides, specification of \( n \), \( \eta \) and \( a \) 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.
(b) Breit-Wigner formula for $\ell = 0$ neutrons and many levels when elastic scattering and radiative capture are the only important processes.

(c) The Bohr-Weiszäcker 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 $\ell$ in the case when only elastic scattering need be considered.

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

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 $\ell$ allowed) can be written in the form, for a reaction proceeding through a single isolated resonance $\lambda$ of spin $J$ and definite parity

$$\sigma_{\ell\ell'} = \frac{\hbar^2}{8\pi^2} \frac{E\Gamma_{\lambda\ell}}{E_{\lambda}^2} \left( \frac{E'\Gamma_{\lambda\ell'}}{E_{\lambda}^2} \right)$$

where the primed sums $\ell_1$, $\ell_2$ are such that

$$\ell + s = \tilde{J} = \ell' + s'$$

-27-
and parity is conserved

\[
\sigma_{aa} = \frac{\pi}{k_a} \left\{ \sum_{\lambda \sigma} \Gamma_{\lambda\sigma} \sin^2 \theta_0 \right\}
\]

\[
\sigma_{a'a'} = -\frac{\pi}{k_a} \sum_{\lambda \sigma} \Gamma_{\lambda\sigma} \left[ \frac{2 \left( \Delta_\lambda + \Delta_\lambda - 2 \right) \sin 2 \theta_0 + \Gamma_\lambda (1 - \cos 2 \theta_0)}{(E_\lambda + \Delta_\lambda - E)^2 + \frac{1}{\Gamma_\lambda^2}} \right]
\]

\[
-\frac{\Gamma_{\lambda\sigma} \Gamma_{\lambda'\sigma'}}{s E}, \quad \frac{s'}{s}, \quad \frac{\Gamma_{\lambda\sigma} \Gamma_{\lambda'\sigma'}}{(E_\lambda + \Delta_\lambda - E)^2 + \frac{1}{\Gamma_\lambda^2}}
\]

(3)

In the formulae

- \( a \) and \( a' \) denote ingoing and outgoing channels respectively so that \( \sigma_{aa} \) is the elastic scattering cross-section.
- \( k_a \) is the wave number for the ingoing channel.
- \( \delta_j = \frac{2I+1}{2(2I+1)} \) is the spin statistical factor.
- \( I \) is the spin of the target nucleus.
- \( J \) is the composite nucleus level \( \lambda \).
- \( s \) is the channel spin \( I \pm \frac{1}{2} \).
- \( \delta_\sigma \) is the hard sphere scattering phase and is independent of \( \sigma \) and \( J \).
- \( E_\lambda \) is an eigenvalue for the internal region.
- \( \Gamma_{\lambda\sigma} \) is the shift factor for the level \( \lambda \).
- \( \Gamma_{\lambda\sigma} \Gamma_{\lambda'\sigma'} \) are level widths for the level \( \lambda \).
- \( \Gamma_\lambda = \Gamma_{\lambda\sigma} \Gamma_{\lambda'\sigma'} \)

The more familiar forms are obtained by a special choice of the boundary conditions for the eigenfunctions corresponding to the \( E_\lambda \).
This gives $E_{\gamma} + \Delta_{\gamma}(E_{\gamma}) = E_{\gamma}$, where $E_{\gamma}$ is the observed resonance energy. We note that, in general, $\Delta_{\gamma}$ is a function of energy as is $\Gamma_{\gamma\gamma}$.

If $J$ is fixed and $\ell = 0$ there is only one value of $\epsilon$ whilst if the internal interaction (nuclear potential) is represented by a square well then $\epsilon_0 = k_{\alpha}a$ for $\epsilon = 0$, where $a$ is the scattering length (or channel radius).

Expanding $E_{\gamma} + \Delta_{\gamma} - E$ about the observed resonance energy $E_{\gamma}$ and setting $\epsilon = 0$, $\sin^2 \theta_0 = k_{\alpha}^2a^2$, we obtain the well known formulae for the contribution to the cross-section from a single resonance

$$\sigma_{\gamma\gamma} = \pi \lambda_{\gamma\gamma} \frac{\Gamma_{\gamma\gamma}^2}{\left(2E_{\gamma}\right)^2 + \Gamma_{\gamma\gamma}^2/4}$$

$$\sigma_{\gamma\gamma} = \pi \lambda_{\gamma\gamma} \frac{\Gamma_{\gamma}}{\left(2E_{\gamma}\right)^2 + \Gamma_{\gamma}^2/4}$$

$$\Gamma = \frac{2\Gamma_{\gamma}}{\pi}$$

$x$ covers emission of gamma radiation or particles. $\lambda$ is the reduced wavelength (centre of mass system).

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

$I, J, E_{\gamma}$

$a$

$\Gamma_{\gamma}$, $\Gamma_{\gamma}$ (all $x$), $\Gamma$ - all evaluated at $E_{\gamma}$.
Additionally it is necessary to know how the partial widths vary with energy - the usual assumption is that \( \Gamma_n \) is independent of energy whilst \( \Gamma_n^Y \) is the reduced neutron width (corresponding to the value of \( \Gamma_n \) at \( E = 1 \text{eV} \)) so that \( \Gamma(E) = \Gamma_n^Y \alpha + \Gamma_n^Y \) 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 \( \Gamma_n \) on energy slightly.

(b) Breit-Wigner Formula for \( E = 0 \) 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

\[
\sigma_{el} = 4\pi a^2 + \pi k^2 g_J \left\{ \sum \frac{\Gamma_n^2}{(E-E_r)^2 + \Gamma_n^2/4} \right\}
\]

\[
+ \sum_f \sum_{\pi^f} \frac{2 \Gamma_n^\pi \Gamma_n}{(E-E_r)^2 + \pi f^2} \left[ (E-E_R^{\pi f}) + (E-E_R^{\pi f}) \right]
\]

\[
\sigma_{nr} = \pi k^2 g_J \sum \frac{\Gamma_n^{\pi f}}{(E-E_r)^2 + \Gamma_n^2/4}
\]

-30-
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-Hoore Formula — a Multilevel Formula with Few Fission Channels for \( \ell = 0 \) Neutrons

The theory is given by Reich and Hoore [16] and has been applied to U233 [17], U235 [18] and Pu239 [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

\[
\sigma_\text{e} = 2\pi \kappa^2 \bar{s}_J R_F (1 - S_{11}) \tag{9}
\]

\[
\sigma_n = \pi \kappa^2 \bar{s}_J |1 - S_{11}|^2 \tag{10}
\]

\[
\sigma_f = \pi \kappa^2 \bar{s}_J (|S_{12}|^2 + |S_{13}|^2) \tag{11}
\]

The expressions for \( S_{11}, S_{12}, S_{13} \) 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.

\( R_\lambda \) (not necessarily equal to \( R_f \))

-31-
\( \Gamma_\lambda, \epsilon(=0), I \)

\( \Gamma_{\lambda\nu} \) the total width

\( \Gamma_{\lambda\nu} \) the neutron width

\( \Gamma_{\lambda\nu} \) the radiation width

\( \Gamma_{\lambda \nu} \) the fission width

\( \beta_{\lambda 2} \) and \( \beta_{\lambda 3} \)

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

\[ |\beta_{\lambda 1}| = (\frac{\Gamma_{\lambda\nu}}{\epsilon})^{\frac{1}{2}} \]  \hspace{1cm} (12)

\[ \Gamma_{\lambda \nu} = 2(\beta_{\lambda 2}^2 \beta_{\lambda 3}^2) \]  \hspace{1cm} (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.

(4) The Vogt Many Channel, Few Level Formula for \( \epsilon = 0 \) Neutrons

The theory is given by Vogt [20] and has been applied to U235, U235 and Fu239 [20] [21]; it was developed to account for the low energy cross-sections of fissile nuclides. Reference [20] gives formulae for elastic, \((n,\gamma)\) and fission cross-sections.

For each resonance \( \lambda \) the following quantities provide a complete specification of the cross-section

\( \Xi_\lambda \) (not necessarily equal to \( \Xi_\nu \))

\( \Gamma_\lambda, \Gamma_{\lambda\nu}, \Gamma_{\lambda \nu} \)

-52-
A c-dimensional vector $g_{\lambda r}$ where c is the number of fission channels - alternatively one need only specify the angles between all pairs $g_{\lambda r} g_{\lambda' r'}$ since $|g_{\lambda r}|^2 = \Gamma_{\lambda r'}$

For simplicity it is probably better to specify the c components of the $g_{\lambda r}$ for each $\lambda$. As in the case of the Reich-Worel formula $1/\nu$ 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 Hidaka

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 $\Gamma \approx \Gamma_{\text{el}}$. The formula for the scattering cross section then becomes (in the case when level widths are much less than spacings)

$$\sigma_{\text{el}} = 4\pi k^2 \sum_r \sum_{\ell} \sum_{\ell'} \frac{1}{2} \Gamma_{\ell} \left( \frac{1}{2} \right) \sin \phi_{\ell} \left( \sin \phi_{\ell'} \right)$$

where $r$ denotes a particular level corresponding to known values of $J$ and $\ell$. $\Gamma_{\ell}$ is the (total) width for resonance $r$ whilst $\phi_{\ell}$ is the hard sphere phase for neutrons of angular momentum $\ell$ on the square well model.

(14) expands into the form (for group of levels having same $\ell$ and $J$)

$$\sigma_{\text{el}} = \sum_{\ell} \left( \frac{\Gamma_{\ell}}{2} \right) |g_{\ell r}|^2 \right) \left( \frac{1}{2} \right) \sin \phi_{\ell} \left( \sin \phi_{\ell'} \right)$$

$$+ \pi k^2 \left( \frac{1}{2} \right) \sum_r \frac{\Gamma_{\ell} \left( \sin \phi_{\ell} \right)}{(2m)^2 + \frac{1}{2} \Gamma_{\ell}^2}$$

$$+ \sum_r \sum_{\ell} \sum_{\ell'} \frac{2\Gamma_{\ell} \Gamma_{\ell'}}{(2m)^2 + \frac{1}{2} \Gamma_{\ell}^2} \left( \frac{1}{2} \right) \sin \phi_{\ell} \left( \sin \phi_{\ell'} \right)$$

$$\left( \phi_{\ell}, \phi_{\ell'} \right) = \left( 2m \right)^2 + \frac{1}{2} \Gamma_{\ell}^2 + \frac{1}{2} \Gamma_{\ell'}^2$$

$$\left[ \frac{1}{2} \Gamma_{\ell} \Gamma_{\ell'} \left( 2m \right)^2 + \frac{1}{2} \Gamma_{\ell'}^2 \right]$$

$$\left( 2m \right)^2 + \frac{1}{2} \Gamma_{\ell}^2 + \frac{1}{2} \Gamma_{\ell'}^2$$

$$-33-$$
There is a fairly obvious relation between (15) and (7).
This formula requires the specification of the following parameters for each resonance
\[ \frac{E_r}{1}, J, \ell \]
\[ \Gamma_r \]
\[ \phi_\ell \] for all \( \ell \) values.
In fact \( \phi_\ell \) may be computed from theoretical formulas based on the square well potential model.

Hidde has applied (15) to analyze resonances in aluminum [22] and in sodium [23].

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

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

\[
\sigma_{nn} = \sum_\ell (2\ell+1) 4\pi \lambda^2 \sin^2 \phi_\ell \]
\[ + \pi \lambda^2 \xi \frac{\Gamma_r^2 - 2\Gamma_r \Gamma \sin^2 \phi_\ell + 2\Gamma (2-2\xi) \sin 2\phi_\ell}{(2-2\xi)^2 + \frac{\Gamma^2}{\Gamma_r}} \]

(16)

\[
\sigma_{nx} = \pi \lambda^2 \xi \frac{\Gamma_r \Gamma x}{(2-2\xi)^2 + \frac{\Gamma^2}{\Gamma_r}} \]

(17)

with \( \Gamma = \Gamma_r + \frac{\Gamma_x}{2} \)

(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 Low Data

Thermal scattering low 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 \( \alpha = [E + E' - 2(E')^{1/2} \cos \theta]/\hbar kT \) and \( \beta = (E' - E)/\hbar kT \). \( E \) is the initial neutron energy, \( E' \) is the final energy and \( \theta \) is the laboratory scattering angle so that \( \alpha \) and \( \beta \) 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

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

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 \( \theta \) is given by

\[
\sigma(E-E', \theta) dE'dcos\theta = \frac{d^2}{2kT} \int \frac{d^2}{dE'dcos\theta} \exp(-\beta/2) S(\alpha, \beta) dE'dcos\theta
\]

\[\beta = \frac{(E' - E)/\hbar kT}{2/kT} \]
where $\sigma_b$ is the bound atom cross-section.

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

where $\sigma_f$ is the free atom cross-section.

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

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

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

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

where $S^*(a, \beta)$ and $\lambda$ are specified in the files.

Two further points require consideration. Firstly in the case of molecules the effective mass (ratio) used to define $a$ is somewhat arbitrary 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.H. = 1002) and the secondary energy distribution is computed using the monatomic gas law of $S(a, \beta)$. 

-36-
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.

<table>
<thead>
<tr>
<th>Field 1</th>
<th>Field 2</th>
<th>Field 3</th>
<th>Field 4</th>
<th>Field 5</th>
<th>Field 6</th>
<th>Label Field 1</th>
<th>Label Field 2</th>
<th>Label Field 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>M.I.M.</td>
<td>Section</td>
<td>Serial</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>No.</td>
<td>No.</td>
<td>No.</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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 fields. Punching is facilitated by using the special data punching sheet shown in figure 3.

-37-
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 (nuclides) 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:

<table>
<thead>
<tr>
<th>Heading cards</th>
<th>Section 00</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neutron data</td>
<td></td>
</tr>
<tr>
<td>01 1001</td>
<td>Total cross-section</td>
</tr>
<tr>
<td>02 1002</td>
<td>Elastic cross-section</td>
</tr>
<tr>
<td>03 2002</td>
<td>Elastic angular distribution</td>
</tr>
<tr>
<td>04 1003</td>
<td>Non-elastic cross-section</td>
</tr>
<tr>
<td>05 1004</td>
<td>( (n, n') ) total cross-section</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Photon interaction data</td>
<td></td>
</tr>
<tr>
<td>X0 8001</td>
<td>Total cross-section</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Photon production data</td>
<td></td>
</tr>
<tr>
<td>W7 11005</td>
<td>Photon production angular</td>
</tr>
</tbody>
</table>

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 peaks 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 identifies the isotope, element or mixture referred to by the data and is identical with the number punched in columns 75-75 (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.

* For further details about nuclide identification numbers see section 2.2
Atomic and Molecular Weights

These are specified as fixed point decimal numbers (10.6) so that for \( ^{238}U \) we have \( A = 238.050760 \). The physical scale in which \( a = 12.000000 \) is used.* Values of \( A \) are given by Kühig 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 Avogadro's number. This is a \( N_0 = 6.02295 \times 10^{23} = 6.023 \times 10^{23} \) for normal purposes since the accuracy of density does not justify more figures.

7. Representation of Neutron Interaction Data on Punched Cards

7.1 Neutron Cross Sections (G.C.H.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 temperature dependence of the cross-sections is not considered this field contains 1.

*Most of the existing data has atomic and molecular weights referred to \( \lambda(0^\circ) = 16.000000 \).
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 31 (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.H.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

1 - Data for centre of mass system
2 - Data for laboratory system.
5,6 Additional information if required.

Card 2

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.J)

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.

-44-
Law 2
Card 3 Field 1 Number of pairs (discrete energy loss, reduction factor) to be considered.
   2 Discrete energy loss ($\nu_d$)
   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 "d"

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

-45-
7.4 Miscellaneous 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, \( \varepsilon = 0 \)
    neutrons, isolated resonance
5152 Single level Breit-Wigner formula for \( \varepsilon = 0 \)
    neutrons and many levels for elastic scattering and radiative capture.
5153 Breit-Wigner 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.

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 \( \Gamma_n^{\text{r}} \), \( \Gamma_x \) etc.
   are to vary with energy
   - e.g., 1 means \( \Gamma_n^{\text{r}} = \Gamma_n^{\text{r, fixed}} \) and \( \Gamma_x \text{ fixed} \) (\( \Gamma_n^{\text{r, fixed}} \) is the reduced neutron width = value at resonance divided by \( Z_n \))
5 A fixed point number indicating the partial widths which are specified and their order on cards 4, 5 etc.
   1 = \( \Gamma_n^{\text{r}} \), \( \Gamma_x \)
   2 = \( \Gamma_n^{\text{r}} \), \( \Gamma_x \), \( \Gamma_x \)
   3 = \( \Gamma_n \)
   etc.
6 Additional information if required

Card 4 Field 1 Energy in MeV
2 Value (barns) of additional \( 1/\nu \) component of elastic cross-section at this energy
3 Energy in MeV
Card 4 Field 4 Value (barns) of additional 1/τ component of first partial non-elastic cross-section at this energy.

5) Similar information for same reactions and in 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 Εₚ, the resonance energy (MeV)

2 J, the angular momentum of the compound nucleus

3 Γ, the total width evaluated at Εₚ

4 onwards Values of the partial widths evaluated at Εₚ (going on to cards 5, 6 etc. 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 raw card. In the most frequently occurring cases the information for one resonance will only occupy one card.

RTN = 5151

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 Γₜₜ', Γₖₖ', Γₕₕ' etc are to vary with energy

   e.g. 1 means Γₜₜ' = Γₜₜ' √E

   Γₖ₂, Γₖ₂', Γₖ₅ 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 $E_\lambda$ (MeV)
2 $J$, the orbital angular momentum of the compound nucleus
3 $\Gamma_\lambda$, the total width evaluated at $E_\lambda$
4 $\Gamma_{\lambda n}$, the neutron width evaluated at $E_\lambda$
5 $\Gamma_{\lambda r}$, the radiative width evaluated at $E_\lambda$
6 $\Gamma_{\lambda f}$, the total fission width evaluated at $E_\lambda$

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 $\beta_{\lambda \ell}$ 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.
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 \(I^R\) varies with energy for given \(J, \ell\)
5 A fixed point number indicating how \(\phi_e\) 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 \(\ell\) for which \(\phi_e\) is needed in this energy range
2 Energy below which \(\phi_1\) is negligible
3 Energy below which \(\phi_2\) is negligible

Card 5 Field 1 \(E_R\), the resonance energy (MeV)
2 \(J\)
3 \(\ell\)
4 \(I^R\)
5, 6 etc. Values of \(\phi_0, \phi_1, \ldots, \phi_{e\max}\) 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 (G.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  $\sigma_0$, the free atom cross-section

4  $\alpha$, 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  $E_0$, the upper energy limit for constant $\sigma_0$. Above
this energy $\sigma_0$ ($RTN = 1002$) must be used in
conjunction with the monotonic gas law.

Card 2  Field 1  Material temperature (degrees absolute) to which
scattering law data is appropriate (leave 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 $\beta$ 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  $\lambda$ the parameter in the $\delta$ - function contribution
e$^{-\lambda\alpha}$ $\delta(\beta)$ to $S(\alpha, \beta)$. If there is no contribution
from this term then $\lambda$ is set equal to zero.

6  Additional information if required

Card 3 onwards contains

$\beta_i$  The $i$th $\beta$ value, $\beta$ values being given in ascending
order

$n_i$  The number of $\alpha$ values corresponding to $\beta_i$
(fixed point)

$\alpha_{ij}  j = 1 \rightarrow n_i$, the values of $\alpha$ being in ascending order
[i.e. $n_i$ values of $\alpha$]

$S(\alpha_{ij}, \beta_i)  j = 1 \rightarrow n_i$  [i.e. $n_i$ values of $S(\alpha, \beta)$]

Each $\beta$ value is in field 1 of a new card and the format of card 3 and
following cards is repeated.
If $n_i = 0$ for some $i$ then the $a$ values are the same as for
the previous value of $\beta$ 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 EBC 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.

-53-
Tapes can be prepared and modified using the IBM 1401 programme NUTP 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 NUTP allow the
(a) Write n nuclides on tape from cards (max. 125)
(b) Copy a tape containing n nuclides.
(c) Modify any specified records (cards) on an existing tape. Reading section cards cannot be modified by NUTP.
(d) Take m (max. 50) nuclides from cards and n (max. 50) nuclides from an existing tape containing p (max) 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 St (Fortran) language programme GEMX [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 monotonically increasing.

*GEMX currently deals only with neutron interaction cross-sections, angular distributions, secondary energies and miscellaneous 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 RDF 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 RDF 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 nuclei. 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 extend 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 AERE Winfrith and designed to allow the extension of Aldermaston data to lower energies is not likely to be of sufficient generality for continued use; it will be superseded eventually by more versatile programmes.

13. **Acknowledgments**

Many workers at both AERE Winfrith (W) and AERE 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. N. Underhill (A), E. D. Pendlebury (A), J. C. Full (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 programs developed by B. A. Brett (A) D. M. Jarman (A), L. W. Hlott (W), V. J. Bell (W) and R. Hines (A).

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

Thanks are due to J. S. Story (W), N. F. James (A), L. W. Hlott (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 SI (Fortran)

Language Programme, REPTON

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, I12, I12)

   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, ZE, ZU, T (format I11, I12, 6E12.6)

   ISN = Section number of following tabulated cross-section
   IRN = Reaction type number of following tabulated cross-section
   Q = Q value for this reaction
IL = 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 5F12.6,
5F12.6) - 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 PRELUDI control card contains IDEM (format 111). IDEM 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. IDEM 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 monotonically increasing).
4. Signs of positive quantities (e.g. energy, atomic weight, temperature (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

-60-
Appendix C

Information Provided by the Data Listing

Programme NDF PRINT

The printout provided by NDF PRINT is arranged as follows:

1. Heading (e.g., "Nuclear Data for 3/123.4.5.6.7.8.9.0.1 = 156").
2. Atomic number, atomic weight, number of reaction types occurring, 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.W'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).
References

1. K. Parker: AWE Report No. 0-27/60
2. K. Parker: AWE Report No. 0-71/60
3. B. R. S. Buckingham, K. Parker and E. D. Pendlebury: AWE Report No. 0-20/60
4. R. B. Wade: AWE Report No. 0-12/63
5. J. H. Towe, D. Sams, W. B. Gilkey and J. B. Parker: To be published
7. J. B. Parker and K. Parker: AWE Report No. 0-20/60
8. K. Parker: AWE Report No. 0-1/61
10. P. F. James: AEWI-2277
11. H. M. Summer: AEWI-1616
12. B. R. S. Buckingham and E. D. Pendlebury: AWE Reports No. 0-64/60 and 0-65/60
13. J. J. Schmidt: FER 120 [ENEO-E-35U]
27. E. König, J. H. E. Nattouch and A. H. Wagner: Nuclear Physics, 2, 18 (1962)
28. T. J. Webster: AWE Report No. 0-71/63
31. WIL 672, p. 5 (1961) and WASH 1001, p. 13 (1962)
32. T. F. Moonhead: AEWI-2254 (1963)
**Nuclear Data File**

**Data for Punching**

<table>
<thead>
<tr>
<th>MATERIAL</th>
<th>WRITTEN BY</th>
<th>DATE</th>
<th>CHECKED BY</th>
<th>DATE</th>
<th>TYPE OF DATA</th>
<th>PUNCHED BY</th>
<th>DATE</th>
<th>CHECKED BY</th>
<th>DATE</th>
<th>CARD COLOUR</th>
<th>NOTES</th>
</tr>
</thead>
</table>

- 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.XXXXXX ± X or X.XXXXXX ± X. If X not specified it is zero.

### Figure 3. Data Punching Sheet

<table>
<thead>
<tr>
<th>Column</th>
<th>Left</th>
<th>Right</th>
<th>...</th>
<th>Left</th>
<th>Right</th>
<th>...</th>
<th>Left</th>
<th>Right</th>
<th>...</th>
<th>Left</th>
<th>Right</th>
<th>...</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Figures 3, 4, 5, and 6**

**Material 1**

**Material 2**

**Material 3**

**Material 4**

**Material 5**

**Material 6**

**Material 7**

**Material 8**

**Material 9**

**Material 10**

**Material 11**

**Material 12**

**Material 13**

**Material 14**

**Material 15**

**Material 16**

**Material 17**

**Material 18**

**Material 19**

**Material 20**

**Material 21**

**Material 22**

**Material 23**

**Material 24**

**Material 25**

**Material 26**

**Material 27**

**Material 28**

**Material 29**

**Material 30**

**Material 31**

**Material 32**

**Material 33**

**Material 34**

**Material 35**

**Material 36**

**Material 37**

**Material 38**

**Material 39**

**Material 40**

**Material 41**

**Material 42**

**Material 43**

**Material 44**

**Material 45**

**Material 46**

**Material 47**

**Material 48**

**Material 49**

**Material 50**

**Material 51**

**Material 52**

**Material 53**

**Material 54**

**Material 55**

**Material 56**

**Material 57**

**Material 58**

**Material 59**

**Material 60**

**Material 61**

**Material 62**

**Material 63**

**Material 64**

**Material 65**

**Material 66**

**Material 67**

**Material 68**

**Material 69**

**Material 70**

**Material 71**

**Material 72**

**Material 73**

**Material 74**

**Material 75**

**Material 76**

**Material 77**

**Material 78**

**Material 79**

**Material 80**

**Material 81**

**Material 82**

**Material 83**

**Material 84**

**Material 85**

**Material 86**

**Material 87**

**Material 88**

**Material 89**

**Material 90**

**Material 91**

**Material 92**

**Material 93**

**Material 94**

**Material 95**

**Material 96**

**Material 97**

**Material 98**

**Material 99**

**Material 100**

**Material 101**

**Material 102**

**Material 103**

**Material 104**

**Material 105**

**Material 106**

**Material 107**

**Material 108**

**Material 109**

**Material 110**

**Material 111**

**Material 112**

**Material 113**

**Material 114**

**Material 115**

**Material 116**

**Material 117**

**Material 118**

**Material 119**

**Material 120**

**Material 121**

**Material 122**

**Material 123**

**Material 124**

**Material 125**

**Material 126**

**Material 127**

**Material 128**

**Material 129**

**Material 130**

**Material 131**

**Material 132**

**Material 133**

**Material 134**

**Material 135**

**Material 136**

**Material 137**

**Material 138**

**Material 139**

**Material 140**

**Material 141**

**Material 142**

**Material 143**

**Material 144**

**Material 145**

**Material 146**

**Material 147**

**Material 148**

**Material 149**

**Material 150**

**Material 151**

**Material 152**

**Material 153**

**Material 154**

**Material 155**

**Material 156**

**Material 157**

**Material 158**

**Material 159**

**Material 160**

**Material 161**

**Material 162**

**Material 163**

**Material 164**

**Material 165**

**Material 166**

**Material 167**

**Material 168**

**Material 169**

**Material 170**

**Material 171**

**Material 172**

**Material 173**

**Material 174**

**Material 175**

**Material 176**

**Material 177**

**Material 178**

**Material 179**

**Material 180**

**Material 181**

**Material 182**

**Material 183**

**Material 184**

**Material 185**

**Material 186**

**Material 187**

**Material 188**

**Material 189**

**Material 190**

**Material 191**

**Material 192**

**Material 193**

**Material 194**

**Material 195**

**Material 196**

**Material 197**

**Material 198**

**Material 199**

**Material 200**

**Material 201**

**Material 202**

**Material 203**

**Material 204**

**Material 205**

**Material 206**

**Material 207**

**Material 208**

**Material 209**

**Material 210**