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ABSTRACT

MIRANDA is the cross-section generation module of the AUS neutronics code system used to prepare multigroup cross-section data which are pertinent to a particular study from a general-purpose multigroup library of cross sections. Libraries have been prepared from ENDF/B which are suitable for thermal and fast fission reactors and for fusion blanket studies. The libraries include temperature dependent data, resonance cross sections represented by subgroup parameters and may contain photon as well as neutron data. The MIRANDA module includes a multiregion resonance calculation in slab, cylinder or cluster geometry, a homogeneous B_L flux solution, and a group condensation facility. This report documents the modifications to an earlier version of MIRANDA [Robinson 1977, AAEC/E410] and provides a complete user's manual.

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The following descriptors have been selected from the INIS Thesaurus to describe the subject content of this report for information retrieval purposes. For further details please refer to IAEA-INIS-12 (INIS: Manual for Indexing) and IAEA-INIS-13 (INIS: Thesaurus) published in Vienna by the International Atomic Energy Agency.

FISSION PRODUCTS; GROUP CONSTANTS; M CODES; MULTIGROUP THEORY; NEUTRON FLUX; NEUTRONS; NUCLEAR DATA COLLECTIONS; RESONANCE; RESONANCE INTEGRALS; TOTAL CROSS SECTIONS

CONTENTS

1. INTRODUCTION

The AUS code system [Robinson 1975a] was developed at Lucas Heights for reactor neutronics computations of a wide range of thermal and fast fission reactor systems. AUS has recently been extended for fusion blanket calculations [Robinson 1984] and is also applicable to many other neutronics applications. MIRANDA is the cross-section generation module for AUS and it is suitable for all the diverse calculations to which AUS is applied. The term 'cross-section generation' is used in the restricted sense of preparing group cross-section data, suitable for a particular subsystem of a reactor or an assembly of material, from an input group cross-section library of wide application.

MIRANDA uses as input data a multigroup cross-section library with group scattering matrices of any P_n order, resonance cross sections in the form of subgroup data, and scattering matrices dependent on potential scattering. All relevant quantities may be temperature dependent. There are two standard libraries for MIRANDA both of which contain data derived mainly from ENDF/B IV. The original 128-group library AUS.ENDFB was developed for fission reactor core calculations and contains neutron data only. The more recent library AUS.ENDF200G, with 200 neutron groups and 37 photon groups, is intended for all applications but currently contains a restricted set of nuclides. The use of these libraries with groups as wide as 0.25 lethargy requires that most major nuclides be given a resonance treatment.

The basic output from MIRANDA is a cross-section data pool containing cross sections for each region of a lattice cell for use in a transport calculation of the cell. Thus, MIRANDA is only the first phase of a normal reactor lattice calculation. The major function of MIRANDA is the resonance theory calculation of nuclide cross sections, in the library group structure, appropriate to the system under study. The multiregion resonance calculation may be performed in slab, cylinder or cluster geometry using the subgroup method. Preliminary group condensation may also be carried out following a homogeneous B_L flux solution. In applications with no cell structure, MIRANDA directly provides cross sections for a global calculation of the system.

An earlier MIRANDA report [Robinson 1977] should be referred to for details of the methods of calculation; only the modifications to those methods are detailed here. In addition, this report is intended as a user's manual. It contains an outline of the code which should be sufficient for most users, a complete description of the input data and the current contents of the cross-section libraries.

A comparison of MIRANDA resonance calculations with numerical solutions using the PEARLS code [Chiarella 1971] was given by Robinson [1977], and a more recent comparison with the MCRP Monte Carlo code [Doherty and Robinson 1985] for thermal reactor lattices has been given by Robinson [1985].

2. OVERVIEW OF THE CODE AND LIBRARIES

2.1 Cross-section Libraries

The cross-section library is in the form of an AUS XSLIB data pool, the structure of which has been given by Robinson [1975a] for neutrons only. The two libraries currently available were generated mainly from ENDF/B IV. The group structure of the libraries and the nuclides included are detailed in **appendix A**. The original 128-group library AUS.ENDFB was directed towards calculations of fission reactor cores and only contains information on neutron reactions. This library includes data for a set of 155 fission products which is normally reduced to a set of 45 fission products, with one pseudo fission product to represent the reactivity effect of the remainder. The library AUS.ENDF200G, with 200 neutron groups and 37 photon groups, was generated during the extension of AUS to fusion blanket applications. In principle, this library can be used in any application, but at present its use for fission reactors is limited because some of the actinide data and all of the fission product data are excluded.

Resonance data in the library are given mainly in the form of subgroup parameters. These data have been obtained from group resonance integrals per unit lethargy I, tabulated as a function of effective potential scattering cross section $\hat{\sigma}_p$, by fits of the form

$$I(\hat{\sigma}_p) = \sum_i w_i \hat{\sigma}_p / (\sigma_i + \hat{\sigma}_p),$$

where σ_i is a parameter representing the total cross section of the nuclide in the i^{th} subgroup, and w_i is the subgroup weight. Most resonance integrals have been obtained by generating cross sections on a fine energy mesh for use in numerical solutions of the neutron slowing-down equation for mixtures of the resonance nuclide and hydrogen.

The calculation also provides the P_0 scattering matrix as a function of $\hat{\sigma}_p$. This treatment has also been applied in the unresolved region, using a ladder of resonances obtained by selecting parameters from the distributions about the average resonance parameters. The alternative treatment of integration over the distributions using a J-function summation has been used above 19.3 keV for all nuclides and throughout the unresolved region on AUS.ENDFB for all nuclides except ^{238}U. Details of the resonance methods for generating data on AUS.ENDFB were given by Robinson [1977]. Details of the modifications to these methods which were used for AUS.ENDF200G are given in **appendix B**.

For non-resonance cross sections, the original data on AUS.ENDFB was generated using the SUPERTOG [Wright *et al.* 1969] and PIXSE [McDougall 1963] codes as outlined by Robinson [1977]. For nuclide data added more recently, a modified version [Robinson 1981] of the XLACS2 code has been used. These recent additions include the moderator nuclides obtained from ENDF/B IV and all of the fission product nuclides. The generation of non-resonance data for AUS.ENDF2000G has been treated in some detail by Robinson [1984]. Again, the modified XLACS2 code was used for neutron data.

2.2 Resonance Treatment

The resonance treatment in MIRANDA is a multiregion calculation which makes use of a set of collision probability routines to obtain subgroup fluxes for each resonance nuclide in turn, then calculates the resonance integrals. Scattering is assumed to be elastic and spherically symmetric in the centre-of-mass system. The collision probability routines included are the numerical integration routines for reflected slab, translational slab and reflected cylinder developed by Doherty [1969], and the approximate routines for cylinders and clusters developed by Robinson [1979]. The approximate routine is normally used for cylinders as it is much faster, gives adequate accuracy, and provides a treatment of polygonal boundaries. Evaluation of the resonance integral does not depend explicitly on an equivalence relation but a numerical equivalence relation is derived to obtain the outscatters of the resonance nuclide.

Corrections to the simple treatment outlined above include the following:

- a λ method to form an equivalence between scattering by different nuclides [see Robinson 1977];
- a non-isolated resonance correction;
- a resonance overlap correction; and
- a dependence of group removals on the group resonance escape probability.

The group reaction rates derived from the resonance integrals are preserved when obtaining effective group cross sections. This involves an iteration on the collision probability formulation of the group equations with an asymptotic source to give a set of cross sections and consistent region fluxes which reproduce the required reaction rate.

Details of the resonance treatment were given by Robinson [1977]. Since then, the treatment has been slightly modified. The changes are discussed in Section 4.

2.3 Homogeneous Flux Calculation

A homogeneous model of the lattice is obtained by spatial averaging, using volume weighting in non-resonance groups and the fluxes obtained for an asymptotic group source in resonance groups. The equations solved are either the transport corrected P_0 equations or the B_L equations for $L > 0$. A search for critical buckling may be performed. The photon flux may be calculated using the photon production from the calculated neutron flux as the source. If bilinear weighting is requested, the adjoint flux equations are also solved. The method of solution has been described by Robinson [1977].

2.4 Condensed Cross-section Output

The flux used in energy condensation is formed by combining the homogeneous group flux with the spatial fluxes available in resonance groups. Only limited condensation should be performed in MIRANDA, because in most cases this flux is very approximate. For flux weighting, the condensation procedures are straightforward except for the transport cross section for which the formulae adopted are based on the use of the derived cross sections in global calculations. The procedures have been detailed by Robinson [1977]. For bilinear weighting, the condensation procedures are the same as those of the EDITAR module [Robinson 1986].

3. USE OF AUS DATA POOLS

MIRANDA normally outputs the following data pools:

- A cross-section data pool on FORTRAN unit 10 containing macroscopic cross sections for the materials of the lattice, and any desired microscopic cross sections.
- A geometry data pool on FORTRAN unit 7.
- A FLUXB data pool on FORTRAN unit 9 giving a P_0 flux in the spatial mesh of the geometry data pool, for the condensed group structure, which serves as a flux guess for the next module.
- Additional entries added to the pair of STATUS data pools, ST1 on FORTRAN unit 4 and ST2 on FORTRAN unit 5.

The purpose of the entries on the STATUS data pool has been outlined in Robinson [1975b]. The following actions are taken by MIRANDA.

If the ST2 data set is empty, both ST1 and ST2 are initiated with TIME entries for time zero. The module then enters the write mode in which data come entirely from the input stream and entries are added to ST1 and ST2. A CELL entry is added to ST2 and CELL, GRPS and material definition entries are added to ST1. A material definition is written for each output material which is not a nuclide on the input cross-section library.

If ST2 is not empty, the last CELL entry acts as a counter of calculations already performed. If there are no more CELL entries for the current time on ST1 than on ST2, the module enters the write mode as above. If there are further CELL entries, the first entry sets the cell name and the following entries are used for material definitions which take precedence over the input stream. When data are obtained from ST1 in this way (which should only occur in burnup calculations), the only STATUS output is a CELL entry on ST2.

4. MODIFICATIONS TO THE RESONANCE TREATMENT

The chief modification is simply the replacement of the collision probability routines for cylinders and rod clusters. The results for cylinders with a white reflective circular boundary are practically unchanged but the new routines provide an approximate treatment of polygonal boundaries. The new cluster routines are a considerable improvement on those used originally.

The inclusion of photon production and kerma factor data in the calculation was easily accommodated. For resonance nuclides, the photon production data stored in the library consists of separate multiplicity matrices for capture, fission and a composite of other reactions. Thus photon production from capture and fission are resonance-shielded in the same way as the neutron reaction data. Similarly, separate kerma factors are stored for capture, fission, elastic scattering and a composite reaction, and thus can be shielded appropriately.

The original MIRANDA resonance treatment relied on resonance nuclides scattering neutrons down through only one energy group. The following changes have been made to generalise that treatment; for continuity, the notation and equation numbers are as used in the earlier report [Robinson 1977]:

$$\phi_0 = 1 / \sum_i V_i \left\{ \sum_m N_{mi} \xi_m \sigma_{pm} + \sum_{m \in L_\ell} N_{mi} \left(\tau \sigma_{rm} (\overline{S}_{mi}) \, \xi_m / \beta_m - \xi_m \sigma_{pm} \right) \right\} \qquad (5.33a)$$

$$\phi_0' = 1 / \sum_i V_i \left\{ \sum_{m \neq \ell} N_{mi} \sigma_{pm} + N_{\ell i} \xi_\ell \sigma_{p\ell} + \sum_{m \in L_\ell} N_{mi} \left(\tau \sigma_{rm} (\overline{S}_{mi}) / \beta_m - \sigma_{pm} \right) \right\} \qquad (5.34a)$$

$$\gamma_\ell = T_0 / \left\{ T_0 + \sum_i V_i N_{\ell i} (\beta_\ell \sigma_{p\ell} - \tau \sigma_r \, (\overline{S}_{\ell i})) \right\} \qquad (5.76)$$

where

$$T_0 = \sum_i V_i \left\{ \sum_{m \in L} N_{mi} \sigma_{pm} \beta_m + \sum_{m \in L} N_{mi} \tau \sigma_{rm} (\overline{S}_{mi}) \right\}$$

The remaining changes relate to the provision of an optional method which may be more suitable than the standard treatment in heavily absorbing systems such as fast reactor assemblies below neutron energies of 1 keV. An option is available to treat some nuclides by a pseudo narrow resonance (NR) treatment. In this

option, the Hill-Schaeffer λ parameter is applied only to the resonance nuclide and the ρ correction factor (equation 5.32 of Robinson [1977]) is not applied. This is as close as possible to an NR treatment, with subgroup parameters fitted to resonance integrals treated as a function of σ_p. The results for mixtures of the resonance nuclide and hydrogen are the same under this option and the standard treatment.

A further option provides a very approximate method of allowing for the effect on resonance overlap of the position of resonances within a neutron group. This effect is based on the group resonance escape probability p, and not on the overlap of resonances at a particular energy. Factors giving the average position within the group of resonance absorption and resonance fission have been included on AUS.ENDF200G for some actinides. Resonance integral weighted values of $\log(E_r/E_g)/\log(E_{g+1}/E_g)$ have been formed using the same resonance integrals as were used to form average λ parameters.

The correction factor applied in MIRANDA to the absorption integral of nuclide ℓ is given by

$$\exp(\sum_m N_m I_m(f_m - f_\ell)\phi) \quad ,$$

and the correction factor for the fission integral is

$$\exp(\sum_m N_m I_m (f_m - f_\ell^f)\phi \quad ,$$

where f_m and f_m^f are position factors of nuclide m for absorption and fission respectively. When not given, the position factors are taken as 0.5.

5. INPUT DATA

5.1 General Layout

Input data to MIRANDA are in free format, with keywords to indicate the data type followed by a string of numeric or alphabetic information. The data are entered in columns 1 to 72 with each keyword starting on a new record. As the data are read with the SCAN input routine [Bennett and Pollard 1967], all the facilities and conventions of SCAN apply. The readability of the data may be improved by including any desired special characters.

Many of the input variables have been given default values. Thus, if the standard value is required, an entire keyword and data may be omitted or trailing data may be left off the end of a data string. There is no set order in which the keywords must be given, but some of the data require information to be previously defined. For example, a material may not be referred to before it is defined. It is, therefore, best to follow the order of keywords given below. When a series of calculations is undertaken, only the data which are to be altered need be given for subsequent calculations.

In the description of entries given below, those that should suffice for most calculations are indicated by an asterisk. Information in upper case in the entry description should be reproduced exactly.

5.2 HEAD Heading Information*

HEAD	Jobname	Heading
where	Jobname	is a word of 1 to 6 alphanumeric characters which provides a unique label for all output including each material on an output cross-section data pool, and
	Heading	is a string of characters, including blanks, also used for labelling.

Example:

HEAD SR5 TEST CALCULATION

5.3 PRELUDE Problem Size Specification

PRELUDE MDEF = md MREQD = mr MAXX = mx MAXBN = mb

with default values

PRELUDE MDEF= 20 MREQD = 0 MAXX = 20 MAXBN = 0

where md is the maximum number of defined materials,
mr is the maximum number of output materials,
i.e. the number of materials on the REQD entry,
mx is the maximum number of geometry intervals, and
mb is the maximum order of a B_L flux solution.

The PRELUDE values of MREQD, MAXX and MAXBN may be exceeded in the first calculation, which serves to redefine these maxima, so that a PRELUDE entry is seldom required. If, however, a subsequent calculation requires a larger value than the first, a PRELUDE entry is necessary.

Example:

PRELUDE MAXBN = 3 MDEF = 30

is required for a B3 calculation following a B1 calculation with 30 materials defined.

5.4 USE Library Selection

USE lib last

with default

USE 8 PFP

where lib is the FORTRAN unit number of the input cross-section library, and
last is the name of the last nuclide on the library to be included.

The specification of 'last' has application only in burnup calculations to alter the set of fission products which are included. The AUS.ENDFB library has a set of 45 individual fission products and a pseudo fission product PFP, followed by a further 110 fission products of low reactivity worth which are not usually included. In normal burnup calculations, MIRANDA uses the decay and yield data of the discarded fission products to modify the yield data of those kept. The PFP fission product is used only if it is the last nuclide included. Thus

USE 8 ALL

may be used to include the 155 individual fission products and discard PFP.

A USE card serves to initialise variables to the standard state, causes a preliminary reading of the cross-section library and causes the STATUS data pool to be read. If a USE card is not given before any input entry except HEAD, PRELUDE (or TEST) is given, the code generates the standard USE entry.

5.5 SELECT Library Selection

SELECT name, source, mod = newname

where name is the name of a library nuclide for which a non-standard set of data is required,
source is the data source of the required data,
mod if given, selects the appropriate data modification, and
newname if given, renames the nuclide so that two versions of a nuclide may be included in a calculation.

The nuclides on the library are labelled by 20 characters consisting of an 8-character simple name, an 8-character data source and a 4-character modifier. The library may include more than one version of a nuclide, and the one having the highest update number is normally used. A number of SELECT entries may be used to choose non-standard versions of nuclide data, but they must immediately follow a USE entry or be the first entries apart from HEAD, PRELUDE or TEST. The nuclide lists for AUS.ENDFB and AUS. ENDF200G are given in **appendix A**.

Example:

SELECT U233 BNL65PHF

selects an old set of ^{233}U data and renames it U233A so that it may be compared with the standard ^{233}U data.

5.6 TEMP Default Temperature*

TEMP t

with default

TEMP 300

where t is the default temperature (K) for any *following* material definitions which do not include a specific temperature value.

5.7 DEFN Material Definition*

DEFN matname t $name_1$, $conc_1$, $name_2$, $conc_2$, ...

where matname is the 1- to 8-character name to be given to the defined material,
t is the temperature (K) of the material, which may be omitted,
$name_i$ is the name of a library nuclide or a previously defined material, and
$conc_i$ is the quantity of $name_i$ to be included, usually in 10^{24} atom cm^{-3}.

The set of nuclides currently included in the libraries is given in **appendix A.** The names they have been given are the obvious isotope or element name. Although a definition in terms of defined materials is permitted, this is only to avoid duplication of input as in the following example:

```
DEFN   UO2    U235   .05   U238   .95   0      2.
DEFN   FUELA  450.   UO2   .022
DEFN   FUELB  600.   UO2   .022   B10   1.E-5
```

5.8 REQD Output Material Selection*

REQD $name_1$ (r_1), $name_2$ (r_2), ...

where $name_j$ is the name of a library nuclide or a defined material which is required for output, and
r_j *if given, selects the resonance geometry interval number for which* the nuclide or material is to be produced.

An interval number r_j is not normally given as the code averages over the required region. The following is a description of the default values. For a defined material, average cross sections are formed over the cell regions occupied by that material (both for materials explicitly in the system, and for intermediate materials such as UO2 above) or over the entire cell for materials not in the cell. For a library nuclide in the cell, a choice may be made between one set of average cross sections or a set of cross sections for each resonance region, which includes the nuclide and is filled by a different material. The choice is made using the REQDREG entry, with the default being the preparation of a number of cross section sets for fuel nuclides only.

Output may be requested for the special material CELL, which has the average properties of the lattice cell. If output of a resonance nuclide is requested for a resonance region in which the nuclide concentration is zero, infinite dilution cross sections will be used. Correct cross sections of a resonance nuclide in such regions may be generated by including a small amount, say 1.E-20, of the nuclide in the material definitions. This procedure is useful in preparing cross sections for a reaction rate scan across the lattice.

If the library order is known, a group of nuclides may be selected using

REQD $name_1$ TO $name_2$, ...

Examples:

REQD FUEL, MOD, U235 TO PU241

REQD FUEL, CAN, MOD, REFL(3)

5.9 XM or RM Geometry Size Specification

XM ibc x_1, x_2, ... , x_n obc
RM ibc x_1, x_2, ... , x_n obc

where XM implies slab geometry,
RM implies cylindrical geometry,
ibc is the inner boundary condition,
x_i is the width of the i^{th} mesh interval in cm, and
obc is the outer boundary condition.

In slab geometry, the boundary conditions have the values 0 for reflective and -1 for translational conditions. In cylindrical geometry,

ibc = 0 for a circular outer boundary,
ibc = n for a polygonal outer boundary with n sides,
ibc = 0 for a white reflective boundary, and
obc = -m for a reflective polygonal boundary,
where m is the number of innermost intervals which are to be treated as fuel. (This boundary condition is limited to a two-region system. The actual geometry is volume smeared into two regions in applying the boundary condition.)

The outermost radius, $\sum_n x_n$, is the radius of a circle having the same area as the polygon.

Either an XM or RM entry is always required, and homogeneous cases should be run as a one-region calculation.

Example:

RM 0 0.5 0.25 0

specifies a two-region cylinder with fuel radius of 0.5 cm and an outer radius of 0.75 cm.

5.10 REG Geometry Layout Specification*

REG [MX] (int_1, ... , int_n, $name_1$),...
or
REG [MR] (int_1, ... , int_n, $name_1$),...

where MX or MR may be included for compatibility with other AUS modules or omitted,
int_1, ...,int_n are the mesh interval numbers which are filled by the defined material, $name_1$, and
$name_1$ may have the form of a material name, or be M(j) which specifies the j^{th} material on the previously given REQD entry.

Examples:

```
REG   1     FUEL          2        MOD
REG   MX    1 3 5 7   MX 2(2)8    M(2)
```

5.11 RODSUB and ARRAY Cluster Specification*

In cluster geometry, the composition and position of fuel rods within the annular geometry given by the RM and REG entries are specified by sets of RODSUB and ARRAY entries. The material specified by the REG entry fills that part of the annulus not occupied by the rods. The boundary conditions specified on the RM entry are applied to the inter-rod boundaries when the synthetic collision probability routine is used. The outer boundary of a cluster is always taken to be a circular white reflecting boundary. The cluster geometry is currently limited to equally spaced rods whose centres lie on a circle. The entries have the form

RODSUB j $(dr_1, \ldots, dr_n)$, $(name_1, \ldots, name_n)$

where j is the number of the ring, numbered from the centre outward,
n is the number of radial subdivisions of a rod in this ring,
dr_i is the width in cm of the i^{th} radial subdivision, and
$name_i$ is the name of the material in the i^{th} subdivison.

ARRAY j, nrod, prod, grod

where j is as defined above,
nrod is the number of rods in the ring,
prod is the radius of the circle on which the rod centres lie, and
grod is the angular displacement of one rod from a reference diameter of the cluster (in radians or degrees).

The angular displacement is not used in MIRANDA but is entered in the AUS geometry data pool.

Example:

```
DEFN      FUELA   U238    .048    U235    .0048
DEFN      FUELB   FUELA   1.
DEFN      MOD     D2O     .033
REQD      FUELA   FUELB   MOD     U235    U238
RM        6       0.985   1.62    5.858   -1
REG       1       2       3       MOD
RODSUB    1       0.825   FUELA
RODSUB    2       0.825   FUELB
ARRAY     1       1       0
ARRAY     2       6       1.875
```

This specifies a 7-rod cluster of unclad fuel pins with a hexagonal boundary applied between pin-cells. Different fuel names are used for the central rod and the rods of the ring, in order that two sets of cross sections will be prepared. Two different sets of ^{235}U and ^{238}U data are also prepared. If one fuel name had been used, average cross sections for the fuel, ^{235}U and ^{238}U, would be produced.

5.12 RESREG Resonance Geometry Specification*

The RESREG entry specifies the geometry to be used in the multiregion resonance calculation and must always be included. A blank RESREG entry indicates that the geometry is that given by the XM or RM and REG entries. However, there is little point in including a large number of mesh intervals in the resonance calculation. Not only can this become rather expensive in computer time, but the results obtained with a single mesh interval in each physical region should be equally reliable in most cases. The collision probability

approximation of a constant source within a mesh interval is completely satisfied for the off-resonance source term of the resonance calculation. Additionally, the Bonalumi approximation normally used in cylindrical geometry becomes worse as the fuel pin is subdivided. A collision probability routine using numerical integration is available for calculations of resonance reaction rate distributions within a fuel pin. A comparison of MIRANDA with Monte Carlo calculations [Robinson 1985a] resulted in a recommendation that one mesh interval per physical region should be used in single-rod lattices.

A RESREG card is used to smear the geometry given by the XM or RM and REG entry. No provision has been made for smearing the rod subdivisions of cluster geometry. The form of the entry is

RESREG ibc, $x_1, ..., x_m$, obc SMEAR $i_1, ..., i_n$

where ibc, $x_1, ..., x_m$, obc — specify an m region geometry to be used in the resonance calculations, with the variables having the same meaning as given on the XM or RM entry,

$i_1, ..., i_n$ — are the resonance region intervals into which each main geometry interval is to be smeared, and

n — is the number of main geometry intervals.

That is the i_j are integers with values between 1 and m.

Example:

```
XM       -1   4*0.5 -1
REG       1   FUELA   3   FUELB   2 4 MOD
RESREG    0   2*0.5   0   SMEAR   1 2 1 2
```

This specifies a 4-region translational slab with 2 different fuel regions, which is treated in the resonance calculation as a 2-region reflected slab in which the fuelled regions are smeared together.

5.13 BUCK Group Buckling*

BUCK [Bℓ] b_1^2, b_2^2, ..., b_n^2

with default

BUCK B0 1.E-20

where Bℓ specifies the order of the Bℓ flux solution and is optional, and
b_i^2 is the buckling for energy group i.

If a short list of b_i^2 is given, the last value in the list is used in the remaining groups. Thus one value is sufficient for a constant group buckling. A transport corrected P_0 calculation is actually performed instead of B_0.

Example:

```
BUCK   B1   .02
```

5.14 SEARCH Search for Critical Buckling*

SEARCH $\frac{\text{OFF}}{\text{ON}}$ BSQ FOR k, δk

with default

```
SEARCH   OFF   BSQ   FOR   1.   .0002
```

where ON,OFF turns the search on or off and the default is 'no search',
k is the value of k_{eff} required, and
δk is the accuracy to which k is required.

The module searches for an eigenvalue λ such that λ times input buckling gives a k_{eff} of k. The buckling in any following calculation is λB_g^2.

Example:

```
SEARCH   ON   BSQ   FOR   1.02
```

5.15 GSCE Group Source

In any calculation which does not include a fissionable nuclide, a ^{235}U fission spectrum is used as the source for the group flux calculation. If this default is not satisfactory, a group source may be specified by

GSCE $S_1, S_2, ..., S_n$

where S_i is the source in group i and a short vector is filled out with zero, or by
GSCE -t
where t is the temperature, in eV, of the simple Maxwellian form of a fission spectrum.

The resulting fluxes are normalised to a total source of 1 neutron cm^{-3} s^{-1}. In fact, the source may be overwritten in this manner in any calculation.

5.16 FSTEMP Nuclide Fission Spectra

The dependence of fission spectra on incident neutron energy is one quantity which is not included in the cross-section library. The library value of the fission spectrum of a nuclide is that appropriate for thermal calculations. Provision has, therefore, been made for fission spectra to be input.
The form is

FSTEMP $name_1, t_1, name_2, t_2, ...$

where $name_1$ is the name of a library nuclide whose fission spectrum is to be altered, and
t_1 is the temperature of the simple Maxwellian form of the fission spectrum in eV.

Example:

```
FSTEMP   U235   1.323E+6
```

This would have no effect as it is the current library value.

5.17 WEIGHT Bilinear Weighting Option*

Flux weighting is normally used to average cross sections and to form printed reaction rates. If bilinear weighting is required, the entry

```
WEIGHT BILINEAR
```

should be included. The bilinear weighting formulae are the same as those used in EDITAR [Robinson 1986].

5.18 OUTPUT Type of Output Required*

```
OUTPUT   XS   RR   AUS   lib   FLUX   GEOM   ZERO   Pn
with default of
OUTPUT   AUS   10   P0   FLUX   GEOM
```

A selection may be made of any of the given parameters. The selection process is additive however, so ZERO must be used to stop any output option previously selected. The options have the meaning

XS	print cross sections,
RR	print reaction rates per unit source, or for bilinear weighting, print material worth components plus a few simple reaction rates,
AUS	write an AUS cross-section data pool on FORTRAN unit lib, and add to the STATUS data pool as necessary,
FLUX	write an AUS FLUXB data pool for the main geometry mesh,
GEOM	write an AUS geometry data pool, and
Pn	scattering matrices on the cross section data pool produced up to order P_n.

All OUTPUT is for the materials on the REQD card in condensed groups.

A series of cases may be performed with output on the same data sets. A composite cross-section data pool is formed automatically by MIRANDA.

Examples:

OUTPUT XS RR

This adds print options to the standard option of writing all data sets.

OUTPUT ZERO RR

This prints reaction rates and nothing else is produced.

5.19 GROUPS Condensed Group Structure*

GROUPS $n, g_1, \ldots, g_{n+1}$

where n is the number of condensed groups,
g_1 is the first library group of condensed group 1, and
g_i for $i > 1$, is the last library group of condensed group $i - 1$.

If $g_1 < 1$, the g_i are taken to be group boundaries in lethargy units. In this case library groups with the nearest lethargy boundary are selected. Although the outer boundaries g_1 and g_{n+1} are specified, they must cover the full energy range of the cross-section library.

Example:

GROUPS 13 1 10(10)120 128

5.20 TRANSPORT Transport Cross Section Option

Transport cross sections following a B_L calculation are normally adjusted to give the correct leakage in a diffusion theory calculation of a reactor. If this is not appropriate, the keyword required is

TRANSPORT P1

5.21 ISOTLIB Specification of Output Nuclides*

ISOTLIB liba $name_1, \ldots, name_n$ BURNUP Pn

with default

ISOTLIB lib ALLMAT P-1

where all quantities are optional,

liba	is the FORTRAN unit on which a nuclide cross-section data pool is written and it may be the same as the main output cross-section data pool.
lib	is the main output cross-section data pool,
$name_i$	is a defined material whose constituent nuclides are to be produced, or is the keyword ALLMAT which causes the constituent nuclides of all REQD defined materials to be produced,
BURNUP	causes the definitions of the set of materials to be modified to include a small amount of all nuclides produced in that material during burnup, and
Pn	is the order of scattering matrices, with the default being no matrices at all.

The default values only apply if an ISOTLIB card is given. The option is turned off in the standard state.

The use of this entry enables nuclide reaction rate editing and burnup calculations to be performed within the AUS system. The connection between macroscopic materials and the nuclides of this cross-section data pool is maintained by information entered in the STATUS data pool by modules of the system.

An ISOTLIB entry which includes the BURNUP specification is normally included in all MIRANDA calculations which form part of a burnup calculation. The entry must be included if the fission-product yields are to be modified (see USE entry).

The entry
ISOTLIB 0
turns off the option after it has been on in a previous case. A series of cases may be run with ISOTLIB output on the same unit.

5.22 REQDREG Nuclide Regions in Output

REQDREG $j_1\ j_2\ j_3$ $name_1, ..., name_n$

with default

REQDREG 2 1 1

where the j_i take the values:

1	which means that cell average nuclide cross sections are produced, or
2	which means that a set of nuclide cross sections is produced for each resonance region in which the nuclide occurs and which is filled by a different material, and
namej	are optional nuclide names for which multiple sets of cross sections are to be produced (n<20),

The three values are for fuel nuclides (atomic mass > 220), normal nuclides and fission products respectively. The nuclides referred to are the library nuclides which are on the REQD entry or which are generated from the ISOTLIB entry.

The names of a set of nuclides which are produced are made distinct by combining the 6-character jobname given on the HEAD entry with a 2-character resonance region number to form the 'source' component of the nuclide name.

5.23 NUCMOD Alternative Label

The form of the material definition written by MIRANDA in the STATUS data pool is, for example,

FUEL, ABCDEFnn, ORIG = U235, ABCDEFnn, ORIG, .003, U238, ABCDEFnn, ORIG,

where	ABCDEF	is the jobname on the HEAD card,
	nn	is two characters which are blank or give a resonance region number, and the input definition of FUEL is

DEFN FUEL U235 .003 U238 .04

In some burnup applications, a common nuclide data pool may suffice for a number of cell types. This is made possible by specifying

NUCMOD name

where name is 1 to 6 characters which are used rather than
jobname on the right hand side of material definitions.

5.24 Resonance Options

RESPARM nrespa, ε_{r1}, ε_{r2}, ε_{r3}, nangle, numer, multi

with default

RESPARM 1 .001 .002 .001 8 0 1

where nrespa is the number of passes to be made throughout the set of light resonance nuclides for each group,

ε_{r1}, ε_{r2}, ε_{r3} are the accuracy criteria of equations (5.6), (5.20) and (5.89), respectively, of Robinson [1977],

nangle is the order of Gaussian quadrature in the collision probability evaluation,

numer is a switch which, for a non-zero value, allows the numerical collision probability routine to be used in cylindrical geometry, and

multi is a switch whereby non-zero means that λ is mesh dependent and it is recommended that zero be used when there is more than one mesh interval per physical region. Weighting by volume and resonance nuclide concentration is used to form the average λ.

RESOPT m n

with default

RESOPT 0 0

where $m \neq o$ results in an additional resonance overlap effect which depends on the average position of resonances in a group and the group resonance escape probability for other resonance reactions,

$n = 1$ if the Hill-Schaeffer λ method is to be replaced by a pseudo NR method for fissile nuclides, and

$n = 2$ if the pseudo NR method is to be used for all nuclides.

In the pseudo NR method, a λ value is applied to the resonance nuclide only; this allows conformity with the derivation of the subgroup parameters on the library but is otherwise an NR method.

EFOFP E_p
with default
EFOFP 5.E+4

where E_p is the energy in eV above which the removal correction factor $f_\ell(p_g)$ given in section 5.8 of Robinson [1977] is not applied.

PEARLS ipearl

with default

PEARLS 0

where	ipearl	takes the values
	0	normal calculation,
	1	a slowing down calculation in which the source term of the homogeneous flux calculation is an asymptotic slowing down source rather than a fission source, and
	2	as for 1 but with a neutron mass of unity.

This entry is used for comparisons with the PEARLS code using a special purpose cross-section library which includes nuclide slowing-down distributions in place of fission spectra.

5.25 Flux Options

GFLUX $\phi_1, \ldots, \phi_{NG}$

or

GFLUX WESTCOTT r

with default

GFLUX WESCOTT .08

where	ϕ_i	is a group flux estimate for the i^{th} library group,
	r(>0)	is the ratio of epithermal to thermal flux in a group flux estimate of Westcott form, and
	r(<0)	gives an estimated flux/lethargy of an integrated fission spectrum times $E^{|r|}$.

This flux estimate is normally used only to weight the fission spectra for use in the homogeneous flux calculation, hence is of no importance.

FLUXPARM limfl, limsea, nscale, ε_f

with default

FLUXPARM 40 10 3 1.E-4

where	limfl	is limit on the number of iterations to converge the group flux calculation,
	limsea	is not used at present,
	nscale	is the number of broad groups used in scaling the thermal flux to improve convergence, and
	ε_f	is the required flux accuracy.

If limfl = 0, a flux calculation is not performed and cross sections may be averaged over an input flux spectrum given by GFLUX.

5.26 TEST Print Control of Intermediate Data

TEST n

with default

TEST 0

where	n = 0	for a normal printout of input data, cross-section library contents, material table, k_{eff}, flux and reaction rates in the library groups
	= 1	prints, additionally, the cross sections of resonance nuclides,
	= 2	prints, additionally to 1, information on the resonance calculation and the flux convergence which is used in debugging,
	= -1	prevents most normal printout, including the library contents if a TEST card is placed first.

5.27 WRITE GEOMLIB Write Geometry

WRITE GEOMLIB

The entry causes a geometry data pool to be written immediately and may be used to create a geometry data pool which is different from the geometry of the MIRANDA calculation.

5.28 Options for Photon Treatment*

The default option is to ignore any photon data on the cross-section library so that neutron-only calculations are not affected by the presence of those data. Treatment of photons is performed if a group structure for photon output is specified. There are three entries which control the photon treatment.

GAMMA n $g_1, \ldots, g_{n+1}$

where |n| is the number of condensed photon groups,
n>0 results in an output AUS cross-section data pool in which photon groups are treated as for neutron groups,
n<0 results in an output AUS cross-section data pool in which photon groups are stored separately (normally such data are used as input to MIRANDA only), and
g_i are photon group boundaries as for the GROUPS entry.

When GAMMA is specified, the default calculation is a B_L calculation of the photon flux of the order specified on the BUCK entry, using a photon production source from the neutron flux calculation. As for the GSCE entry for neutrons, this default may be altered by using a GASCE entry to specify the source in each photon group.

GAFLUX $\phi_1, \ldots, \phi_N$
or
GAFLUX -1

cause the B_L photon flux calculation to be bypassed, ϕ_i specifies the flux in the i^{th} photon group, and -1 causes a constant in energy flux to be used. A blank GAFLUX entry restores the default B_L calculation.

The default order of P_n scattering expansion for photon interaction data on output is the same as that for neutrons. To modify this default, GAP n is included on the OUTPUT entry.

5.29 START Begin Calculation*

START

The entry causes the calculation which has been set up by the previous entries to begin.

5.30 Control of STATUS Data Pool

READ STATUS

This entry causes the STATUS data pool to be read immediately. This will set up a succeeding calculation which is specified by the STATUS data pool.

STATOFF

This entry causes nothing to be written on either STATUS data pool. It is useful for perturbations on a burnup calculation. The normal usage would be

(a) burnup to a required time,

(b) perform perturbed calculations with STATOFF,

(c) perform standard calculations and continue burnup.

5.31 STOP*

STOP

This entry causes termination of the module.

5.32 Example

A sample of input for a lattice calculation using the modules MIRANDA, ANAUSN [Clancy 1982] and EDITAR [Robinson 1986] is given below. The calculation includes

(i) MIRANDA - 3-region resonance calculation, B_3 flux calculation and condensation to 26 groups;

(ii) ANAUSN - 26-group k_∞ spatial calculation in S_6 with P_1 scattering; and

(iii) EDITAR - edit of ANAUSN fluxes, B_3 flux calculation to give final k_{eff} and two-group reaction rates.

```
// EXEC AUS
//GO.SYSIN  DD *
*DD1
STEP *
          LINK MIRANDA
          LINK ANAUSN(1,3)
          LINK EDITAR(1,4)
          END
STOP
*DD2
HEAD TRX1 REF ENDF-202
DEFN FUEL U235 6.253-4 U238 4.7205-2
DEFN VOID O 1.-10
DEFN CLAD AL .06025
DEFN MOD H2O .03338
REQD FUEL VOID CLAD MOD U235 U238
RM 0 5*.0983 .0127 .0711 5*.0745836 0
REG 1(1)5 FUEL 6 VOID 7 CLAD 8(1)12 MOD
RESREG 0 .4915 .0838 .372918 0 SMEAR 5*1 2 2 5*3
BUCK B3 5.7-3
OUTPUT P3
GROUPS 26 1 3(2)11(6)41 51 61 71 80(4)128
START
STOP
*DD3
TRX
AUS NL 1 NSN 6 END
*DD4
BUCK B3 5.7-3   SEARCH OFF
GROUPS 2 1 15 26
OUTPUT RR START
```

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APPENDIX A

CONTENTS OF THE CROSS-SECTION LIBRARIES

TABLE A1

NEUTRON GROUP BOUNDARIES FOR AUS.ENDF200G

Group	Lower Energy (MeV)	Lethargy	Group	Lower Energy (MeV)	Lethargy	Group	Lower Energy (keV)	Lethargy
0	15.488	-0.43750						
1	15.012	-0.40625	34	2.231	1.5000	67	283.68	3.5625
2	14.550	-0.37500	35	2.096	1.5625	68	266.49	3.6250
3	14.102	-0.34375	36	1.969	1.6250	69	250.35	3.6875
4	13.668	-0.31250	37	1.850	1.6875	70	235.18	3.7500
5	13.248	-0.28125	38	1.738	1.7500	71	220.93	3.8125
6	12.840	-0.25000	39	1.632	1.8125	72	207.54	3.8750
7	12.062	-0.18750	40	1.534	1.8750	73	194.97	3.9375
8	11.331	-0.12500	41	1.441	1.9375	74	183.16	4.0000
9	10.645	-0.06250	42	1.353	2.0000	75	172.06	4.0625
10	10.000	0.0	43	1.271	2.0625	76	161.63	4.1250
11	9.394	0.06250	44	1.194	2.1250	77	151.84	4.1875
12	8.825	0.12500	45	1.122	2.1875	78	142.64	4.2500
13	8.290	0.18750	46	1.054	2.2500	79	125.88	4.3750
14	7.788	0.25000	47	0.990	2.3125	80	111.09	4.5000
15	7.316	0.31250	48	0.930	2.3750	81	98.04	4.6250
16	6.873	0.37500	49	0.874	2.4375	82	86.52	4.7500
17	6.456	0.43750	50	0.821	2.5000	83	76.35	4.8750
18	6.065	0.50000	51	0.771	2.5625	84	67.38	5.0000
19	5.698	0.56250	52	0.724	2.6250	85	59.46	5.1250
20	5.353	0.62500	53	0.681	2.6875	86	52.48	5.2500
21	5.028	0.68750	54	0.639	2.7500	87	46.31	5.3750
22	4.724	0.75000	55	0.601	2.8125	88	40.87	5.5000
23	4.437	0.81250	56	0.564	2.8750	89	36.07	5.6250
24	4.169	0.87500	57	0.530	2.9375	90	31.83	5.7500
25	3.916	0.93750	58	0.498	3.0000	91	28.09	5.8750
26	3.679	1.00000	59	0.468	3.0625	92	24.79	6.0000
27	3.456	1.06250	60	0.439	3.1250	93	21.87	6.1250
28	3.247	1.12500	61	0.413	3.1875	94	19.30	6.2500
29	3.050	1.18750	62	0.388	3.2500	95	17.04	6.3750
30	2.865	1.25000	63	0.364	3.3125	96	15.03	6.5000
31	2.691	1.31250	64	0.342	3.3750	97	13.27	6.6250
32	2.528	1.37500	65	0.321	3.4375	98	11.71	6.7500
33	2.375	1.43750	66	0.302	3.5000	99	10.33	6.8750

TABLE A1 (cont'd)

Group	Lower Energy (eV)	Lethargy	Group	Lower Energy (eV)	Lethargy	Group	Lower Energy (eV)	Lethargy
100	9118.82	7.000	134	13.7096	13.50	168	0.18602	17.8
101	8047.33	7.125	135	10.6770	13.75	169	0.16832	17.9
102	7101.74	7.250	136	8.3153	14.00	170	0.15230	18.0
103	6267.27	7.375	137	6.4760	14.25	171	0.13781	18.1
104	5530.84	7.500	138	5.0435	14.50	172	0.12469	18.2
105	4880.95	7.625	139	3.9279	14.75	173	0.11283	18.3
106	4307.42	7.750	140	3.0590	15.00	174	0.10209	18.4
107	3801.29	7.875	141	2.7679	15.10	175	0.09237	18.5
108	3354.63	8.000	142	2.5045	15.20	176	0.08358	18.6
109	2960.45	8.125	143	2.2662	15.30	177	0.07563	18.7
110	2612.59	8.250	144	2.0505	15.40	178	0.06843	18.8
111	2305.60	8.375	145	1.8554	15.50	179	0.06192	18.9
112	2034.68	8.500	146	1.6788	15.60	180	0.05603	19.0
113	1795.60	8.625	147	1.5191	15.70	181	0.05070	19.1
114	1584.61	8.750	148	1.3745	15.80	182	0.04587	19.2
115	1398.42	8.875	149	1.2437	15.90	183	0.04151	19.3
116	1234.10	9.000	150	1.1254	16.00	184	0.03756	19.4
117	961.12	9.250	151	1.0183	16.10	185	0.03398	19.5
118	748.52	9.500	152	0.9214	16.20	186	0.03075	19.6
119	582.95	9.750	153	0.8337	16.30	187	0.02782	19.7
120	454.00	10.000	154	0.7544	16.40	188	0.02517	19.8
121	353.57	10.250	155	0.6826	16.50	189	0.02278	19.9
122	275.36	10.500	156	0.6176	16.60	190	0.02061	20.0
123	214.45	10.750	157	0.5588	16.70	191	0.01865	20.1
124	167.02	11.000	158	0.5057	16.80	192	0.01688	20.2
125	130.07	11.250	159	0.4575	16.90	193	0.01527	20.3
126	101.30	11.500	160	0.4140	17.00	194	0.01382	20.4
127	78.89	11.750	161	0.3746	17.10	195	0.01250	20.5
128	61.44	12.000	162	0.3390	17.20	196	0.00758	21.0
129	47.85	12.250	163	0.3067	17.30	197	0.00460	21.5
130	37.27	12.500	164	0.2775	17.40	198	0.00279	22.0
131	29.02	12.750	165	0.2511	17.50	199	0.00169	22.5
132	22.60	13.000	166	0.2272	17.60	200	0.00001	27.6
133	17.60	13.250	167	0.2056	17.70			

TABLE A2
NEUTRON GROUP BOUNDARIES FOR AUS.ENDFB

Group	Lower Energy (keV)	Lethargy	Group	Lower Energy (eV)	Lethargy
0	12640.25	-0.25			
1	10000.00	0.0	33	3354.63	8.00
2	7788.01	0.25	34	2612.59	8.25
3	6065.30	0.50	35	2034.68	8.50
4	4723.66	0.75	36	1584.61	8.75
5	3678.79	1.00	37	1234.10	9.00
6	2865.05	1.25	38	961.12	9.25
7	2231.30	1.50	39	748.52	9.50
8	1737.74	1.75	40	582.95	9.75
9	1353.35	2.00	41	454.00	10.00
10	1053.99	2.25	42	353.57	10.25
11	820.85	2.50	43	275.36	10.50
12	639.28	2.75	44	214.45	10.75
13	497.87	3.00	45	167.02	11.00
14	387.74	3.25	46	130.07	11.25
15	301.97	3.50	47	101.30	11.50
16	235.18	3.75	48	78.89	11.75
17	183.16	4.00	49	61.44	12.00
18	142.64	4.25	50	47.85	12.25
19	111.09	4.50	51	37.27	12.50
20	86.52	4.75	52	29.02	12.75
21	67.38	5.00	53	22.60	13.00
22	52.48	5.25	54	17.60	13.25
23	40.87	5.50	55	13.71	13.50
24	31.83	5.75	56	10.68	13.75
25	24.79	6.00	57	9.19	13.90
26	19.30	6.25	58	8.32	14.00
27	15.03	6.50	59	7.52	14.10
28	11.71	6.75	60	6.81	14.20
29	9.12	7.00	61	6.16	14.30
30	7.10	7.25	62	5.57	14.40
31	5.53	7.50	63	5.04	14.50
32	4.31	7.75	64	4.56	14.60

TABLE A2 (cont'd)

Group	Lower Energy (eV)	Lethargy	Group	Lower Energy (eV)	Lethargy
65	4.1292	14.7	97	0.16832	17.9
66	3.7363	14.8	98	0.15230	18.0
67	3.3807	14.9	99	0.13781	18.1
68	3.0590	15.0	100	0.12469	18.2
69	2.7679	15.1	101	0.11283	18.3
70	2.5045	15.2	102	0.10209	18.4
71	2.2662	15.3	103	0.09237	18.5
72	2.0505	15.4	104	0.08358	18.6
73	1.8554	15.5	105	0.07563	18.7
74	1.6788	15.6	106	0.06843	18.8
75	1.5191	15.7	107	0.06192	18.9
76	1.3745	15.8	108	0.05603	19.0
77	1.2437	15.9	109	0.05070	19.1
78	1.1254	16.0	110	0.04587	19.2
79	1.0183	16.1	111	0.04151	19.3
80	0.9214	16.2	112	0.03756	19.4
81	0.8337	16.3	113	0.03398	19.5
82	0.7544	16.4	114	0.03075	19.6
83	0.6826	16.5	115	0.02782	19.7
84	0.6176	16.6	116	0.02517	19.8
85	0.5588	16.7	117	0.02278	19.9
86	0.5057	16.8	118	0.02061	20.0
87	0.4575	16.9	119	0.01865	20.1
88	0.4140	17.0	120	0.01688	20.2
89	0.3746	17.1	121	0.01527	20.3
90	0.3390	17.2	122	0.01382	20.4
91	0.3067	17.3	123	0.01250	20.5
92	0.2775	17.4	124	0.00758	21.0
93	0.2511	17.5	125	0.00460	21.5
94	0.2272	17.6	126	0.00279	22.0
95	0.2056	17.7	127	0.00169	22.5
96	0.1860	17.8	128	0.00103	23.0

TABLE A3
PHOTON GROUP BOUNDARIES

Group	Lower Energy (MeV)	Group	Lower Energy (keV)
0	20.0		
1	14.0	20	1000
2	12.0	21	800
3	10.0	22	700
4	8.0	23	600
5	7.5	24	512
6	7.0	25	510
7	6.5	26	450
8	6.0	27	400
9	5.5	28	300
10	5.0	29	200
11	4.5	30	150
12	4.0	31	100
13	3.5	32	70
14	3.0	33	60
15	2.5	34	45
16	2.0	35	30
17	1.66	36	20
18	1.5	37	10
19	1.33		

TABLE A4
NUCLIDES IN AUS.ENDF200G

Name	Source		Pn Order	Temperature Range	Resonance Data?	Photon Data?
ZZ999	ZZ999	ORIG	-			No
CH2	ENDFB4	ORIG	7	296		
H2O	ENDFB4	ORIG	7	296-1000		
D2O	ENDFB4	ORIG	7	296-1000		
HE3	ENDFB4	ORIG	3	300		No
C	ENDFB4	ORIG	7	296-1600		
BE	ENDFB4	ORIG	7	296-1000		
O	ENDFB4	ORIG	7	296-3000		
LI6	ENDFB4	ORIG	7	300		
LI7	ENDFB4	ORIG	7	300		
B10	ENDFB4	ORIG	3	300		
B11	ENDFB4	ORIG	3	300		
N	ENDFB4	ORIG	3	300		
F	ENDFB4	ORIG	3	300		No
NA	ENDFB4	ORIG	7	300	Yes	
AL	ENDFB4	ORIG	7	300	Yes	
SI	ENDFB4	ORIG	7	300		
CA	ENDFB4	ORIG	7	300		
TI	ENDFB4	ORIG	3	300		
V	ENDFB4	ORIG	3	300		
CR	ENDFB4	ORIG	7	300	Yes	
MN	ENDFB4	MOD1	3	300	Yes	
FE	ENDFB4	ORIG	7	300	Yes	
FE54D	ENDFB4	ORIG	-			No
CO	ENDFB4	ORIG	3	300		No
NI	ENDFB4	ORIG	7	300	Yes	
NI58	ENDFB503	ORIG	-			No
CU	ENDFB4	ORIG	3	300		No
ZR	ENDFB4	MOD1	7	300		
NB	ENDFB4	ORIG	3	300		
MO	ENDFB4	ORIG	3	300		
CD	ENDFB4	ORIG	3	300		No
I	ENDFB4	ORIG	3	300		
GD	ENDFB4	ORIG	3	300		No
W182	ENDFB4	ORIG	3	300		
W183	ENDFB4	ORIG	3	300		
W184	ENDFB4	ORIG	3	300		
W186	ENDFB4	ORIG	3	300		
PB	ENDFB4	ORIG	7	300		

TABLE A4 (cont'd)

Name	Source		Pn Order	Temperature Range	Resonance Data?	Photon Data?
BI	ENDL8400	ORIG	3	300		
U234	ENDFB4	G128	3	300	Yes	No
U235	ENDFB4	ORIG	7	300-2100	Yes	
U236	ENDFB4	G128	3	300	Yes	No
U237	ENDFB5	ORIG	3	300		No
U238	ENDFB4	ORIG	7	300-2100	Yes	
NP237	ENDFB5	ORIG	3	300		No
NP239	ZAX325	ORIG	-			No
PU238	ENDFB4	ORIG	3	300		No
PU239	ENDFB4	ORIG	3	300-2100	Yes	
PU240	ENDFB4	ORIG	3	300-2100	Yes	
PU241	ENDFB4	ORIG	3	300-2100	Yes	No
PU242	ENDFB4	ORIG	3	300-2100	Yes	No
AM241	ENDFB5	ORIG	3	300		No
AM242M	ENDFB5	ORIG	3	300		No
AM243	ENDFB5	ORIG	3	300		No
CM242	ENDFB502	ORIG	3	300		No
CM243	ENDFB5	ORIG	3	300		No
CM244	ENDFB5	ORIG	3	300		No
CM245	ENDFB5	ORIG	3	300		No

NOTES ON NUCLIDES IN AUS.ENDF 200G

(a) The nuclides CH2, H20, D20, C, BE include S(α,β) data from ENDF/B

(b) The Pn order is that for neutrons. Photon data is of order P_5. A Pn order of 7 implies P_7 for neutron energies above 142 keV and P_3 below that.

(c) Kerma factor data are included only when photon data are given.

(d) Photon production data for deuterium in D20 and B11 are not included.

(e) Photon production data for ZR is from the ENDL library [Howerton 1975].

(f) ZZ999 is a 1/v absorber with a cross section of 1 barn at 0.0253 eV.

(g) Data for U234 and U236 were expanded in a simple manner from AUS.ENDFB.

(h) FE54D is from the dosimetry file. Only (n,p) is given.

TABLE A5
NUCLIDES IN AUS.ENDFB

Name	Source		Pn Order	Temperature Range	Resonance Data?
TH232	ENDFB4	ORIG	3	300	Yes
PA233	PHF68	MOD3	0	300- 900	Yes
U232	NDXD40	ORIG	0	300	
U233	BNL65PHF	MOD2	0	300- 900	Yes
U233	ENDFB4	ORIG	3	300	
U234	ENDFB4	ORIG	3	300	Yes
U235	ENDFB4	ORIG	3	300- 900	Yes
U235	ENDFB4	MOD1	3	300- 900	Yes
U236	ENDFB4	ORIG	3	300	Yes
U237	ZAX325	ORIG	-		
NP237	ENDFB4	ORIG	3	300	
U238	ENDFB4	ORIG	3	300- 900	Yes
U238	ENDF45	ORIG	3	300- 900	Yes
NP239	ZAX325	ORIG	-		
PU238	ENDFB4	ORIG	3	300	
PU239	ENDFB4	ORIG	3	300- 900	Yes
PU240	ENDFB4	MOD1	3	300- 900	Yes
PU241	ENDFB4	ORIG	3	300- 900	Yes
PU242	ENDFB4	ORIG	3	300- 900	Yes
AM241	ENDFB4	ORIG	3	300	
AM242M	BNL325	ORIG	-		
AM243	ENDFB4	ORIG	3	300	
CM242	BNL325	ORIG	-		
CM243	BNL325	ORIG	-		
CM244	ENDFB4	ORIG	3	300	
CM245	BNL325	ORIG	-		
CH2	ENDFB3	ORIG	3	296	
H2O	ENDFB3	MOD1	3	296- 600	
H2O	ENDFB4	MOD1	3	296-1000	
D2O	ENDFB3	ORIG	3	296- 400	
D2O	ENDFB4	MOD1	3	296-1000	
C	ENDFB4	ORIG	3	296	
C	ENDFB4	MOD1	3	296-1600	
O	ENDFB3	ORIG	3	296-1200	
O	ENDFB4	MOD1	3	296-3000	
BEO	NDXD40	MOD1	0	1200	
BE	ENDFB3	ORIG	3	296	
NA	ENDFB3	MOD1	3	300	Yes
MG	ENDFB4	ORIG	3	300	

TABLE A5 (cont'd)

Name	Source		Pn Order	Temperature Range	Resonance Data?
AL	ENDFB4	MOD1	3	300	Yes
K	ENDFB4	ORIG	3	300	
CR	ENDFB4	MOD1	3	300	Yes
FE	ENDFB4	MOD1	3	300	Yes
NI	ENDFB4	MOD1	3	300	Yes
ZIRC2	ENDFB4	ORIG	3	300	
LI6	AEEW69	ORIG	-		
HE3	AEEW69	ORIG	-		
T3	NDXD4C	ORIG	-		
ZZ999	NDXD127G	ORIG	-		
XX999	NDXD127G	ORIG	-		
B10	ENDFB4	ORIG	3	300	
B11	ENDFB4	ORIG	3	300	
N	AEEW69	ORIG	-		
F	ENDFB4	ORIG	3	300	
SI	ENDFB4	ORIG	3	300	
CL	AEEW69	ORIG	-		
CA	AEEW69	ORIG	-		
V	ENDFB4	ORIG	3	300	
TI	AEEW69	ORIG	-		
MN	ENDFB4	ORIG	3	300	
FE56	ENDFB4	ORIG	-		
CO	ENDFB4	ORIG	3	300	
CU	ENDFB4	MOD1	3	300	Yes
GA	AEEW69	ORIG	-		
CU63	ENDFB4	ORIG	-		
NB	ENDFB4	ORIG	3	300	
MO	ENDFB4	ORIG	3	300	
RH	ENDFB4	ORIG	3	300	
AG107	BNL66	ORIG	-		
CD	AEEW69	ORIG	-		
ER166	BNL73	ORIG	-		
ER167	BNL73	ORIG	-		
LU176	ENDFB4	ORIG	3	300	
TA	ENDFB4	ORIG	3	300	
W	AEEW69	ORIG	-		
W186	BNL66PHF	MOD1	-		
AU	ENDFB4	ORIG	3	300	
PB	ENDFB4	ORIG	3	300	

NOTES ON NUCLIDES IN AUS.ENDFB

(a) Nuclides not from ENDF/B have been obtained mainly from the UKAEA nuclear data file AEEW69 [Norton 1968] for those labelled or BNL 325 for those labelled ZAX325, BNL325, BNL66, BNL73.

(b) The nuclides CH2, H20, D20, C, BE include S(α,β) data from ENDF/B. The ENDFB4 MOD1 versions were prepared using XLACS2.

(c) ZIRC2 is zircaloy 2 (or 4).

(d) ZZ999 is a 1/v absorber with a cross section of 1 barn at 0.0253 eV.

(e) XX999 has a resonance integral of 1 barn

(f) FE56, CU63, and IN115 are from the dosimetry file and have the important reaction only, as AUS reaction 7.

(g) U235 ENDFB4 MOD1 was prepared using the modified methods used for AUS.ENDF200G.

(h) U238 ENDF45 is from ENDF/B IV but with the resonance parameters replaced by those of de Saussure et al. [1978].

TABLE A6
FISSION PRODUCTS IN AUS.ENDFB

Mass numbers and possible isometric state for each element

	Normal Set	Extended Set
GE		72 73 74 76
AS		75
SE		76 77 78 80 82
BR		81
KR	83	82 84 85 86
RB		85 87
SR		86 88 89 90
Y		89 91
ZR	95	90 91 92 93 94 96
NB	95	
MO	95	96 97 98 99 100
TC	99	
RU	100 101 102 103	104 106
RH	103 105	
PD	104 105 106 107 108	110
AG	109	111
CD	113	110 111 112 114 115M 116
IN		115
SN		116 117 118 119 120 122 123 124 126
SB		121 123 124 125
TE		122 123 124 125 126 127M 128 129M 130
I		127 129 131 135
XE	131 133 135	128 130 132 134 136
CS	133 134 135	136 137
BA		134 136 137 138 140
LA		139 140
CE	144	140 141 142 143
PR	143	141
ND	143 144 145 146 147 148	142 150
PM	147 148M 148 149	151
SM	147 149 150 151 152	148 153 154
EU	153 154 155	156
GD	157	154 155 156 158 160
TB		159 160
DY		160 161 162 163 164
HO		165

(a) A pseudo fission product PFP is used with the normal set to represent the reactivity effect of the extended set.

(b) All cross section data from ENDF/B IV.

(c) Only P_0 scattering matrices are given.

(d) Resonance subgroup data are not given.

(e) Yields taken from Crouch [1977] are included for ^{233}U, ^{235}U, ^{238}U, ^{239}Pu, ^{241}Pu and ^{239}Pu in a fast neutron spectrum.

APPENDIX B
MODIFICATIONS TO THE METHODS OF PREPARING RESONANCE DATA FOR THE LIBRARY

The modifications given below have been used in the generation of the AUS.ENDF200G library. These modifications are given with respect to the methods detailed in appendix B of Robinson [1977], which were used to generate AUS.ENDFB. There are a number of errata to that appendix :

In appendix B2

$$k = 2.196771\times10^{-3}\ E^{1/2}A'/(A'+1)$$

$$x_r = 2(E-E_r)/\Gamma_r$$

In appendix B3

$$F = \left(1 - \frac{1}{\langle D_s\rangle}\int_0^\infty P_n(r)\int_0^\infty P_k(t)\Gamma_s\, J(\theta,\beta)\,dt\,dr\right)(1-2\sin^2\Phi_\ell)$$

$$I_x = \frac{1}{5}\sum_i \frac{\sigma_p\,(\langle\sigma_x(E_i)\rangle + \sigma_{Bx}(E_i))}{\sigma_p + \langle\sigma_\gamma(E_i)\rangle + \langle\sigma_f(E_i)\rangle + \langle\sigma_s(E_i)\rangle + \sigma_{Btot}(E_i)}$$

In appendix B5

$$\hat{\sigma}_{pi} = (\sigma_{Hi} + \lambda_{\ell i}\,\sigma_{p\ell})\ \frac{I_a^\infty + I_s^\infty}{I_a^\infty + \lambda_{\ell i}\, I_s^\infty}$$

The only modification in the method for generating point cross sections in the resolved resonance range [appendix B2, Robinson 1977] is to the treatment of distant resonance levels. In the new treatment, the contribution from distant levels is evaluated using the standard formulae but the evaluation is performed at a reduced number of points. Linear interpolation of the distant level contribution is used between these evaluated points. The formulae of appendix B2 [Robinson 1977] for single level Breit-Wigner parameters have also been used in the unresolved resonance range. In that range a fixed number of resonances has been summed at each point. Sufficient resonances were included to give better than 0.6 per cent accuracy in group cross sections.

The method of calculating group resonance integrals in the unresolved resonance range by direct integration over the width distributions [appendix B3, Robinson 1977] has been little changed, but it is now only applied above 19.3 keV. The change is to renormalise the results to the infinitely dilute cross sections obtained by a refinement of the method. In the refinement, a ten-point integration over fission and neutron width distributions is performed to evaluate the average cross sections at each energy at which average resonance parameters are given in ENDF/B. Then cross sections interpolated from these average point cross sections are group-averaged using 100 equal lethargy intervals in each group. The refined method follows the ENDF/B IV prescription. As well as being used to renormalise the direct integration results, the infinitely dilute average cross sections are used to normalise the resonance ladder method discussed below.

The main method used in the unresolved range is the ladder method, in which a ladder of resonances is constructed by sampling from the resonance spacing and level width distributions. A ladder has been chosen which reproduces the infinitely dilute group cross sections.

To achieve this for each group for each ℓ ,J state:

- infinitely dilute group cross sections are calculated as above;
- a ladder of resonances is generated and the infinitely dilute group cross sections calculated for these resonances;
- the ladder is accepted if the error contributed to the total fission, capture and scattering cross sections is less than an error criterion;
- if the error is exceeded, further ladders are generated till one is satisfactory or a maximum number of ladders is reached; and
- the best ladder is used if the maximum is reached.

Final agreement with the infinitely dilute group cross sections is obtained by normalisation of the point cross sections generated from the selected resonance parameters. In practice, 0.5 per cent accuracy has been requested with a maximum of 500 ladders tested. The final normalisation has not differed from 1.0 by more than a few per cent. the method has been applied to ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu and ^{242}Pu but only s wave parameters were generated for ^{235}U and ^{241}Pu. The procedure for ladder selection was performed for 0.25 lethargy width groups.

Two modifications have been made to the calculation of group data from a slowing down calculation using point cross section data [appendix B4, Robinson 1977]. The first is simply to allow the resonance nuclide to scatter through more than one group. The second modification makes the calculation of the factor F_g, which accounts for the non-asymptotic value of the group source, conform with the MIRANDA group removal correction factor. The formula for the S_g term in the F_g formula becomes

$$S_g = \sigma_H(E_g - E_{g+1})\left\{ \frac{\phi_{00}}{E_1} + \sum_{h=1}^{g-1} \left[\frac{1}{E_{h+1}} - \frac{1}{E_h} \right] R'_h \phi_{oh} \bar{p}_h f_H(Q_h) \right\}$$

$$+ \sum_{h=1}^{g-1} \sigma_{\ell,h\to g} R'_h \tau_h \phi_{oh} \bar{p}_h f_\ell(Q_h)$$

where

$$\bar{p}_g = p(E_g)\left[\frac{Q_g E_g - E_{g+1}}{E_g - E_{g+1}} + \frac{1-Q_g}{\tau_g} \right]$$

and

$$Q_g = p(E_{g+1})/p(E_g) \quad .$$