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SAMMY User Guidance for ENDF Formats

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ACKNOWLEDGMENTS

Many of the pages of this document were borrowed from the ENDF-102 manual and modified slightly to provide more clarity to SAMMY users. The author gratefully acknowledges the debt owed to the many authors and editors of the ENDF-102 manual.

Members of the Oak Ridge Nuclear Data Group have provided encouragement and assistance in the development of this document, and their contributions are greatly appreciated. Special thanks go to Royce Sayer, whose ^{35}Cl evaluation created the ENDF File 2 and File 32 shown in examples number 17 and 18 of this document, and to Dorothea Wiarda, who patiently assisted in debugging the SAMMY implementation of the newer ENDF formats.

ABSTRACT

The purpose of this document is to gather into one location information relevant to the use of ENDF formats in the resolved resonance region, with emphasis on the use of those formats within the SAMMY evaluation code. This document contains those portions of the ENDF formats manual (ENDF-102) relevant to the resolved resonance region, with a few corrections and occasional comments interjected into the text (in blue ink, to distinguish from the original ENDF-102 verbiage) to highlight the usage within SAMMY. Examples of ENDF File 2 (resonance parameters) and File 32 (covariances for resonance parameters) are also included.

I. INTRODUCTION

The SAMMY code [Ref. 1] is widely used for analysis and evaluation of neutron-induced time-of-flight experimental data in the resonance region.   One important product of such evaluations is a set of R-matrix parameters and the associated covariance matrix which provide the best description of the experimental data. For these data to be useful for reactor or criticality calculations, the resonance parameters and covariance matrix must be written into appropriate formats and reported to appropriate groups such as the Cross Section Evaluation Working Group (CSEWG) [Ref. 2] for inclusion in the Evaluated Nuclear Data Files [Ref. 3].

The SAMMY code contains post-processing capability for creating the relevant portions of the ENDF files. This report serves as documentation of the ENDF formats written and/or read by SAMMY. Much of the information contained in this report is also included in the official ENDF document ENDF-102 [Ref. 4]. One major exception is the examples given in Section VI, which are not in the ENDF-102 manual.

Pages in this report are formatted somewhat differently from those in ENDF-102, for easier legibility. Short sections, for example, are printed on one page rather than divided across two. References to sections of the ENDF-102 manual that are not repeated in this report are so noted in the text. Within this report, sections of the ENDF-102 manual may contain comments added by this author to clarify usage with regard to SAMMY; these comments are printed in blue to distinguish them from the original ENDF-102 verbiage.

This report covers only "File 2" and "File 32" of the many files included in an ENDF file. Moreover, only the resolved resonance portions of these two files are discussed.

Section II of this document corresponds to ENDF-102 Section 0.7 (General Description). Section III corresponds to ENDF-102 Section 2 (File 2, Resonance Parameters).   Section IV corresponds to ENDF-102 Section 32 (File 32, Covariances of Resonance Parameters). Section V corresponds to ENDF-102 Appendix D.1 (Resolved Resonance Region Formulae). Section VI contains realistic annotated examples for both File 2 and File 32, for four different resonance parameter formats (LRF = 1, 2, 3, and 7) and three different representations of the covariance matrix (LCOMP = 0, 1, and 2).

This document will not be published on paper, but instead will be made available only in electronic format, fully bookmarked and interlinked.   The file is downloadable from the SAMMY section of the ORNL Nuclear Data Group's web site http://www.ornl.gov/sci/nuclear_science_technology/nuclear_data/sammy/.
For anyone who wishes to print hard copy, a second version of the file will be available. This version has blank pages inserted as necessary so that double-sided copy will be properly paginated.

The latest version of the SAMMY code was released in October, 2006. Updates for errors uncovered in the code subsequent to that release are available from the author at LarsonNM@ornl.gov. Because some of the updates pertain to the new ENDF formats, anyone using sammy-7.0.0 to create ENDF File 2 or File 32 will want to have the updates.

II. GENERAL DESCRIPTION OF ENDF-102 FORMATS

In order for this report to be sufficiently complete that the user need not constantly refer to the ENDF-102 manual [Ref. 4], portions of that document are repeated here. Information in the remainder of this section is taken essentially verbatim from Section 0.7 of the ENDF-102 manual. However, the layout of the pages has been reformatted to make it easier to read and to make the outline style more prominent. Subsections are as follows:

0.7. General Description of Data Formats

An ENDF "tape" is built up from a small number of basic structures called "records," such as TPID, TEND, CONT, TAB1, and so on. These "records" normally consist of one or more 80-character FORTRAN records. It is also possible to use binary mode, where each of the basic structures is implemented as a FORTRAN logical record. The advantage of using these basic ENDF "records" is that a small library of utility subroutines can be used to read and write the records in a uniform way.

0.7.1. Structure of an ENDF Data Tape

The structure of an ENDF data tape (file) is illustrated schematically in Fig. 0.3. The tape contains a single record at the beginning that identifies the tape. The major subdivision between these records is by *material*. The data for a material is divided into *files*, and each file (MF number) contains the data for a certain class of information. A file is subdivided into *sections*, each one containing data for a particular reaction type (MT number). Finally, a section is divided into records. Every record on a tape contains three identification numbers: MAT, MF, and MT. These numbers are always in increasing numerical order, and the hierarchy is MAT, MF, MT. The end of a section, file, or material is signaled by special records called SEND, FEND, and MEND, respectively.

Figure 0.3

Structure of an ENDF data tape
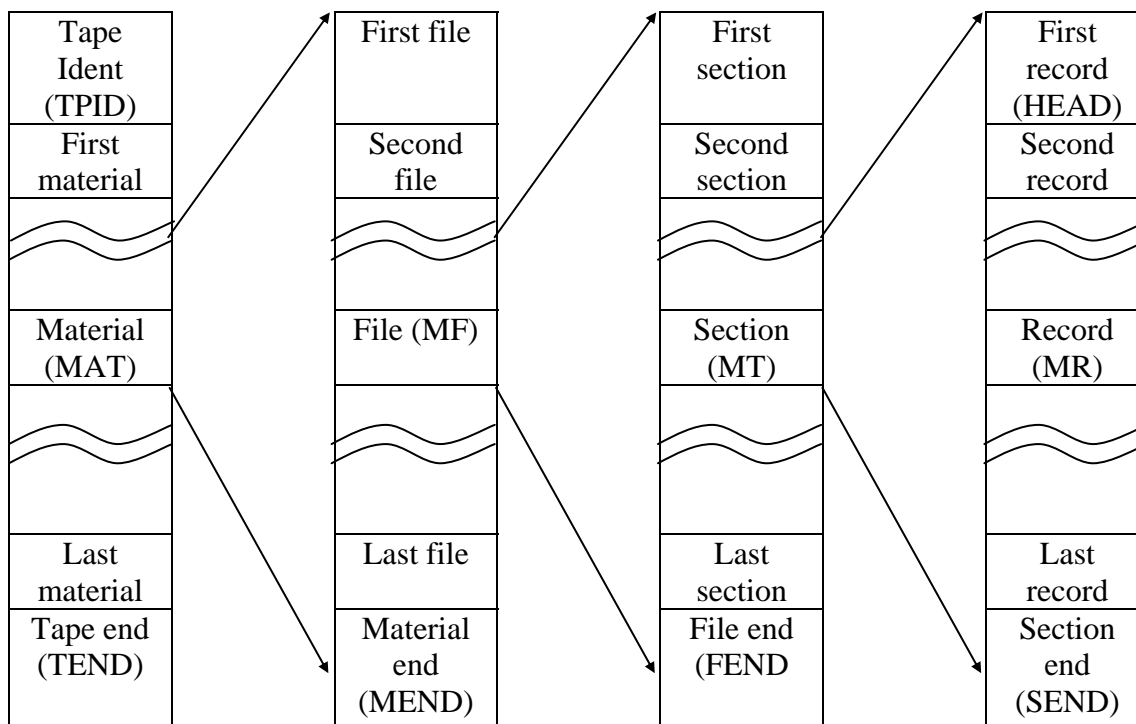
0.7.2. Format Nomenclature

An attempt has been made to use an internally consistent notation based on the following rules.

a) Symbols starting with the letter I, J, K, L, M, or N are integers. All other symbols refer to floating-point (real) numbers.
b) The letter I or a symbol starting with I refers to an interpolation code (see Section 0.6.2 of the ENDF-102 manual, which is not repeated in this report).
c) Letters J, K, L, M, or N when used alone are indices.
d) A symbol starting with M is a control number. Examples are MAT, MF, and MT.
e) A symbol starting with L is a test number.

A symbol starting with N is a count of items.

All numbers are given in fields of 11 columns. In character mode, floating-point numbers should be entered in one of the following forms:

$\pm 1.234567 \pm n$

$\pm 1.23456 \pm nn$, where $nn \le 38$

depending on the size of the exponent. Both of these forms can be read by the "E11.0" format specification of FORTRAN. However, a special subroutine available to the NNDC must be used to output numbers in the above format. If evaluations are produced using numbers written by "1PE11.5" (that is, $1.2345E \pm nn$), the numbers will be standardized into 6- or 7-digit form, but the real precision will remain at the 5-digit level.

In the resolved resonance region, the five significant digits provided by this format are often inadequate, especially for the resonance energies for nuclides such as ^{235}U for which the density of resonances is high. SAMMY generally produces ENDF File 2 with ten significant digits. In cases for which it is important to retain the large numbers of significant digits, evaluators should take care when submitting a SAMMY-generated ENDF File 2 to be used in the evaluated nuclear data files, to be sure that subsequent processing of the file does not truncate the values.

0.7.3. Types of Records

All records on an ENDF tape are one of six possible types, denoted by TEXT, CONT, LIST, TAB1, TAB2, and INTG. The CONT record has six special cases called DIR, HEAD, SEND, FEND, MEND, and TEND. The TEXT record has the special case TPID. Every record contains the basic control numbers MAT, MF, and MT, as well as a sequence number. The definitions of the other fields in each record will depend on its usage as described below.

0.7.4. TEXT Records

This record is used either as the first entry on an ENDF tape (TPID) or to give the comments in File 1. It is indicated by the following shorthand notation:

    [MAT, MF, MT/ HL] TEXT

where HL is 66 characters of text information. The TEXT record can be read with the following FORTRAN statements:

        READ(LIB,10)HL,MAT,MF,MT,NS
     10 FORMAT(A66,I4,I2,I3,I5)

where NS is the sequence number.[1] For a normal TEXT record, MF = 1 and MT = 451. For a TPID record, MAT contains the tape number NTAPE, and MF and MT are both zero.

---

[1] Records are sequentially numbered within a given MAT/MF/MT.

0.7.5. Control Records

0.7.5.1. CONT Records

The smallest possible record is a control (CONT) record. For convenience, a CONT record is denoted by

```
[MAT,MF,MT/C1,C2,L1,L2,N1,N2]CONT
```

The CONT record can be read with the following FORTRAN statements:

```
   READ(LIB,10)C1,C2,L1,L2,N1,N2,MAT,MF,MT,NS
10 FORMAT(2E11.0,4I11,I4,I2,I3,I5).
```

The actual parameters stored in the six fields C1, C2, L1, L2, N1, and N2 will depend on the application for the CONT record.

0.7.5.2. HEAD Records

The HEAD record is the first in a section and has the same form as CONT, except that the C1 and C2 fields always contain ZA and AWR, respectively.

0.7.5.3. END Records

The SEND, FEND, MEND, and TEND records use only the three control integers, which signal the end of a section, file, material, or tape, respectively. In binary mode, the six standard fields are all zero. In character mode, the six are all zero as follows:

```
[MAT,MF,99999/  0.0,  0.0,   0,   0,   0,   0] SEND²
[MAT, 0,    0/  0.0,  0.0,   0,   0,   0,   0] FEND
[  0, 0,    0/  0.0,  0.0,   0,   0,   0,   0] MEND
[ -1, 0,    0/  0.0,  0.0,   0,   0,   0,   0] TEND
```

0.7.5.4. DIR Records

The DIR records are described in more detail in Section 1.1.1. The only difference between a DIR record and a standard CONT record is that the first two fields in the DIR record are blank in character mode.

---

[2] The SEND record has the sequence number 99999.

0.7.6. LIST Records

This type of record is used to list a series of numbers B1, B2, B3, etc. The values are given in an array B(n), and there are NPL of them. The shorthand notation for the LIST record is

```
[MAT,MF,MT/ C1, C2, L1, L2, NPL, N2/ Bn] LIST
```

The LIST record can be read with the following FORTRAN statements:

```
    READ(LIB,10)C1,C2,L1,L2,NPL,N2,MAT,MF,MT,NS
 10 FORMAT(2E11.0,4I11,I4,I2,I3,I5)
    READ(LIB,20)(B(N),N=1,NPL)
 20 FORMAT(6E11.0)
```

The maximum for NPL varies with use (see Appendix G of the ENDF-102 manual, which is not repeated in this document).

0.7.7. TAB1 Records

These records are used for one-dimensional tabulated functions such as *y(x)*. The data needed to specify a one-dimensional tabulated function are the interpolation tables NBT(N) and INT(N) for each of the NR ranges, and the NP tabulated pairs of *x(n)* and *y(n)*. The shorthand representation is

```
[MAT,MF,MT/ C1, C2, L1, L2, NR, NP/xint/y(x)]TAB1
```

The TAB1 record can be read with the following FORTRAN statements:

```
    READ(LIB,10)C1,C2,L1,L2,NR,NP,MAT,MF,MT,NS
 10 FORMAT(2E11.0,4I11,I4,I2,I3,I5)
    READ(LIB,20)(NBT(N),INT(N),N=1,NR)
 20 FORMAT(6I11)
    READ(LIB,30)(X(N),Y(N),N=1,NP)
 30 FORMAT(6E11.0)
```

The limits on NR and NP vary with use (see Appendix G of the ENDF-102 manual, which is not repeated here). The limits must be strictly observed in primary evaluations in order to protect processing codes that use the simple binary format. However, these limits can be relaxed in derived libraries in which resonance parameters have been converted into detailed tabulations of cross section versus energy. Such derived libraries can be written in character mode or a non-standard blocked-binary mode.

0.7.8. TAB2 Records

The last record type is the TAB2 record, which is used to control the tabulation of a two-dimensional function $y(x, z)$. It specifies how many values of z are to be given and how to interpolate between the successive values of z. Tabulated values of $y_l(x)$ at each value of z_l are given in TAB1 or LIST records following the TAB2 record, with the appropriate value of z in the field designated as C2. The shorthand notation for TAB2 is

```
[MAT,MF,MT/ C1, C2, L1, L2, NR, NZ/ Zint]TAB2,
```

The TAB2 record can be read with the following FORTRAN statements:

```
    READ(LIB,10)C1,C2,L1,L2,NR,NZ,MAT,MF,MT,NS
 10 FORMAT(2E11.0,4I11,I4,I2,I3,I5)
    READ(LIB,20)(NBT(N),INT(N),N=1,NR)
 20 FORMAT(6I11)
```

For example, a TAB2 record is used in specifying angular distribution data in File 4. In this case, NZ in the TAB2 record specifies the number of incident energies at which angular distributions are given. Each distribution is given in a LIST or TAB1 record.

0.7.9 INTG records

INTG, or INTeGer, records are used to store a correlation matrix in integer format. The shorthand notation is

```
[MAT,  MF,  MT / II, JJ, KIJ ] INTG
```

where II and JJ are position locators, and KIJ is an array whose dimension is specified by the number of digits NDIGIT to be used for representing the values. NDIGIT can have any value from 2 to 6; the corresponding dimensions (NROW) are 18, 13, 11, 9, and 8, respectively.

The INTG record can be read with the following FORTRAN statements:

```
DIMENSION KIJ(NROW)
IF (NDIGIT.EQ.2) READ (LIB,20) II, JJ, KIJ, MAT, MF, MT, NS
IF (NDIGIT.EQ.3) READ (LIB,30) II, JJ, KIJ, MAT, MF, MT, NS
IF (NDIGIT.EQ.4) READ (LIB,40) II, JJ, KIJ, MAT, MF, MT, NS
IF (NDIGIT.EQ.5) READ (LIB,50) II, JJ, KIJ, MAT, MF, MT, NS
IF (NDIGIT.EQ.6) READ (LIB,60) II, JJ, KIJ, MAT, MF, MT, NS
 20 FORMAT (2I5, 1X, 18I3, 1X,  I4, I2, I3, I5)
 30 FORMAT (2I5, 1X, 13I4, 3X,  I4, I2, I3, I5)
 40 FORMAT (2I5, 1X, 11I5,      I4, I2, I3, I5)
 50 FORMAT (2I5, 1X,  9I6, 1X,  I4, I2, I3, I5)
 60 FORMAT (2I5,       8I7,     I4, I2, I3, I5)
```

See File 32, LCOMP = 2, for details regarding the use of this format. The NDIGIT = 2 format was approved by CSEWG for use in ENDF in 2004; the general case (NDIGIT = 2 through 6) was approved during the November 2006 CSEWG meeting.

III. INTRODUCTION TO ENDF FILE 2: PARAMETERS FOR RESOLVED RESONANCE REGION

In this section are given the various ENDF formats for presentation of R-matrix parameters in the resolved resonance region. Information in the remainder of this section is taken essentially verbatim from Section 2.0 of the ENDF-102 manual. However, the layout of the pages has been reformatted to make it easier to read and to make the outline style more prominent. Subsections are as follows:

2   Resonance Parameters
2.1   General Description
2.2   Resolved Resonance Parameters
2.2.1   Formats
2.2.1.1   Single and Multilevel Breit Wigner
2.2.1.2   So-called Reich-Moore Format
2.2.1.3   Adler-Adler (not used in SAMMY, so not reproduced in this report)
2.2.1.4 to 2.2.1.6   Deleted in ENDF-102
2.2.1.7   R-Matrix Limited Format, General
2.2.1.7.1   Specifics for basic RML
2.2.1.7.2   Optional extensions to RML
2.2.1.7.2.1   Different R-Matrix Formulations
2.2.1.7.2.2   Background R-Matrix
2.2.1.7.2.3   Tabulated Phase Shifts (not used in SAMMY)
2.3   Unresolved Resonance Parameters (not included in this report)

Note that information on the unresolved resonance region is absent from this report. The current ENDF format for the unresolved region is inadequate and will likely soon be replaced.

2. FILE 2. RESONANCE PARAMETERS

2.1. General Description

The primary function of File 2 is to contain data for both resolved and unresolved resonance parameters. It has only one section, with the reaction type number MT = 151. A File 2 is required for incident-neutron evaluations, but it may be omitted in other cases. The use of File 2 is controlled by the parameter LRP (see Section 1.1 of ENDF-102, which is not reproduced in this report):

LRP = −1 No File 2 is given. Not allowed for incident neutrons. This option is not relevant for SAMMY.

LRP = 0 No resonance parameters are given except for the scattering radius AP. This option is not available for SAMMY and therefore is not discussed in this report.

AP is included for the convenience of users who need an estimate of the potential scattering cross section. It is not used to calculate a contribution to the scattering cross section, which in this case is represented entirely in File 3.

LRP = 1 Resonance contributions for the total, elastic, fission, and radiative capture cross sections are to be computed from the resonance parameters and added to the corresponding cross sections in File 3.[1] This is the only relevant LRP option for SAMMY.

The File 2 resonance contributions should also be added to any lumped reactions included in File 3. For single-level Breit Wigner (SLBW) and multilevel Breit Wigner (MLBW), any other competing reactions in the resonance range must be given in their entirety in File 3 and included in the background for the total cross section. The effects of the competing reactions on the resonance reactions are included using a single competitive width, Γ_x. This width is given explicitly in the unresolved resonance region, and implicitly in the resolved region. In the latter region, it is permissible for the total width to exceed the sum of the neutron, radiative capture, and fission widths. The difference is interpreted as the competitive width,

$$\Gamma_x = \Gamma - \left(\Gamma_n + \Gamma_\gamma + \Gamma_f\right) \quad .$$

For the so-called Reich-Moore (LRF = 3) or Adler-Adler (LRF = 4) formalisms, competitive reactions are not used.   For the R-Matrix Limited format (LRF = 7), competitive reactions are included as separate channels.

LRP = 2 Resonance parameters are given in File 2 but are not to be used in calculating cross sections, which are assumed to be represented completely in File 3. Used for certain derived libraries only. This option is irrelevant for SAMMY.

---

[1] In the unresolved resonance region, the evaluator may, optionally, specify a different procedure, which uses the unresolved resonance parameters in File 2 solely for the purpose of computing an energy-dependent self-shielding factor. This option is governed by a flag, LSSF, defined in Section 2.3.1 of ENDF-102, and discussed in Section 2.4.21 of ENDF-102; neither of these sections is included in this report. When this option is specified, File 3 is used to specify the entire infinitely dilute cross section, and the function of File 2 is to specify the calculation of self-shielding factors for shielded pointwise or multigroup values.

The resonance parameters for a ***material*** are obtained by specifying the parameters for each ***isotope*** in the ***material***. The data for the various ***isotopes*** are ordered by increasing ZAI values (charge and isotopic mass number). The resonance data for each isotope may be divided into several incident neutron energy ranges, given in order of increasing energy. The energy ranges for an isotope should not overlap; each may contain a different representation of the cross sections.

In addition to these parameterized resonance ranges, the full energy range may contain two additional non-resonance ranges, also non-overlapping. Comments on these ranges follow:

1. The low energy region (LER) is one in which the cross sections are tabulated as smooth functions of energy. Doppler effects must be small enough so that the values are essentially zero degrees Kelvin. For light elements, that is, those whose natural widths far exceed their Doppler widths and hence undergo negligible broadening, the entire energy range can often be represented in this way.   For heavier materials, this region can sometimes be used below the lowest resolved resonances. With a good multilevel resonance fit, the LER can often be omitted entirely, and this is preferred.   An important procedure for the LER is described in Section 2.4.6.4 of ENDF-102, which is not reproduced here.

2. The resolved resonance region (RRR) is one in which resonance parameters for individual resonances are given. Usually this implies that experimental resolution is good enough to "see" the resonances, and to determine their parameters by area or shape analysis, but an evaluator may choose to supply fictitious resolved parameters if he so desires. If the evaluator does this, the resonances must have physically allowed quantum numbers, and be in accord with the statistics of level densities (Appendix D, Section D.2.2 of ENDF-102, which is not reproduced in this report).   A File 3 background may be given. The essential point is that resonance self-shielding can be accounted for by the user for each resonance individually.

3. The unresolved resonance region (URR) is that region in which the resonances still do not actually overlap, so that self-shielding is still important, but experimental resolution is inadequate to determine the parameters of individual resonances. In this situation, self-shielding must be handled on a statistical basis. A File 3 may be given. The interpretation of this cross section depends on the flag LSSF (see Sections 2.3.1 and 2.4.21 of ENDF-102, which is not reproduced in this report). It may be interpreted either as a partial background cross section, to be added to the File 2 contribution, as in the resolved resonance region or it may be interpreted as the entire dilute cross section, in which case File 2 is to be used solely to specify the self-shielding appropriate to this energy region. It is important to choose the boundary between the RRR and the URR so that the statistical assumptions underlying the unresolved resonance treatments are valid. This problem is discussed further in Section 2.4 of ENDF-102, which is not reproduced in this report.

4. The high-energy region (HER) starts at still higher energies where the resonances overlap and the cross sections smooth out, subject only to Ericson fluctuations. The boundary between the URR and HER should be chosen so that self-shielding effects are small in the HER.

File 3 may contain "background cross sections" in the resonance ranges resulting from inadequacies in the resonance representation (e.g., SLBW), the effects of resonances outside the energy range, the average effects of missed resonances, or competing cross sections. If these background cross sections are nonzero, there must be double energy points in File 3 corresponding to each resonance range boundary (except 10^{-5}eV). See Section 2.4 of ENDF-102 (which is not reproduced in this report) for a more complete discussion of backgrounds.

Several representations are allowed for specifying resolved resonance parameters. The flag LRF indicates the representation used for a particular energy range:

LRF = 1   Single-level Breit-Wigner; (no resonance-resonance interference; one single-channel inelastic competitive reaction is allowed). Use of this format is discouraged for new evaluations, which should use the Reich Moore approximation (LRF = 3 or 7).

LRF = 2   Multilevel Breit-Wigner (resonance-resonance interference effects are included in the elastic scattering and total cross sections; one single-channel inelastic competitive reaction is allowed). Use of this format is discouraged for new evaluations, which should use the Reich Moore approximation (LRF = 3 or 7).

LRF = 3   Reich-Moore (multilevel multichannel R-matrix; no competitive reactions allowed).

It is possible to define partial widths $\Gamma_{l\ s_1\ J}$ and $\Gamma_{l\ s_2\ J}$ with two different values of the channel spin, as is required when both the target spin and the orbital angular momentum are greater than zero. This is accomplished by setting the resonance spin parameter AJ to a positive value for the larger channel spin ($s = I + 1/2$) and negative for the smaller channel spin ($s = I - 1/2$). (See definition of AJ in 2.2.1 of ENDF-102, which *is* reproduced in this document.) Older ENDF files have not used this feature, but instead have only positive AJ; in this case, all resonances of a given *l,J* are assumed to have the same channel spin.

For a given resonance, the only rigorously conserved quantities are *J* (total angular momentum) and π (total parity). Nevertheless, this format assumes that both *l* (orbital angular momentum) and *s* (channel spin) are also conserved quantities.

The LRF = 3 format permits only a limited subset of Reich-Moore evaluations, but is adequate for some situations.

LRF = 4   Adler-Adler (level-level and channel-channel interference effects are included in all cross sections via "effective" resonance parameters; usually applied to low-energy fissionable materials; no competitive reactions).

LRF = 5   This option is no longer available.
LRF = 6   This option is no longer available.

LRF = 7   R-Matrix Limited format, which contains all the generality of LRF = 3 plus unlimited numbers and types of channels. This format is appropriate for SAMMY evaluations.

Preferred formalisms for evaluation are discussed in Section 2.4.17 of ENDF-102, which is not reproduced in this report. Further discussion of the above formalisms is contained in the Procedures Section 2.4 of ENDF-102, which is not reproduced in this report. LRF = 7 (or, in some situations, LRF = 3) is the format of choice for SAMMY users.

Each resonance energy range contains a flag, LRU, that indicates whether it contains resolved or unresolved resonance parameters. LRU = 1 means resolved, LRU = 2 means unresolved.

Only one representation is allowed for the unresolved resonance parameters, namely, average single-level Breit-Wigner. However, several options are permitted, designated by the flag LRF. With the first option, LRF = 1, only the average fission width is allowed to vary as a function of incident neutron energy. The second option, LRF = 2, allows the following average parameters to vary: level spacing, fission width, reduced neutron width, radiation width, and a width for the sum of all competitive reactions.

The data formats for the various resonance parameter representations are given in Sections 2.2.1 (resolved) and 2.3.1 (unresolved). (Section 2.2.1 is reproduced in this document; Section 2.3.1 is not.) Formulae for calculating cross sections from the various formalisms are given in Appendix D of ENDF-102, which is reproduced in Section V of this report.

The following quantities have definitions that are the same for all resonance parameter representations:

NIS	Number of isotopes in the material (NIS $\leq$ 10).
ZAI	(Z,A) designation for an isotope.
NER	Number of resonance energy ranges for this isotope.
ABN	Abundance of an isotope in the material. This is a number fraction, not a ***weight*** fraction, nor a ***percent***.

LFW	Flag indicating whether ***average fission widths*** are given in the unresolved resonance region for this isotope:
	
	    LFW = 0, average fission widths ***are not*** given;
	    LFW = 1, average fission widths ***are*** given.

NER	Number of resonance energy ranges for isotope.
EL	Lower limit for an energy range.[2]
EH	Upper limit for an energy range.[2]

LRU	Flag indicating whether this energy range contains data for resolved or unresolved resonance parameters:
	
	    LRU = 0, only the scattering radius is given (LRF = 0, NLS = 0, LFW = 0 are
	             required with this option);
	    LRU = 1, resolved resonance parameters are given.
	    LRU = 2, unresolved resonance parameters are given.

---

[2] These energies are the limits to be used in calculating cross sections from the parameters. Some resolved resonance levels, for example, bound levels, will have resonance energies outside the limits.

LRF	Flag indicating which representation has been used for the energy range. The definition of LRF depends on the value of LRU:
	
	If LRU = 1 (resolved parameters), then
	    LRF = 1, single-level Breit-Wigner (SLBW);
	    LRF = 2, multilevel Breit-Wigner (MLBW);
	    LRF = 3, Reich-Moore (RM);
	    LRF = 4, Adler-Adler (AA);
	    LRF = 5, no longer available;
	    LRF = 6, no longer available;
	    LRF = 7, R-Matrix Limited (RML). This is the recommended format.
	
	If LRU = 2 (unresolved parameters), then
	    LRF = 1, only average fission widths are energy dependent;
	    LRF = 2, average level spacing, competitive reaction widths, reduced neutron
	        widths, radiation widths, and fission widths are energy dependent.

NRO	Flag designating possible energy dependence of the scattering radius:
	    NRO = 0, radius is energy independent;
	    NRO = 1 (not allowed in the ENDF/B-VI library).[3]

NAPS	Flag controlling the use of the two radii, the ***channel radius*** a and the ***scattering radius*** AP.
	
	For NRO = 0 (AP energy-independent), if
	    NAPS = 0, calculate a from Equation (D.0) given in Appendix D, and read
	        AP as a single energy-independent constant on the subsection
	        CONT (range) record; use a in the penetrabilities and shift
	        factors, and AP in the hard-sphere phase shifts;
	    NAPS = 1, do not use Equation (D.0); use AP in the penetrabilities and shift
	        factor as well as in the phase shifts.
	
	For NRO = 1 (AP energy-dependent), if
	    NAPS = 0, calculate a from the above equation and use it in the
	        penetrabilities and shift factors. Read AP(E) as a TAB1 quantity
	        in each subsection and use it in the phase shifts;
	    NAPS = 1, read AP(E) and use it in all three places, P_l, S_l, φ_l;
	    NAPS = 2, read AP(E) and use it in the phase shifts. In addition, read the
	        single, energy-independent quantity AP, see following, and use it
	        in P_l and S_l, overriding the above equation for a.

---

[3] Formerly used for radius expressed as a table of energy, radius pairs.

File 2 contains a single section (MT=151) containing subsections for each energy range of each isotope in the material.

Two versions of the File 2 format structure are presented here. The first one, denoted a *special case*, is instead merely a particular instance of the general case with the particular values NER = 1, LRU = 0, LRF = 0, and NRO = 0.

(1) The structure of File 2, for the *special case* in which just a scattering radius is specified (no resolved or unresolved parameters are given), is as follows (such a material is not permitted to have multiple isotopes or an energy-dependent scattering radius):

```
[MAT, 2,151/  ZA, AWR,   0,   0, NIS,    0] HEAD                    (NIS=1)
[MAT, 2,151/ ZAI, ABN,   0, LFW, NER,    0] CONT
                                           (ZAI=ZA,ABN=1.0,LFW=0,NER=1)
[MAT, 2,151/  EL,  EH, LRU, LRF, NRO, NAPS] CONT
                                           (LRU=0,LRF=0,NRO=0,NAPS=0)
[MAT, 2,151/ SPI,  AP,   0,   0, NLS,    0] CONT                    (NLS=0)
[MAT, 2,  0/ 0.0, 0.0,   0,   0,   0,    0] SEND
[MAT, 0,  0/ 0.0, 0.0,   0,   0,   0,    0] FEND
```

(2) If resonance parameters are given, the structure of File 2 is as follows:

```
[MAT, 2,151/  ZA, AWR,   0,   0, NIS,    0] HEAD
[MAT, 2,151/ ZAI, ABN,   0, LFW, NER,    0] CONT                    (isotope)
[MAT, 2,151/  EL,  EH, LRU, LRF, NRO, NAPS] CONT                    (range)
<Subsection for the first energy range for the first isotope>
(depends on LRU and LRF)
[MAT, 2,151/   EL,  EH, LRU, LRF, NRO, NAPS] CONT                   (range)
<Subsection for the second energy range for the first isotope>
   -------------------------------
   -------------------------------
[MAT, 2,151/   EL,  EH, LRU, LRF, NRO, NAPS] CONT                   (range)
    <Subsection for the last energy range for the last isotope for this material>
[MAT, 2,  0/ 0.0,  0.0,   0,   0,   0,    0] SEND
```

The data are given for all ranges for a given isotope, and then for all isotopes. The data for each range start with a CONT (range) record; those for each isotope, with a CONT (isotope) record. The specifications for the subsections that include resonance parameters are given in Sections 2.2.1 for the resolved resonance region and 2.3.1 for the unresolved resonance region. (Section 2.3.1 is not included in this report.) A multi-isotope material is permitted to have *some*, but not all, isotopes specified by a scattering radius only. The structure of a *subsection* for such an isotope is:

```
[MAT, 2,151/ SPI,  AP,   0,   0, NLS,    0] CONT                    (NLS = 0)
```

and as above LFW = 0, NER = 1, LRU = 0, LRF = 0, NRO = 0, and NAPS = 0 for this isotope.

In the case that NRO ≠ 0, the "range" record preceding each subsection is immediately followed by a record giving the energy dependence of the scattering radius, AP.

[MAT, 2,151/ 0.0,   0.0,   0,   0,   NR,   NP/ E_{int} / AP(E)] TAB1

If NAPS is 0 or 1, the value of AP on the next record of the subsection should be set to 0.0. If NAPS is 2, the value of AP should be set equal to the desired value of the channel radius.

2.2. Resolved Resonance Parameters (LRU = 1)

2.2.1. Formats

Six different resonance formalisms are allowed to represent the resolved resonance parameters. Formulae for the various quantities, and further comments on usage, are given in Appendix D of ENDF-102, which is reproduced in Section V of this report. The flag LRU = 1, given in the CONT (range) record, indicates that resolved resonance parameters are given for a particular energy range. Another flag, LRF, in the same record specifies which resonance formalism has been used.

The following quantities are defined for use with all formalisms:

SPI	Spin, I, of the target nucleus.
AP	Scattering radius in units of 10^{-12} cm. For LRF = 1 through 4, AP is assumed to be independent of the channel quantum numbers.
NLS	Number of *l*-values (neutron orbital angular momentum) in this energy region. For LRF = 1 through 4, a set of resonance parameters is given for each *l*-value. Currently, NLS ≤ 4. When higher *l*-values are needed, use LRF = 7.
AWRI	Ratio of the mass of a particular isotope to that of a neutron.
QX	Q-value to be added to the incident particle's center-of-mass energy to determine the channel energy for use in the penetrability factor. The conversion to laboratory system energy depends on the reduced mass in the exit channel. For inelastic scattering to a discrete level, the Q-value is minus the level excitation energy. QX = 0.0 if LRX = 0.
L	Value of *l*.
LRX	Flag indicating whether this energy range contains a competitive width: For LRX = 0, no competitive width is given, and $\Gamma = \Gamma_n + \Gamma_\gamma + \Gamma_f$ in the resolved resonance region, while $\langle\Gamma_x\rangle = 0$ in the unresolved resonance region; LRX must be 0 for LRF = 3 or 4; For LRX = 1, a competitive width is given and is an inelastic process to the first excited state. In the resolved region, it is determined by subtraction, $\Gamma_x = \Gamma - [\Gamma_n + \Gamma_\gamma + \Gamma_f]$ This parameter is irrelevant for LRF = 7.
NRS	Number of resolved resonances for a given *l*-value. (NRS ≤ 600)
ER	Resonance energy (in the laboratory system).

AJ	The absolute value of AJ is the floating-point value of *J* (the spin, or total angular momentum, of the resonance).
	When two channel spins are possible, if the sign of AJ is negative, the lower value for the channel spin is implied; if positive, the higher value is implied.
	When AJ is zero, only one value of channel spin is possible so there is no ambiguity; the channel spin *s* is equal to the orbital angular momentum *l*.
GT	Resonance total width, Γ, evaluated at the resonance energy ER.
GN	Neutron width evaluated at the resonance energy ER.
GG	Radiation width, Γ_γ, a constant.
GF	Fission width, Γ_f, a constant.
GX	Competitive width, Γ_x, evaluated at the resonance energy ER.
	It is not given explicitly for LRF = 1 or 2 but is to be obtained by subtraction, $GX = GT - (GN + GG + GF)$, if $LRX \neq 0$.
a	***Channel*** radius, in 10^{-12} cm. An uppercase symbol is not defined because it is not an independent library quantity. Depending on the value of NAPS, it is either calculated from the equation given earlier (and in Appendix D of ENDF-102, which is reproduced in Section V of this report) or read from the position usually assigned to the ***scattering radius*** AP.

2.2.1.1. <u>SLBW and MLBW (LRU=1, LRF=1 or 2)</u>

The structure of a *subsection* is as follows:

```
[MAT, 2,151/  0.0, 0.0,   0,      0,     NR,   NP/ Eint / AP(E)] TAB1
```
$$\text{(if } NRO \neq 0)$$
```
[MAT, 2,151/  SPI,  AP,   0,      0,    NLS,    0] CONT
```
Use AP = 0.0, if AP(E) is supplied and NAPS=0 or 1.
```
[MAT, 2,151/ AWRI,  QX,    L,    LRX, 6*NRS, NRS/
            .ER1,  AJ1,  GT1,    GN1,   GG1,  GF1,
            .ER2,  AJ2,  GT2,    GN2,   GG2,  GF2,
            --------------------------------
            ERNRS, AJNRS, GTNRS,  GNNRS,  GGNRS, GFNRS] LIST
```

The LIST record is repeated until each of the NLS *l*-values has been specified in order of increasing *l*. The values of ER for each *l*-value are given in increasing order.

Use of either of the Breit-Wigner formats is discouraged for new evaluations. The recommended format is LRF = 7.

2.2.1.2. Reich-Moore (LRU = 1, LRF = 3)

The following additional quantities are defined:

LAD	Flag indicating whether these parameters can be used to compute angular distributions.
	    LAD = 0 do not use
	    LAD = 1 can be used if desired. Do **not** add to File 4.

NLSC	Not relevant.
APL	l-dependent scattering radius. If zero, use APL = AP.
GFA	First partial fission width, a constant.
GFB	Second partial fission width, a constant.

GFA and GFB are signed quantities, their signs being determined by the relative phase of the width amplitudes in the two fission channels. In this case, the structure of a subsection is similar to LRF = 1 and 2, but the total width is eliminated in favor of an additional partial fission width. GFA and GFB can both be zero, in which case, Reich-Moore reduces to an R-function.

The structure for a subsection is as follows:

```
[MAT, 2,151/  0.0, 0.0,   0,   0,    NR,   NP/ Eint / AP(E)] TAB1
                                                           (if NRO ≠ 0)
[MAT, 2,151/  SPI,  AP, LAD,   0,  NLS, NLSC] CONT
[MAT, 2,151/ AWRI, APL,   L,   0, 6*NRS,  NRS/
             ER1,  AJ1,  GN1, GG1,  GFA1, GFB1,
             ER2,  AJ2,  GN2, GG2,  GFA2, GFB2,
            -------------------------------
           ERNRS,AJNRS, GNNRS,GGNRS,GFANRS,GFBNRS] LIST
```

The LIST record is repeated until each of the NLS l-values has been specified in order of increasing l. The values of ER for each l-value are given in increasing order.

2.2.1.3. Adler-Adler (LRU = 1, LRF = 4)

Because SAMMY does not use the Adler-Adler formalism, this section is not reproduced in this document.

2.2.1.4. (LRU = 1, LRF = 5) no longer available
2.2.1.5. (deleted)
2.2.1.6. (LRU = 1, LRF = 6) no longer available

2.2.1.7 <u>R-Matrix Limited Format (LRU = 1, LRF = 7)</u>

In R-matrix scattering theory, a channel is defined by the two particles inhabiting that channel and by the quantum numbers for the combination. The two particles are hereafter referred to as a particle-pair (PP), and are defined by their properties: neutron (or other particle) plus target nuclide (in ground or excited state), with individual identifiers such as mass, spin, parity, and charge. The additional quantum numbers defining the channel include orbital angular momentum l, channel spin s and associated parity, and total spin and parity J^{π}.

NOTE: This format is NOT restricted to one neutron (entrance) channel and two exit channels. There may be several entrance channels and a multitude of exit channels. Charged-particle exit channels are not excluded.

The term "spin group" may be used to define the set of resonances with the same channels and quantum numbers. For any given spin group, only total spin and parity are constant; there may be several entrance channels and/or several reaction channels (and, hence, several values of l or s, etc.) contributing to the spin group.

The "R-Matrix Limited" (RML) format was designed to accommodate the features of R-Matrix theory as implemented in analyses codes being used for current evaluations. In this format, relevant parameters appear only once. Particle-pairs are given first: the masses, spins and parities, and charges for the two particles are specified, as well as the Q-value and the MT value (which defines whether this particle-pair represents elastic scattering, fission, inelastic, capture, etc.). Two particle-pairs will always be present: gamma + compound nucleus and neutron + target nucleus in ground state. Other particle-pairs are included as needed.

The list of resonance parameters is ordered by J^{π}, which (as stated above) is the only conserved quantity for any spin group. For each spin group, the channels are first specified in the order in which they will occur in the list of resonances. For each channel, the particle-pair number and the values for l and s are given, along with the channel radii.

2.2.1.7.1 Formats for the basic RML subsection

Additional quantities are defined (or, in some cases, redefined):

KRM	Flag to specify which formulae for the R-matrix are to be used. KRM = 1 for single-level Breit Wigner, KRM = 2 for multilevel Breit Wigner, KRM = 3 for Reich Moore, KRM = 4 for full R-matrix. (Others may be added at a later date.)
KRL	Flag is zero for non-relativistic kinematics, 1 for relativistic.
NJS	Number of values of J^π to be included.
NPP	Total number of particle-pairs.
IA	Spin (and parity, if non-zero) of one particle in the pair (the neutron or projectile, if this is an incident channel).
IB	Spin of the other particle in the pair (target nuclide, if this is an incident channel). IB is set to zero and ignored if the first particle is a photon.
PA	Parity for first particle in the pair, used only in the case where IA is zero and the parity is negative. (Value = +1.0 if positive, −1.0 if negative.)
PB	Parity for second particle, used if IB= 0 and parity is negative.
MA	Mass of first particle in the pair (in units of neutron mass).
MB	Mass of second particle (in units of neutron mass).
ZA	Charge of first particle.
ZB	Charge of second particle.
QI	Q-value for this particle-pair. (See Section 3.3.2 of ENDF-102 for details; this section is not reproduced in this report.)
PNT	Flag is 1 if penetrability is to be calculated; −1 if not. If PNT is set to zero, the default value for MT = 102 (capture) or 19 (fission) is PNT = −1; the default value for other MT values (excluding fission or capture) is generally PNT = +1. To be safe, give the value explicitly.
SHF	Flag is 1 if shift factor is to be calculated, −1 if not (default = not, so SHF = 0 is equivalent to SHF = −1).
MT	Reaction type associated with this particle-pair; see Appendix B.
AJ	Floating point value of J (spin); sign indicates parity.
PJ	Parity (used only if AJ = 0.0).
NCH	Number of channels for the given J^π.
IPP	Particle-pair number for this channel (written as floating-point number).
L	Orbital angular momentum (floating-point value).
SCH	Channel spin (floating-point value).
BND	Boundary condition for this channel (needed when SHF = +1)

APE	Effective channel radius (scattering radius), used for calculation of phase shift only. Units are 10^{-12} cm.
APT	True channel radius (scattering radius), used for calculation of penetrability and shift factors. Units are 10^{-12} cm.
KBK	Non-zero if background R-matrix exists; see Subsection 2.2.1.7.2. (Often set to 0.)
KPS	Non-zero if non-hard-sphere phase shift are to be specified. (Often set to 0.)
NRS	Number of resonances for the given J^{π}.
NX	Number of lines required for all resonances for the given J^{π}, assuming each resonance starts on a new line; equal to (NCH/6+1)*NRS (using FORTRAN integer arithmetic). If there are no resonances for a spin group, then NX = 1.
ER	Resonance energy in eV.
IFG	Flag is 0 if GAM is channel width in eV, 1 if reduced-width amplitude in $eV^{1/2}$.
GAM	Channel width in eV or reduced-width amplitude in $eV^{1/2}$.

NOTE:

For IFG = 0, the input quantity GAM is the width at the energy of the resonance; reduced-width amplitudes are calculated from Eq. (7) of D.1.7 (Section V of this report), with E set to E_λ. (For negative-energy dummy resonances, the convention is that the input quantity is the width evaluated at the absolute value of the resonance energy.) In all cases, if the value GAM given in File 2 for the partial width is negative, the standard convention is assumed: the negative sign is to be associated with the reduced-width amplitude $\gamma_{\lambda c}$ rather than with $\Gamma_{\lambda c}$ (since $\Gamma_{\lambda c}$ is always a positive quantity). More specifically, $\Gamma_{\lambda c} = |GAM|$ and $\gamma_{\lambda c} = \text{sign}(GAM) \times \sqrt{GAM / 2 P}$, with P evaluated at the energy of the resonance.

If IFG = 1, the input quantity is the reduced-width amplitude $\gamma_{\lambda c}$.

Formats are as follows:

```
[MAT,2,151/  0.0,    0.0,    IFG,   KRM,   NJS,      KRL ]  CONT
```

(The following record provides all particle-pair descriptions. For KRM = 1, 2, or 3, the first particle-pair is the gamma-plus-compound-nucleus pair.)

```
[MAT,2,151/  0.0,    0.0,    NPP,   0,     12*NPP,   2*NPP/
             MA₁,    MB₁,    ZA₁,   ZB₁,   IA₁,      IB₁,
             Q₁,     PNT₁,   SHF₁,  MT₁,   PA₁,      PB₁,
             MA₂,    MB₂,    ZA₂,   ZB₂,   IA₂,      IB₁,
             Q₂,     PNT₂,   SHF₂,  MT₂,   PA₂,      PB₁,
             ------------------------------------------
             MA_NPP, MB_NPP, ZA_NPP, ZB_NPP, IA_NPP,  IB_NPP,
             Q_NPP,  PNT_NPP, SHF_NPP, MT_NPP, PA_NPP, PB_NPP ] LIST
```

SAMMY users should be aware that the original sammy-7.0.0 release contained an error in the implementation of this format – variables PNT and SHF were interchanged. Be sure to ask the SAMMY author for the update before using sammy-7.0.0 to create LRF = 7 files.

(The following record provides the channel descriptions for one spin group. This record and the next one are repeated together, once for each of the NJS spin groups.)

```
[Mat,2,151/  AJ,     PJ,     KBK,   KPS,   6*NCH,    NCH/
             IPP₁,   L₁,     SCH₁,  BND₁,  APE₁,     APT₁,
             IPP₂,   L₂,     SCH₂,  BND₂,  APE₂,     APT₂,
             ------------------------------------------
             IPP_NCH, L_NCH,  SCH_NCH, BND_NCH, APE_NCH, APT_NCH] LIST
```

(The following record gives the values for resonance energy and widths for each resonance in this spin group.)

```
[Mat,2,151/  0.0,    0.0,    0,     NRS,       6*NX,     NX/
             ER₁,    GAM₁,₁,  GAM₂,₁   GAM₃,₁,      GAM₄,₁,   GAM₅,₁,
             GAM₆,₁, GAM_NCH,₁,
             ER₂,    GAM₁,₂,  GAM₂,₂,  GAM₃,₂,      GAM₄,₂,   GAM₅,₂,
             GAM₆,₂, …,       GAM_NCH,₂,
             ------------------------------------------
             ER_NRS,  GAM₁,_NRS, GAM₂,_NRS,  GAM₃,_NRS,    GAM₄,_NRS, GAM₅,_NRS,
             GAM₆,_NRS,…,GAM_NCH,_NRS                                   ] LIST
```

(If the number of resonances is zero for a spin group, then NRS = 0 but NX = 1 in this record.)

Other records may be included here, as described below in Section 2.2.1.7.2. If KBK is greater than zero, a "background R-matrix" is given. If KPS is greater than zero, tabulated values exist for phase shifts. If KBK = 0 and KPS = 0, no additional records are needed.

The above two records, beginning with "channel descriptions," are repeated until each of the NJS J^π spin groups has been fully specified.

2.2.1.7.2 Formats for optional extensions to the RML

The formats described in the previous section are sufficient for most evaluations currently (2003) available (using KRM = 3, KBK = 0, and KPS = 0). For the sake of generality, and to accommodate expected future developments in R-matrix analysis codes, additional capabilities are included in the RML format.

2.2.1.7.2.1 Different R-Matrix formulations (KRM = 1,2,4)

Equations given in Appendix D.1.7 (Section V of this report) are relevant to the Reich-Moore approximation to R-Matrix theory. The format, however, can also be used for single-level Breit Wigner (KRM = 1), multilevel Breit Wigner (KRM = 2), or R-Matrix without approximations (KRM = 4). Equations for KRM = 1 or 2 will be written up if/when the need arises. Equations for KRM = 4 are identical to those given in Appendix D.1.7 with the elimination of the imaginary term in the denominator of Eq. (6), and the inclusion of each gamma-channel on a equal basis with all other channels.

2.2.1.7.2.2 Background R-matrix (KBK > 0):

As described in Appendix D (D.1.7.5 of ENDF-102, which is reproduced in Section V of this report), a background R-Matrix can be defined in a variety of different methods.

For KBK = 0, Option 0 is used everywhere (that is, for all channels for this spin group) for the background R-Matrix. No additional formats are required and no additional records need to be written; the dummy resonances are included along with the physical resonances in the list record described above.

For KBK > 0, one LIST record (and two TAB1 records, for tabulated values) is included for each channel of the current spin group, for a total of NCH records. The particular option to be used for the channel is identified by parameter **LBK**. The formats for the four options are as follows:

Option 0. Dummy resonances (**LBK** = 0)

No additional information is conveyed in this record, other than LBK = 0. No terms are added to the R-matrix for this channel.

```
[Mat,2,151/ 0.0,   0.0,    0,       0,      LBK,     1/
            0.0,   0.0,    0.0,    0.0,     0.0,     0.0 ] LIST
```

Option 1. Tabulated complex function of energy (**LBK** = 1)

Notation:

RBR	Value of real part of tabulated function
RBI	Value of imaginary part of tabulated function

```
[Mat,2,151/ 0.0,   0.0,   0,     0,     LBK,    1/
            0.0,   0.0,   0.0,   0.0,   0.0,    0.0] LIST
[Mat,2,151/ 0.0,   0.0,   0,     0,     NR,     NP/ E_int / RBR(E) / TAB1
[Mat,2,151/ 0.0,   0.0,   0,     0,     NR,     NP/ E_int / RBR(E) / TAB1
```

(Recall that NR and NP are parameters which define the interpolation scheme for TAB1 records, as defined in Section 0.7.7 of ENDF-102, which is reproduced in Section II of this report. Energy values given by E_{int} are in units of eV.)

Option 2. SAMMY's logarithmic parameterization (**LBK** = 2)

Notation [See Eq. (40) of Section D.1.7.5 of ENDF-102, which is reproduced in Section V of this report, for meanings of these quantities]:

R0	$\bar{R}_{con,c}$	**S0**	$\bar{s}_{con,c}$
R1	$\bar{R}_{lin,c}$	**S1**	$\bar{s}_{lin,c}$
R2	$\bar{R}_{q,c}$		
EU	E_c^{up}	**ED**	E_c^{down}

```
[Mat,2,151/  ED,     EU,     0,     0,     LBK,    1/
             R0,     R1,     R2,    S0,    S1,     0.0] LIST
```

Option 3. Fröhner's parameterization (**LBK** = 3)

Notation [See Eqs. (41) and (42) of Section D.1.7.5 of ENDF-102, which is reproduced in Section V of this report, for meanings of these quantities]:

R0	$\bar{R}_c$	**S0**	$\bar{s}$
GA	Γ_γ		
EU	E_c^{up}	**ED**	E_c^{down}

```
[Mat,2,151/  ED,     EU,     0,     0,     LBK,    1/
             R0,     SO      GA,    0.0,   0.0,    0.0] LIST
```

2.2.1.7.2.3 <u>Tablulated phase shifts (KPS = 1)</u> (not used in SAMMY)

When phase shifts are calculated externally (from optical model potentials, for example), rather than generated from the usual hard-sphere phase shift formulae, then the phase shifts must be presented in tabular form.

If parameter KPS is equal to 0, all phase shifts are calculated from the hard-sphere phase shift formulae; see Table D.1.7.1 for non-Coulomb and Section D.1.7.2 for Coulomb hard-sphere phase shifts. Section D.1.7 of ENDF-102 is reproduced in this report. The Coulomb hard-sphere phase shift information was inadvertently omitted from both ENDF-102 and the original version of this document; it has been added as Section D.1.7.6.

For KPS > 0, one LIST record (and two TAB1 records, for tabulated values) is included for each channel of the current spin group, for a total of NCH records. The particular option to be used for the channel is identified by parameter **LPS**. The formats for the two options are as follows:

Option 0. Hard-sphere phase shifts (**LPS** = 0)

No additional information is conveyed in this record, other than LPS = 0.

```
[Mat,2,151/   0.0,     0.0,     0,       0,          LPS,       1/
              0.0,     0.0,     0.0,     0.0,        0.0,       0.0] LIST
```

Option 1. Phase shift is a tabulated complex function of energy (**LPS** = 1)

Notation:
   PSR   Value of real part of tabulated phase shift
   PSI   Value of imaginary part of tabulated phase shift

```
[Mat,2,151/ 0.0,    0.0,    0,       0,       LPS,    1/
            0.0,    0.0,    0.0,     0.0,     0.0,    0.0] LIST
[Mat,2,151/ 0.0,    0.0,    0,       0,       NR,     NP/ Eint / PSR (E) / TAB1
            0.0,    0.0,    0,       0,       NR,     NP/ Eint / PSR (E) / TAB1
```

(Recall that NR and NP are parameters which define the interpolation scheme for TAB1 records, as defined in Section 0.7.7 of ENDF-102, which is reproduced in Section II of this report. Energy values given by E_{int} are in units of eV.)

2.3. Unresolved Resonance Parameters (LRU = 2)

Information for the unresolved resonance region is not included in this report.

IV. INTRODUCTION TO ENDF FILE 32: COVARIANCE MATRIX ASSOCIATED WITH RESONANCE PARAMETERS

In this section are presented the various ENDF formats for presentation of covariance matrix associated with the R-matrix parameters in the resolved resonance region. Information in the remainder of this section is taken essentially verbatim from Section 32.0 of the ENDF-102 manual. However, the layout of the pages has been reformatted to make it easier to read and to make the outline style more prominent. Subsection topics are as follows:

Information on the unresolved resonance region is included here simply because it was readily available. The reader should be aware, however, that current ENDF formats for the unresolved region are woefully inadequate and will likely soon be replaced. When that occurs, this document will also be modified.

32. FILE 32. COVARIANCES OF RESONANCE PARAMETERS

32.1. General Description

File 32, MT = 151, contains the variances and covariances of the resonance parameters given in File 2, MT = 151. The resonance parameters, used with the appropriate resonance formulae, provide an efficient way to represent the complicated variations in the magnitudes of the different resonant partial cross sections, compared to the use of File 3 alone. Similarly for File 32, the use of the covariances of the resonance parameters of individual resonances provides an efficient way of representing the rapid variation over the individual resonances of the covariances of the partial cross sections. The covariance data of the processed cross sections include the effects of both File 32 and File 33 within a given energy region, similar to the way the cross sections themselves are the sum of contributions from File 2 and File 3.

In the resonance region, the covariances of the partial cross sections are often characterized by a) "long-range" components that affect the covariances over many resonances and b) "short-range" components affecting the covariances of the different partial cross sections in the neighborhood of individual resonances. The former often can best be represented in File 33, while the latter can be given in File 32. In SAMMY, only the short-range components are used since they can be accurately generated rather than crudely estimated.

When the material composition is dilute in the nuclide of concern and the cross sections are to be averaged over an energy region that includes many resonances, the effects of "short-range" components are unimportant and the covariances of the averaged cross sections can be well represented by processing the long-range components given in File 33. Therefore, the covariances of the cross sections in the unresolved resonance energy region should be given entirely by means of File 33 unless resonance self-shielding in this energy region is thought to be of practical significance for a particular nuclide. For many nuclides these conditions may also be valid in the high-energy portion of the resolved resonance energy region.

In the resolved resonance region it may be necessary to calculate covariances for the resonance self-shielding factors to obtain the uncertainty in the Doppler effect. As another example, one may require group cross-section covariances where the groups are narrow compared to the resonance width or where only a few resonances are within a group. In these cases File 32 should be used. Because this situation may be important only in the lower energy portion of the resolved resonance region, File 32 need not include the whole set of resonances given in File 2. File 33 remains available for use in combination with File 32.

The ENDF-6 formats for File 32 are structured to maintain compatibility with those of ENDF/B-V, and there are new features to permit representation of covariance components among the parameters of different resonances. Covariances between resonance energies and widths are now also allowed. While File 32 was limited in ENDF-5 to the Breit-Wigner representations (LRF = 1 or 2), in ENDF-6 formats, covariances may also be given for the Reich-Moore (LRF = 3), Adler-Adler (LRF = 4), and R-Matrix Limited (LRF = 7) formulations. A limited representation is offered for unresolved resonance parameter covariance data. The conventions are retained that the cross section

covariances for the resonance region are combined from covariance data in File 32 and File 33, and that relative covariances given in File 33 apply to the cross sections reconstructed from File 2 plus File 3 when that option is specified in File 2. (There is a partial exception for LRF = 4.) Since the ENDF-6 formats do not allow a continuous range of values for the total angular momentum J of a resonance, covariance data for the resonance spin are no longer recognized.

Note that File 32 formats retain many restrictions. For example, there is no provision for representing covariances between the parameters of resonances in two different materials or in two isotopes within the same elemental evaluation. Since File 32 can become cumbersome if many resonances are treated, evaluators will do so only for nuclides of greatest practical importance. (The LCOMP = 2 format is available for use in the case of very many resonances; this format provides a compact but approximate representation for the resonance parameter covariance matrix. Details are given in Section 32.3 of ENDF-102, which is included in this document.)

The strategy employed for File 32 is similar to that for smooth cross sections in that the variance of a resonance parameter or the covariance between two such parameters can be given as a sum of several components. Some contributions can be labeled by resonance energy and parameter type, while others can arise from long-range covariances among parameters of the same type for different resonances in the same isotope. The latter are labeled by energy bands, and the same uncertainty characteristic is applied to the indicated parameter of all the File 2 resonances in a given band.

The idea of assigning the same relative covariance to all parameters of a given type in an energy region has limited validity. One limit arises because long-range uncertainties in reaction yields do not generally carry over proportionately to uncertainties in the corresponding reaction widths. However, gamma-ray widths are sometimes known only for resonances at low neutron energy, and then the average of these values is used for the resonances at higher energy. This situation motivates formats resembling File 33 except that a relative uncertainty in the file applies to the indicated parameter (e.g., Γ_γ) of every resonance in the indicated energy range. The approach here is to allow the long range correlations to extend over any energy interval in which consistent resolved resonance formulations are utilized.

The definitions of common quantities are as given in Section 2 of ENDF-102 (Section III of this report).

Caveat: Resonance parameter covariance matrices reported in File 32 are written in terms of the parameters given in the File 2 listing; this is true even when a given parameter is not the actual quantity used in the calculation. In particular, if the value GAM given in File 2 for the partial width is negative, the negative sign is to be associated with the reduced width amplitude $\gamma_{\lambda c}$ rather than with $\Gamma_{\lambda c}$ (since $\Gamma_{\lambda c}$ is always a positive quantity). More specifically, $\Gamma_{\lambda c}$ = |GAM| and $\gamma_{\lambda c} = \text{sign}(\text{GAM}) \times \sqrt{\text{GAM}/2\,\text{P}}$, with P evaluated at the energy of the resonance. In this case, the covariance matrix is written in terms of GAM rather than $\Gamma_{\lambda c}$. [See Section 2.2.1.7.1 of ENDF-102 (in Section III of this report) for details; however, the rule applies for LRF = 1, 2, and 3 as well as LRF = 7.]

32.2. Formats

The format for File 32, MT = 151, parallels the format for File 2, MT = 151, with the restriction to LRF = 1, 2, 3, 4, or 7 for LRU = 1 (resolved parameters) and to LRF = 1 for LRU = 2 (unresolved parameters). The File 32 formats for LRU = 1, LRF = 7 may omit some of the File 2 information.

The general structure of File 32 is as follows:

```
[MAT,32,151/   ZA, AWR,   0,   0, NIS,   0] HEAD
[MAT,32,151/  ZAI, ABN,   0, LFW, NER,   0] CONT          (isotope)
[MAT,32,151/   EL,  EH, LRU, LRF, NRO, NAPS] CONT             (range)
        <subsection for the first energy range for the first isotope>
[MAT,32,151/   EL,  EH, LRU, LRF, NRO, NAPS] CONT             (range)
        <subsection for the second energy range for the first isotope>
                ------------------------------
                ------------------------------
[MAT,32,151/   EL,  EH, LRU, LRF, NRO, NAPS] CONT             (range)
        <subsection for the last energy range for the first isotope>
                ------------------------------
                ------------------------------
[MAT,32,151/  ZAI, ABN,   0, LFW, NER,   0] CONT          (isotope)
[MAT,32,151/   EL,  EH, LRU, LRF, NRO, NAPS] CONT             (range)
        <subsection for the first energy range for the last isotope>
                ------------------------------
                ------------------------------
[MAT,32,151/ EL,  EH, LRU, LRF, NRO, NAPS] CONT               (range)
        <subsection for the last energy range for the last isotope>
                ------------------------------
                ------------------------------
[MAT,32,  0/  0.0, 0.0,   0,   0,   0,   0] SEND
[MAT, 0,  0/  0.0, 0.0,   0,   0,   0,   0] FEND
```

Data are given for all ranges for a given isotope, then for successive isotopes. The data for each isotope start with a CONT (isotope) record; those for each range start with a CONT (range) record. File segments need not be included for all isotopes represented in the corresponding File 2.

If the "range" record preceding a subsection has NRO≠0, indicating that the energy dependence of the scattering radius is given in File 2, the initial file segment within the subsection has the form

```
[MAT,32,151/ 0.0, 0.0,   0,   0,   0,   NI] CONT
```
          <NI sub-subsections as defined in Chapter 33.2 for the
            energy-dependent covariances of the scattering radius>

The next record of a subsection (the first record if NRO=0) has the form

```
[MAT,32,151/ SPI,  AP,   0, LCOMP, NLS,   0] CONT
```

If the compatibility flag, LCOMP, is zero, NLS is the number of L-values for which lists of resonances are given in a form compatible with that used in ENDF-5, as described in Section 32.2.1. If LCOMP = 1, then NLS = 0 and subsection formats are as shown in Section 32.2.2. If LCOMP = 2, the covariance matrix is expressed in compact form as described in Sections 32.3 and 32.4.

32.2.1 Compatible resolved resonance subsection format (LCOMP = 0).

This format differs from that used for ENDF-5 only in that covariances of the resonance spin are all zero. It is applicable only for resolved parameters (LRU=1) and for the Breit-Wigner formalisms (LRF = 1 or 2). While this format is available for reading and writing via SAMMY, its use is discouraged. The following covariance quantities are defined:

DE^2	Variance of the resonance energy in units eV^2.
DN^2	Variance of the neutron width GN in units eV^2.
$DNDG$	Covariance of GN and GG in units eV^2.
DG^2	Variance of the gamma-ray width in units eV^2
$DNDF$	Covariance of GN and GF in units eV^2.
$DGDF$	Covariance of GG and GF in units eV^2.
DF^2	Variance of the fission width GF in units eV^2.
$DJDN$	(null) covariance of resonance J-value and GN.
$DJDG$	(null) covariance of resonance J-value and GG.
$DJDF$	(null) covariance of resonance J-value and GF.
DJ^2	(null) variance of resonance J-value.

A complete subsection for LCOMP = 0 has the following form:

<If NRO is not 0, a control record and NI sub-subsections for energy-dependent
covariances of the scattering radius>

```
[MAT,32,151/ SPI,      AP,        0,   LCOMP,      NLS,        0] CONT (LCOMP=0)
[MAT,32,151/AWRI,     0.0,        L,       0, 18*NRS,      NRS/
             ER₁,     AJ₁,      GT₁,     GN₁,      GG₁,      GF₁,
             DE₁²,    DN₁²,    DNDG₁,     DG₁²,    DNDF₁,    DGDF₁,
             DF₁²,   DJDN₁,    DJDG₁,    DJDF₁,     DJ₁²,      0.0,
                              (DJDN₁,DJDG₁,DJDF₁ = 0.0)
```

<three physical records for each resonance through resonance NRS> **]** **LIST**
<a similar list record for each additional value of L through NLS>

Note that in this compatible format, no covariance can be given between parameters of different resonances even if they overlap. This format therefore permits only a relatively crude approximation to the true resonance parameter covariance matrix. Although SAMMY can read this format in general and write specific cases of this format, use of this format for new evaluations is nevertheless strongly discouraged.

32.2.2 General resolved resonance subsection formats for LCOMP = 1.

Following the record that starts with the target spin, SPI, if it states LCOMP = 1, the next card of a subsection defines for that isotope and energy range how many (NSRS) subsections will occur for covariances among parameters of specified resonances and how many (NLRS) subsections are to contain data on long-range parameter covariances. The complete structure of an LCOMP = 1 subsection is as follows:

<if NRO≠0, a control record and NI sub-subsections for energy-
dependent covariances of the scattering radius>

```
[MAT,32,151/ SPI,  AP, IFG, LCOMP,  NLS,    0] CONT   (LCOMP=1,NLS=0)
[MAT,32,151/AWRI, 0.0,   0,    0, NSRS, NLRS] CONT
```

<NSRS sub-subsections each giving covariances among specified
parameters of enumerated sets of resonances>

<NLRS sub-subsections each giving long-range covariances contributions
for stated energy regions for a particular type of resonance parameter>

(For LRF = 7, NLS in the first of these formats is to be interpreted as NJS. Parameter IFG is relevant only for LRF = 7 and has the same meaning as in File 2.)

Covariance formats for NSRS-type sub-subsections

The formats here differ from the LCOMP = 0 formats of Section 32.2.1 in that covariances between parameters of different resonances appear, resonance representations LRF = 1 to 4 and 7 are allowed, there is no segregation by L-value (or by *J* and parity for LRF = 7), and the number of parameters considered per resonance is declared in each sub-subsection primarily to avoid tabulating zero covariances for fission widths in files concerning structural materials. The listed resonances must be present in File 2, but there is no requirement that all resonances be included in File 32 that are given in File 2.

The following paragraphs cover the formats for the NSRS sub-subsections for the various (LRF) resonance formulations for resolved parameters (LRU = 1). LRF = 1, 2, 3, 4, and 7 are allowed.

LRF = 1, 2, LRU = 1, LCOMP = 1. These cases have the same formats. All the resonances for which covariances are to be included are divided into blocks. Covariances between parameters can only be included for resonances in the same block. (A given resonance can appear in more than one block.) A sub-subsection covers the data for a block. Within each such block, the parameters are given of those resonances for which covariances are included, and the upper triangular representation of the parameter covariance matrix is included for the whole block of resonances. For each block, one specifies the number MPAR of parameters to be included for each listed resonance in the block, since for most cases there is, for example, no fission width and the size of the covariance matrix can therefore be minimized.

The NSRS-type subsections have the form below for LRF = 1 and 2:

```
[MAT,32,151/  0.0,  0.0, MPAR,   0, NVS+6*NRB, NRB/
Parameters for        ER₁,  AJ₁,  GT₁,  GN₁,  GG₁,  GF₁,
each resonance for    ...
which there is        ...
covariance data.      ER_NRB, AJ_NRB, GT_NRB, GN_NRB, GN_NRB, GG_NRB, GF_NRB,
Resonance parameter   V₁₁, V₁₂, .... V₁,MPAR*NRB,  V₂₂,
variances and         ..., V₂,NPAR*NRB,     V₃₃,
covariances for all   ...,          V_MPAR*NRB,MPAR*NB, 0.0, 0.0] LIST
resonances listed.
```

Note that the record first lists all the parameters of resonances in the group, for positive identification, and then lists the covariance terms.

MPAR	Number of parameters per resonance in this block which have covariance data (in order: ER, GN, GG, GF, GX, indices 1-5).
NVS	Number of covariance elements listed for this block of resonances, NVS = [NRB×MPAR×(NRB×MPAR+1)]/2.
NRB	Number of resonances in this block and for which resonance parameter and covariance data are given in this subsection.
ER	Lab system energy of the kth resonance (in this block).
AJ$_k$	Floating-point value of the spin for the kth resonance.
GT$_k$	Total width (eV) for the kth resonance. GT = GN + GG + GF + GX.
GN$_k$	Neutron width of the kth resonance.
GG$_k$	Gamma-ray width for the kth resonance.
GF$_k$	Fission width of the kth resonance.
V$_{mn}$	Variance (eV^2) or covariance matrix element, row m and column n, with n ≥ m. If j ≤ MPAR is the parameter index (j = 4 for fission width) for the kth resonance in the block, then m = j + (k−1) × MPAR. The indexing is the order defined above under MPAR.

LRF = 3, LRU = 1, LCOMP=1.   The representation for the Reich-Moore resonance formulation is very similar. The listing of the parameters among which covariance terms are allowed takes the form used in File 2, namely,

ER, AJ, GN, GG, GFA, GFB.

Similarly, in interpreting the indices for the covariance matrix of the parameters in a given block of resonances, the order when LRF = 3 is ER, GN, GG, GFA, GFB and the largest possible value of MPAR is 5.

LRF = 4, LRU = 1, LCOMP=1. [This is not used in SAMMY.] The Adler-Adler resonance representation includes background constants as well as resonance parameters. The uncertainty in the background constants is to be treated indirectly just as the smooth background given in File 3. (That is, in the energy region EL, EU for LRF = 4 any relative uncertainty data in File 33 applies to the sum of the cross section in File 3 and the contribution of the cross sections computed from the Adler-Adler background constants. Great care will be required if this uncertainty representation for Adler-Adler fits is used in other than single-isotopes evaluations.) The inherent assumption is that covariance data will be detailed for the largest resonances, and those representing the Adler-Adler backgrounds. It is assumed that LI = 7.

An LRF = 4 NSRS sub-subsection takes the following form, using the previous definitions where possible:

```
     [MAT,32,151/  0.0,    0.0, MPAR,    0,NVS+6*NRB,   NRB/
                    DET₁,   DWT₁,   GRT₁, GIT₁,       DEF₁,   DWF₁,
Parameters for     GRF₁,   GIF₁,   DEC₁, DWC₁,       GRC₁,   GIC₁,
each reference     -------------------------------------
in the block.      DET_NRB, DWT_NRB, GRT_NRB, GIT_NRB, DEF_NRB, DWF_NRB,
                   GRF_NRB, GIF_NRB, DEC_NRB, DWC_NRB, GRC_NRB, GIC_NRB,
Resonance parameter V₁₁,    V₁₂, -------------,   V₁,MPAR*NRB,    V₂₂,
variances for all   ----------------------,   V₂,NPAR*NRB,    V₃₃,
resonances listed.  ----------, V_MPAR*NRB,MPAR*NB,        0.0,    0.0] LIST
```

The Adler-Adler parameters of the selected list of resonances are given in the same redundant style indicated in Section 2.2.1.3 (which is not reproduced in this report). For LRF = 4 the maximum value of MPAR is 8 and for a given resonance the covariance matrix indexing is in the order:

μ = DET = DEF = DEC,   DWT = DWF = DWD = v,
GRT, GIT, GRF, GIF, GRC, GIC

     <u>LRF = 7, LRU = 1, LCOMP = 1.</u> No long-range subsections are allowed for LRF = 7. For each short-range section, it is not sufficient to give merely the number of resonances in the block (as is done for LRF = 3, for example). Instead, because the LRF = 7 format permits different numbers of channels for different spin-and-parity (J^{π}) groups, both the number of spin groups in the block and the number of channels for each spin group must be specified. As with the other LRF values, not all resonances need to be included in this listing; further, not all J^{π} groups need be included here. NJSX is the number of J^{π} groups that are included in this short-range section; the format for specifying NJSX is

```
[MAT,2,151/        0.0,   0.0,   NJSX,  0,        0,  0      ] CONT
```

     For each spin group, the number of channels (NCH), the number of included resonances (NRB), and the number of lines per resonance (NX) must be specified. In addition, the number of values to be read (6 times the number of lines) must also be given in the LIST record, along with the resonance parameters:

```
[Mat,2,151/   0.0,   0.0,     NCH,      NRB,        6*NX,    NX/
              ER₁,    GAM₁,₁,   GAM₂,₁    GAM₃,₁,     GAM₄,₁,   GAM₅,₁,
              GAM₆,₁, GAMNCH,₁,
              ER₂,    GAM₁,₂,   GAM₂,₂,   GAM₃,₂,     GAM₄,₂,   GAM₅,₂,
              GAM₆,₂, …,        GAMNCH,₂,
              -------------------------------------------------
              ERNRB,  GAM₁,NRB,GAM₂,NRB,  GAM₃,NRB,    GAM₄,NRB,  GAM₅,NRB,
              GAM₆,NRB,…,GAMNCH,NRB                                      ] LIST
```

The above two records are repeated once for each included J^{π} group.

     Parameters are numbered in the order in which they appear in the listing; the total number of parameters (NPARB) is the sum (over all included J^{π} values) of (NCH+1)*NRB, where NRB is the number of resonances from this J^{π} group in this covariance block. Following the final resonance for the final J^{π} group in this block, the triangular half of the covariance matrix is presented as a LIST record with N entries, where N = (NPARB*(NPARB+1))/2.

     The covariance matrix is given in the following format:

```
[MAT,32,151/  0.0,  0.0, 0, 0, N, NPARB/
Resonance parameter      V₁₁, V₁₂, .... V₁,NPARB,   V₂₂,
variances and            ..., V₂,NPARB,      V₃₃,
covariances for all      ...,          VNPARB,NPARB, 0.0, 0.0] LIST
resonances listed.
```

<u>Format for Long-Range Covariance Sub-subsections (LRU = 1)</u> <u>[not used in SAMMY]</u>.

Here are described the forms that the sub-subsections may take to represent long-range (in energy) covariances among parameters of a given type. The strategy is to use formats that resemble those for File 33 but refer to a particular parameter and equally to all resonances of a given isotope within the indicated energy regions.

Here each sub-subsection must identify the resonance parameter considered (Γ_n, Γ_γ, etc.) via the parameter IDP, indicate the covariance pattern via a value of LB, and give the energy regions and covariance components. The following table defines the permitted values of LB. Note the definition of one LB value not defined in File 33, and that LB = 3 and 4 are not employed in File 32 because of LB = 5 is typically much more convenient. The term $Cov[\Gamma_\alpha(i),\Gamma_\alpha(j)]$ is defined as the covariance between the Γ_α parameters for two different resonances (indexed i and j) in the same nuclide.

LB = −1   Relative variance components entirely uncorrelated from resonance-to-resonance but having constant magnitude within the stated energy intervals.

$$Cov\left[\Gamma_a(i)\Gamma_a(j)\right] = \delta_{ij} \sum_{k=1}^{NE-1} S_i^k \, F_{\alpha k}^{(-1)} \, \Gamma_\alpha^2(i)$$

LB = 0   Absolute covariance components correlated only within each E interval.

$$Cov\left[\Gamma_a(i)\Gamma_a(j)\right] = \sum_{k=1}^{NE-1} P_{j,k}^{i,k} \, F_{\alpha k}^{(0)}$$

LB = 1   Relative covariance components correlated only within each E interval.

$$Cov\left[\Gamma_a(i)\Gamma_a(j)\right] = \sum_{k=1}^{NE-1} P_{j,k}^{i,k} \, F_{\alpha k}^{(1)} \, \Gamma_\alpha(i) \, \Gamma_\alpha(j)$$

LB = 2   Fractional covariance components fully correlated over all E intervals with variable magnitude.

$$Cov\left[\Gamma_a(i)\Gamma_a(j)\right] = \sum_{k,k'=1}^{NE-1} P_{j,k'}^{i,k} \, F_{\alpha k}^{(2)} \, F_{\alpha k'}^{(2)} \, \Gamma_\alpha(i)\Gamma_\alpha(j)$$

LB = 5   Relative covariance components in an upper triangular representation of a symmetric matrix.

$$Cov\left[\Gamma_a(i)\Gamma_a(j)\right] = \sum_{k,k'=1}^{NE-1} P_{j,k'}^{i,k} \, F_{\alpha k k'}^{(5)} \, \Gamma_\alpha(i)\Gamma_\alpha(j)$$

Note that the $F^{(-1)}$, $F^{(1)}$, and $F^{(5)}$ parameters have the dimensions of relative covariances, the $F^{(0)}$ are absolute covariances, and the $F^{(2)}$ are relative standard deviations.

The *S* and *P* are dimensionless operations defined in Section 33.2 of ENDF-102, which is not reproduced in this report.

The sub-subsection format for LB = −1, 0, 1, or 2 is

[MAT,32,151/ 0.0, 0.0, IDP, LB, 2*NE, NE/{E$_k$,F$^{(LB)}$}] LIST

For LB = 5 the requisite format is

[MAT,32,151/ 0.0, 0.0, IDP, LB, NT, NE/{E$_k$},{F$_{kk}$$^{(5)}$}] LIST(LB=5)

In the above, the following definitions hold:

LB	Indicator of covariance pattern as defined above.
NE	Number of energies in the parameter table for a given subsection.
NT	NE*(NE+1)/2.
IDP	Identification number of a resonance parameter type. This index depends on the resonance formulation used, as summarized in the table below. This table is consistent with the order of parameters used in the NSRS-type sub-subsections to define the parameter covariances included, the first NPAR parameters in the list for the given LRF value.

<table>
<tr><th></th><th colspan="4">LRF</th></tr>
<tr><th>IDP</th><th>1</th><th>2</th><th>3</th><th>4</th></tr>
<tr><td>1</td><td>E_r</td><td>E_r</td><td>E_r</td><td>$E_r=\mu$</td></tr>
<tr><td>2</td><td>Γ_n</td><td>Γ_n</td><td>Γ_n</td><td>ν</td></tr>
<tr><td>3</td><td>Γ_γ</td><td>Γ_γ</td><td>Γ_γ</td><td>GRT</td></tr>
<tr><td>4</td><td>Γ_f</td><td>Γ_f</td><td>Γ_f</td><td>GIT</td></tr>
<tr><td>5</td><td>Γ_x</td><td>Γ_x</td><td>Γ_x</td><td>GRF</td></tr>
<tr><td>6</td><td></td><td></td><td></td><td>GIF</td></tr>
<tr><td>7</td><td></td><td></td><td></td><td>GRC</td></tr>
<tr><td>8</td><td></td><td></td><td></td><td>GIC</td></tr>
</table>

For LB = 0, ±1, 2, and 5, the energy values in the tables are monotonically increasing and cover the range EL to EH. For LB = 5, the F-values are given in the upper triangular representation of a symmetric matrix by rows, i.e., F_{11}, F_{12}, ..., $F_{1,NE-1}$; F_{22}, $F_{2,NE-1}$; $F_{NE-1,NE-1}$.

32.2.3 Unresolved resonance subsection format (LRU = 2)

For the unresolved resonance region, a simplified covariance formulation is permitted. For the purposes of covariance representation, no energy dependence is specified for the average parameter relative covariances, even though in File 2 the unresolved region may be represented with energy-dependent average Breit-Wigner parameters using LRF = 2. Relative covariance elements are tabulated, unlike the cases above.

If the evaluator wishes to represent the relative covariance of the unresolved resonance parameters, the subsection for a given isotope has the following form.:

```
[MAT,32,151/  SPI,   AP,      0,    0,    NLS,     0] CONT
[MAT,32,151/ AWRI,  0.0,      L,    0, 6*NJS,   NJS/
             D₁,    AJ₁,   GNO₁,  GG₁,     GF₁,   GX₁,
            ------------------------------------
             D_NJS, AJ_NJS, GNO_NJS, GG_NJS,   GF_NJS,  GX_NJS] LIST
          <NJS card images for each L value in successive LIST records>
[MAT,32,151/  0.0,   0.0,  MPAR,    0,(NPAR*(NPAR+1))/2,NPAR/
             RV₁₁,  RV₁₂, -------------------------,
            ----------, RV₁,NPAR,--------, RN_NAPR,NPAR] LIST
```

MPAR is the number of average parameters for which relative covariance data are given for each L and J, in the order D, GNO, GG, GF, and GX, for a maximum of 5. That is, relative covariance values for the first MPAR of these are tabulated for each (L,J) combination. If MPAR is given as 4 when LFW=0 on the CONT (isotope) record, then the four covariance matrix indices per (L,J) combination represent D, GNO, GG, and GX.

NPAR = MPAR∗(sum of the values of NJS for each L).

The LSSF flag is defined in Section 2.3.1, which is not reproduced in this report.

RV_{ij} is the relative covariance matrix element ~~quantities~~ among these average unresolved parameters for the given isotope. The final LIST record contains the upper triangular portion of the symmetric relative covariance matrix by rows.

32.3. General Description of Compact Covariance Matrix (LCOMP = 2).

This format was developed in order to provide a means of communicating the actual resonance-parameter covariance matrix (as determined during the data-evaluation process) in a compact, legible, and accurate form, for those situations in which it is not practical to provide the entire covariance matrix using the LCOMP = 1 format. The covariance matrix is specified as uncertainties plus correlation matrix. The correlation coefficients (whose values range from −1 to 1) are presented in a compact representation as an integer with NDIGIT digits plus a sign; each approximated correlation coefficient differs from the original value by at most $0.5 \times 10^{-\text{NDIGIT}}$ (0.005 if NDIGIT = 2). Allowed values for NDIGIT are 2 through 6.

If the covariance matrix element connecting parameter number i with parameter number j is denoted by V_{ij}, the uncertainty on parameter i by D_i, and the correlation coefficient by C_{ij}, then these quantities are related by

$$D_i^2 = V_{ii} \qquad\qquad V_{ij} = D_i \, C_{ij} \, D_j$$

Values for C_{ij} range from −1 to +1; values for D_i are always positive. Note that the diagonal elements of C_{ij}, those for which $i = j$, are always exactly 1.0 and therefore are never specified explicitly. Compacting the off-diagonal correlation coefficients is accomplished as follows:

1. Drop (set to zero) all values of C_{ij} between $-10^{-\text{NDIGIT}}$ and $+10^{-\text{NDIGIT}}$.
2. Multiply the remaining coefficients by 10^{NDIGIT}.
3. Map all positive values greater than K and less than or equal to K+1 to the integer K.
4. Map all negative values less than −K and greater than or equal to −K−1 to the integer −K.

The reverse mapping takes the integer to the center of the range. For example, with NDIGIT = 2, the positive integer 87 (which corresponds to original correlation coefficients in the range from 0.87 up to and including 0.88) maps to 0.875. The negative integer −12 (which corresponds to original correlation coefficients in the range from −0.12 inclusive down to −0.13 exclusive) maps to correlation coefficient −0.125.

In the LCOMP = 2 format, parameters for one resonance are given first (on one line in a LIST record), followed directly by the uncertainties on those parameters, followed by values and uncertainties for the next resonance. After parameters and uncertainties for all resonances have been specified, the correlation coefficients are given.

Two types of records are used for the mapped correlation coefficients. A CONT record reads NDIGIT, NNN (the number of parameters), and NM (the number of lines of INTG records that follow). NDIGIT can have any of the values 2, 3, 4, 5, or 6; the corresponding number NROW of correlation coefficients that can be displayed on one INTG record is 18, 13, 11, 9, and 8, respectively.

```
[MAT,  32,  151 /  0.0,  0.0,  NDIGIT,  NNN,  NM,  0]    CONT
[MAT,  MF,  MT / II,  JJ,  KIJ  ]   INTG
[MAT,  MF,  MT / II,  JJ,  KIJ  ]   INTG
```
< Continue until a total of NM INTG records are read >

The information stored in the INTG records may be summarized as follows: Let i and j represent two of the parameters in the numbering scheme defined above, with $i > j$. All those correlation coefficients mapped to non-zero integers K_{ij} are printed in File 32; zero-valued K_{ij} are printed (as blanks or zeros) only when they occur on the same record with non-zero values. Each line (record) in the file begins by specifying the location (i.e., by specifying i and j, with $i > j$); other K's on the same line correspond to $(i, j + 1)$, $(i, j + 2)$, ... $(i, j + \text{NROW} - 1)$, with the restriction that $j + \text{NROW} - 1 < i$. If there are more non-zero K's for the same i, they are given on another line, again beginning with the next non-zero K.

The following FORTRAN can be used to read the mapped correlation coefficients and reconstruct the correlation matrix:

```
      DIMENSION K(18), CORR(n,n)
C     Note that n must be greater than or equal to NNN
      READ (LIB,10) NNN, NM, NX, MAT, MF, MT, NS
   10 FORMAT (33X, 3I11, I4, I2, I3, I5)
C     The CONT record: NNN is dimension of CORR(NNN,NNN), and
C               NM is the number of lines to follow in the file
      DO I=1,NNN
         DO J=1,I-1
            CORR(J,I) = 0.0
         END DO
         CORR(I,I) = 1.0
      END DO
      DO M=1,NM
         IF (Ndigit.EQ.2) THEN
            READ (LIB,20) I, J, (K(N),N=1,18), MAT, MF, MT, NS
            Nmax = 18
   20       FORMAT (I5, I5, 1X, 18I3, 1X, I4, I2, I3, I5)
         ELSE IF (Ndigit.EQ.3) THEN
            READ (LIB,30) I, J, (K(N),N=1,13), MAT, MF, MT, NS
            Nmax = 13
   30       FORMAT (I5, I5, 1X, 13I4, 3X, I4, I2, I3, I5)
         ELSE IF (Ndigit.EQ.4) THEN
            READ (LIB,40) I, J, (K(N),N=1,11), MAT, MF, MT, NS
            Nmax = 11
   40       FORMAT (I5, I5, 1X, 11I5, I4, I2, I3, I5)
         ELSE IF (Ndigit.EQ.5) THEN
            READ (LIB,50) I, J, (K(N),N=1,9), MAT, MF, MT, NS
            Nmax = 9
   50       FORMAT (I5, I5, 1X, 9I6, 1X, I4, I2, I3, I5)
         ELSE IF (Ndigit.EQ.6) THEN
            READ (LIB,60) I, J, (K(N),N=1,7), MAT, MF, MT, NS
            Nmax = 8
   60       FORMAT (I5, I5, 8I7, I4, I2, I3, I5)
         END IF
         JP = J - 1
         Factor =10.0**(-Ndigit)
         DO N=1,Nmax
            JP = JP + 1
            IF (JP.GE.I) GO TO 30
            IF (K(N).NE.0) THEN
               IF (K(N).GT.0) THEN
                  CORR(JP,I) = (K(N)+0.5)*Factor
               ELSE
                  CORR(JP,I) = -(-K(N)+0.5)*Factor
               END IF
```

```
            END IF
         END DO
      END DO
```


Only the upper-triangular portion of the correlation matrix [CORR(J,I) for J < I] is defined by this procedure.   The lower-triangular portion can be found by invoking symmetry [CORR(I,J) = CORR(J,I)].

32.4 Formats for Compact Covariance Matrix

The compact format for covariances uses File 32, MT = 151, with LCOMP = 2 (with LRF = 1, 2, 3, and 7) for LRU = 1 (resolved-resonance parameters). The format parallels the format for File 2, MT = 151, with parameter uncertainties specified along with parameter values. Correlation coefficients are given separately.

The general structure of File 32 is as given in Section 32.2.

```
[MAT, 32, 151 /  ZA, AWR,    0,    0, NIS,     0]HEAD
[MAT, 32, 151 / ZAI, ABN,    0, LFW, NER,     0]CONT (isotope)
[MAT, 32, 151 /  EL,   EH, LRU, LRF, NRO, NAPS]CONT  (range)
    <subsection for the first energy range for the first isotope>
[MAT, 32, 151 /  EL,   EH, LRU, LRF, NRO, NAPS]CONT  (range)
    <subsection for the second energy range for the first isotope>
    ---------------------------------------------------------------
    ---------------------------------------------------------------
[MAT, 32, 151 /  EL,   EH, LRU, LRF, NRO, NAPS]CONT  (range)
    <subsection for the last energy range for the first isotope>
    ---------------------------------------------------------------
    ---------------------------------------------------------------
[MAT, 32, 151 / ZAI, AWR,    0, LFW, NER,     0]CONT (isotope)
[MAT, 32, 151 /  EL,   EH, LRU, LRF, NRO, NAPS]CONT  (range)
    <subsection for the first energy range for the last isotope>
    ----------------------------------------------------------------
    ----------------------------------------------------------------
[MAT, 32, 151 /  EL,   EH, LRU, LRF, NRO, NAPS]CONT  (range)
    <subsection for the last energy range for the last isotope>
[MAT, 32,   0 / 0.0, 0.0,    0,    0,    0,     0]SEND
[MAT,  0,   0 / 0.0, 0.0,    0,    0,    0,     0]FEND
```

Formats for the individual subsections differ depending on the value of LRF and are discussed in Section 32.4.1.

32.4.1 Compact covariance matrix formats for subsections of a particular energy range and isotope

In the format descriptions to follow, the notation is as defined in Section 2 of ENDF-102, which is reproduced in Section III of this report. Uncertainties are denoted by parameters whose names begin with "D" but are otherwise identical to the parameter of Section 2. For example, ER represents the resonance energy in the laboratory system, in units of eV. Therefore, DER represents the uncertainty (square root of the variance) associated with the resonance energy; DER has the same units as ER.

Parameters that are not variables (i.e., those that are not searchable parameters in the analysis process) do not have uncertainties associated with them. For example, the total spin of a resonance, denoted by parameter AJ, has no associated uncertainty DAJ. In File 32, the value 0.0 is given instead of DAJ (for LRF = 1,2,3).

For LRF = 1 and 2, the redundant parameter GT (which is equal to GN + GG + GF) has no corresponding uncertainty DGT specified explicitly. Instead, if needed, DGT may be calculated using values for DGN, DGG, and DGF, and the correlation matrix.

During the evaluation process, not all potential variables are treated as searchable parameters. For example, if no capture cross section data were available, the evaluator might choose to set all capture widths GG to a constant value. The associated uncertainty DGG is then specified in File 32 as 0.0, indicating that this parameter's uncertainty is not known. (The proper procedure to be used in evaluating the effect of these unvaried parameters on the final covariance matrix remains an open question and is not addressed in this document.)

In order to express the correlation matrix as compactly as possible, the resonance parameters (those which may be varied during the evaluation process) are implicitly numbered, in the order in which they occur in the listing of File 2. For LRF = 1, 2, or 3, the non-searchable parameter AJ is included in the list but is NOT included in this numbering, nor (for LRF = 1 or 2) is the redundant parameter GT. Parameters whose value is given but whose uncertainty is unknown (as described in the previous paragraph) are nevertheless included in the numerical ordering. For completely non-fissile nuclides, fission widths are not included in the numbering scheme; likewise, for fissile or fissionable nuclides for which the evaluator chose to use only one fission width, the second fission width (for LRF = 3) would not be counted.

Notation used here not previously defined:

NRSA   For LRF = 1, 2, or 3, the total number of resonances (for all L values) to be included in the covariance matrix
For LRF = 7, the number of resonances from a particular J^{π} group to be included in the covariance matrix

NJSX   For LRF = 7 only, the number of J^{π} groups with resonances to be included in the covariance matrix

NDIGIT   Number of digits to be used in writing the LCOMP = 2 INTG record

32.4.1.1 SLBW and MLBW (LRU = 1, LRF = 1 or 2, LCOMP = 2)

The structure of the *subsection* (assuming NRO = 0) is as follows:

```
[MAT, 32, 151 / SPI,    AP,       0,LCOMP,        0,     0 ]CONT
[MAT, 32, 151 /AWRI,    QX,       0,    0,12*NRSA, NRSA /
               ER₁,    AJ₁,    GT₁,    GN₁,      GG₁,   GF₁,
               DER₁,   0.0,    0.0,   DGN₁,     DGG₁,  DGF₁,
               ER₂,    AJ₂,    GT₂,    GN₂,      GG₂,   GF₂,
               DER₂,   0.0,    0.0,   DGN₂,     DGG₂,  DGF₂,
               -------------------------------------------------
               ERₙᵣₛₐ,  AJₙᵣₛₐ,  GTₙᵣₛₐ,  GNₙᵣₛₐ,  GGₙᵣₛₐ, GFₙᵣₛₐ
               DERₙᵣₛₐ,   0.0,    0.0, DGNₙᵣₛₐ, DGGₙᵣₛₐ, DGFₙᵣₛₐ]LIST
[MAT, 32, 151 / 0.0,  0.0,NDIGIT,   NNN,     NM, 0      ] CONT
[MAT,  MF,  MT / II, JJ, KIJ ] INTG
[MAT,  MF,  MT / II, JJ, KIJ ] INTG
```
< Continue until a total of NM INTG records are read >

Note that NNN is the total number of unique resonance parameters included in this listing, not including AJ or GT. For fissile nuclides, NNN = NRSA × 4; for non-fissile nuclides, NNN = NRSA × 3.

32.4.1.2 Reich Moore (LRU = 1, LRF = 3, LCOMP = 2)

The structure of the *subsection* is

```
[MAT, 32, 151/ SPI,    AP,   0,  LCOMP,        0,    0]CONT
[MAT, 32, 151/AWRI,    0,    0,      0, 12*NRSA, NRSA /
               ER₁,    AJ₁,  GN₁,  GG₁,    GFA₁,  GFB₁,
               DER₁,   0.0 , DGN₁, DGG₁,   DGFA₁, DGFB₁,
               ER₂,    AJ₂,  GN₂,  GG₂,    GFA₂,  GFB₂,
               DER₂,   0.0 , DGN₂, DGG₂,   DGFA₂, DGFB₂,
               -------------------------------------------------
               ERₙᵣₛₐ,    AJₙᵣₛₐ, GNₙᵣₛₐ, GGₙᵣₛₐ, GFAₙᵣₛₐ,GFBₙᵣₛₐ,
               DERₙᵣₛₐ,    0.0, DGNₙᵣₛₐ, DGGₙᵣₛₐ, DGFAₙᵣₛₐ,DGFBₙᵣₛₐ] LIST
[MAT, 32, 151 /  0.0, 0.0,NDIGIT, NNN,    NM,  0    ]CONT
[MAT,  MF,  MT / II, JJ, KIJ ] INTG
[MAT,  MF,  MT / II, JJ, KIJ ] INTG
```
< Continue until a total of NM INTG records are read >

Only one LIST record is to be read here; it contains parameter values and uncertainties for all resonances which contribute to the covariance matrix. NNN is the total number of resonance parameters to be included (again not including AJ). For non-fissile nuclides, NNN = NRSA × 3. For fissile nuclides, NNN = NRSA × 4 if only one fission channel is used and NNN = NRSA × 5 if both are used.

32.4.1.3 R-Matrix Limited (LRU = 1, LRF = 7, LCOMP = 2)

The structure of the *subsection* is

```
[MAT,32,151/ 0.0,  0.0,      0,LCOMP,     NJS,        0  ] CONT
[MAT,32,151/ 0.0,  0.0,    NPP, NJSX, 12*NPP,    2*NPP/
            MA₁,    MB₁,      ZA₁,    ZB₁,     IA₁,      IB₁,
             Q₁,   PNT₁,    SHF₁,    MT₁,     PA₁,      PB₁,
            MA₂,    MB₂,      ZA₂,    ZB₂,     IA₂,      IB₂,
             Q₂,   PNT₂,    SHF₂,    MT₂,     PA₂,      PB₂,
            -------------------------------------------------
            MA_NPP, MB_NPP,   ZA_NPP,  ZB_NPP,   IA_NPP,   IB_NPP,
            Q_NPP, PNT_NPP,  SHF_NPP,  MT_NPP,   PA_NPP,   PB_NPP    ] LIST
```

<Note that the parameter NJSX is included here but not in File 2>

```
[MAT,32,151/AJ,    PJ,        0,       0,   6*NCH,    NCH/
            IPP₁,   L₁,      SCH₁,   BND₁,    APE₁,    APT₁,
            IPP₂,   L₂,      SCH₂,   BND₂,    APE₂,    APT₂,
            -------------------------------------------------
            IPP_NCH, L_NCH,   SCH_NCH, BND_NCH,  APE_NCH,  APT_NCH    ] LIST
```

```
[MAT,32,151/0.0,  0.0,       0,   NRSA,   12*NX,   NX/
            ER₁ ,   GAM₁,₁,  GAM₂,₁,   GAM₃,₁,    GAM₄,₁,  GAM₅,₁,
            GAM₆,₁,            ...,      GAM_NCH,₁,
            DER₁ ,  DGAM₁,₁, DGAM₂,₁,  DGAM₃,₁,  DGAM₄,₁, DGAM₅,₁,
            DGAM₆,₁,           ...,      DGAM_NCH,₁,
            ER₂,    GAM₁,₂,  GAM₂,₂,   GAM₃,₂,    GAM₄,₂,  GAM₅,₂,
            GAM₆,₂,            ...,      GAM_NCH,₂,
            DER₂,   DGAM₁,₂, DGAM₂,₂,  DGAM₃,₂,  DGAM₄,₂, DGAM₅,₂,
            DGAM₆,₂,           ...,      DGAM_NCH,₂,
            --------------------------------------------------
            ER_NRSA, GAM₁,_NRSA, GAM₂,_NRSA,  GAM₃,_NRSA,  GAM₄,_NRSA,  GAM₅,_NRSA,
            GAM₆,_NRSA,           ...,      GAM_NCH,_NRSA
            DER_NRSA,DGAM₁,_NRSA,DGAM₂,_NRSA,DGAM₃,_NRSA,DGAM₄,_NRSA,DGAM₅,_NRSA,
            DGAM₆,_NRSA,          ...,      DGAM_NCH,_NRSA                  ] LIST
```

<The above two list records are repeated until each of the NJSX J^{π} states has been specified.>

```
[MAT, 32, 151 / 0.0,  0.0,NDIGIT,   NNN,    NM, 0      ] CONT
[MAT, 32, 151 / II, JJ, KIJ ] INTG
[MAT, 32, 151 / II, JJ, KIJ ] INTG
```

< Continue until a total of NM INTG records are read >

For LRF = 7 (unlike other formats), the number of channels may vary from one spin group to another. The number of resonance parameters NNN is therefore given by the sum (from 1 to NJS) of (NCH × NRSA).

V. FORMULAE FOR THE VARIOUS R-MATRIX REPRESENTATIONS

In this section are presented the formulae for representing cross sections in terms of R-matrix parameters in the resolved resonance region. Information in the remainder of this section is taken essentially verbatim from Appendix D of the ENDF-102 manual. However, the layout of the pages has been reformatted to make it easier to read and to make the outline style more prominent. Corrections have been made where needed.

Subsections are as follows:

ENDF-102 APPENDIX D

Resonance Region Formulae

D.1. The resolved resonance region

The following resonance formalisms are given for a particular isotope in the laboratory system, without Doppler broadening.

D.1.1. Single-Level Breit-Wigner (SLBW): LRU=1, LRF=1

D.1.1.1. Elastic Scattering Cross Sections[1]

$$\sigma_{n,n}\left(E\right)= \sum_{l=0}^{\text{NLS}-1} \sigma_{n,n}^{l}\left(E\right)\left(E\right) \quad, \tag{D.1.1-1}$$

where

$$\sigma_{n,n}^{l}\left(E\right)= \left(2l+1\right)\frac{4\pi}{k^{2}}\sin^{2}\phi_{l}$$
$$+\frac{\pi}{k^{2}}\sum_{J}g_{J}\sum_{r=1}^{\text{NR}_{J}}\frac{\Gamma_{nr}^{2}-2\Gamma_{nr}\Gamma\sin^{2}\phi_{l}+2\left(E-E'_{r}\right)\Gamma_{nr}\sin 2\phi_{l}}{\left(E-E'_{r}\right)^{2}+\frac{1}{4}\Gamma_{r}^{2}} \quad. \tag{D.1.1-2}$$

The hard-sphere phase shifts ϕ_l, the wave number k, the primed resonance energy E'_r, the neutron width Γ_{nr}, and through it the total width Γ_r, are all functions of energy, $\phi_l\left(E\right)$, $k(E)$, $E'_r(E)$, $\Gamma_{nr}(E)$, and $\Gamma_r(E)$, but this dependence is not shown explicitly. Also, each resonance parameter carries the implicit quantum numbers l and J, determined by the appropriate entries in the ENDF/B file. In case a given pair (l,J) is compatible with two different values of the channel spin, s, the width is a sum over the two partial channel spin widths. This allows one to omit an explicit sum over channel spin when defining the cross sections.

D.1.1.2. Radiative Capture Cross Section

$$\sigma_{n,\gamma}\left(E\right)= \sum_{l=0}^{\text{NLS}-1}\sigma_{n,\gamma}^{l}\left(E\right) \quad, \tag{D.1.1-3}$$

where

$$\sigma_{n,j}^{l}\left(E\right)= \frac{\pi}{k^{2}}\sum_{J}g_{J}\sum_{r=1}^{\text{NR}_{J}}\frac{\Gamma_{nr}\Gamma_{\gamma r}}{\left(E-E'_{r}\right)+\frac{1}{4}\Gamma_{r}^{2}} \tag{D.1.1-4}$$

and $\mathbf{\Gamma_{\gamma r}}$, the radiative capture width, is constant in energy.

---

[1] Processing codes should sum the cross section, as shown, from $l = 0$ to $l = \text{NLS} - 1$, including any "empty" or "non-resonant" channels, in order to get the potential-scattering contribution. If higher l-values contribute to the scattering in the resonance region, it is the responsibility of the evaluator to provide a suitable File 3 contribution. (See Sections 2.4.23 and 2.4.24, which are not reproduced in this report.)

D.1.1.3. Fission Cross Section

$$\sigma_{n,f}\left(E\right)= \sum_{l=0}^{NLS-1}\sigma_{n,f}^{l}\left(E\right) \quad , \tag{D.1.1-5}$$

where

$$\sigma_{n,f}^{l}\left(E\right)=\frac{\pi}{k^{2}}\sum_{J}g_{J}\sum_{r=1}^{NR_{J}}\frac{\Gamma_{nr}\Gamma_{fr}}{\left(E-E'_{r}\right)^{2}+\frac{1}{4}\Gamma_{r}^{2}} \tag{D.1.1-6}$$

and Γ_{fr}, the fission width, is constant in energy.

D.1.1.4. The Competitive Reaction Cross Section

The competitive reaction cross section, $\sigma_{n,x}(E)$, is given in terms of analogous formulas involving Γ_{xr}, the competitive width. By convention, the cross section for the competitive reaction is given entirely in File 3 and is not to be computed from the resonance parameters. The reason for this is that the latter calculation can be done correctly only for a single competitive channel, since the file can define only one competitive width.

The statistical factor $g_J = (2J+1) / (2(2I+1))$ is obtained from the target spin I and the resonance spin J given in File 2 as SPI and |AJ|, respectively.

The sum on l extends over all l-values for which resonance parameters are supplied. There will be NLS terms in the sum. NLS is given in File 2 for each isotope. In general, ENDF/B resonance files are limited to $l = 0$, 1, and 2, so that the potential-scattering contribution will be represented by hard-sphere scattering up to the energy where f-wave ($l = 3$) potential scattering starts. At that point, the evaluator may have to supply File 3 scattering to simulate the higher l-values. He may also require a File 3 contribution at lower energies to represent any differences between hard-sphere scattering and experiment.

The sum on J extends over all possible J-values for a particular l-value. NR_J is the number of resonances for a given pair of l and J values and may be zero. NRS is the total number of resonances for a given l-value and is given in File 2 for each l-value.

$$NRS = \sum_{J=JMIN}^{J=JMAX} NR_{J} ,$$

where

$$JMAX = l + I + \tfrac{1}{2}$$

and

$$JMIN = \begin{cases} \left| l-I-\tfrac{1}{2} \right| & \text{if } l \geq I \\ \left| I-l-\tfrac{1}{2} \right| & \text{if } I \geq l \end{cases} = \left| l-I \right| - \tfrac{1}{2} \quad .$$

$\Gamma_{nr}(|E_r|) \equiv GN_r$ is the neutron width, for the rth resonance for a particular value of l and J, evaluated at the resonance energy E_r. For bound levels, the absolute value $|E_r|$ is used.

$$\Gamma_{nr} = \frac{P_l(E)\Gamma_{nr}(|E_r|)}{P_l(E_r)} \tag{D.1.1-7}$$

$\Gamma_r = \Gamma_{nr}(E) + \Gamma_{\gamma r} + \Gamma_{fr} + \Gamma_{xr}$ is the total width, a function of energy through Γ_{nr} and Γ_{xr}, since $\Gamma_{\gamma r}$ and Γ_{fr} are constant with respect to energy. The "competitive" width Γ_{xr} is not entered explicitly in File 2. It is calculated from the equation

$$\Gamma_{xr} = \Gamma_r - \Gamma_{nr} - \Gamma_{\gamma r} - \Gamma_{fr} \quad \text{at} \ \ E = E_r \quad . \tag{D.1.1-8}$$

The following quantities are given in File 2 for each resonance:

E_r	= ER, the resonance energy
J	= AJ, the angular momentum ("spin") of the resonance state
I	= SPI, the angular momentum ("spin") of the target nucleus
g_J	= statistical factor $(2J+1)/(2(2I+1))$
$\Gamma_{nr}(|E_r|)$	= GN, the neutron width
$\Gamma_{\gamma r}$	= GG, the radiation width
Γ_{fr}	= GF, the fission width and
$\Gamma_r(|E_r|)$	= GT, the total width evaluated at the resonance energy

Since the competitive width Γ_{xr} is not given, Γ_r should be obtained from File 2 directly and *not* by summing partial widths.

For p-, d- and higher l-values, the primed resonance energy E'_r is energy dependent:

$$E'_r = E_r + \frac{S_l(|E_r|) - S_l(|E|)}{2P_l(|E_r|)}\Gamma_{nr}(|E_r|) \quad . \tag{D.1.1-9}$$

The fact that the shift is zero at *each* E_r is an artifact of the SLBW formalism and implies a different R-matrix boundary condition for each resonance.

The neutron wave number in the center-of-mass system is given as

$$k = \frac{\sqrt{2m_n}}{\hbar}\frac{\text{AWRI}}{\text{AWRI}+1.0}\sqrt{|E|} \quad , \tag{D.1.1-10}$$

where

　　　　　AWRI = ratio of the mass of a particular isotope to that of the neutron, and
　　　　　E　　= laboratory energy in eV.

The energy is written with absolute value signs so that the same formula can be used for positive incident neutron energies and for negative (bound state) resonance energies. (When inelastic scattering can occur, resonances below the level threshold are at "negative energy" in the inelastic channel.)

S_l is the shift factor,

$$S_0 = 0, \qquad\qquad S_2 = -\frac{18 + 3\rho^2}{9 + 3\rho^2 + \rho^4},$$

$$S_1 = -\frac{1}{1 + \rho^2}, \qquad S_3 = -\frac{675 + 90\rho^2 + 6\rho^4}{225 + 45\rho^2 + 6\rho^4 + \rho^6}. \qquad (D.1.1\text{-}11)$$

(The quantity ρ is defined below.)

For higher l-values, S_l is defined by Equation (2.9) in Reference 1 of ENDF-102 (Ref. 5 of this report). See also the SAMMY manual [Ref. 1]. In conventional R-matrix theory, the shift factors are defined differently for negative energies (Reference 1, Equations 2.11a-c). In ENDF, the positive-energy formulas are used, but the absolute value of E is used in SLBW and MLBW. For the R-Matrix Limited format, Section D.1.7 (in Section V of this report), a flag indicates whether shifts are to be calculated or assumed to be zero for each particle-pair.

P_l is the penetration factor,

$$P_0 = \rho, \qquad\qquad P_2 = \frac{\rho^5}{9 + 3\rho^2 + \rho^4},$$

$$P_1 = \frac{\rho^3}{1 + \rho^2}, \qquad P_3 = \frac{\rho^7}{225 + 45\rho^2 + 6\rho^4 + \rho^6}. \qquad (D.1.1\text{-}12)$$

For higher l-values, the P_l are defined by Equation (2.9) in Reference 1 of ENDF-102 [Ref. 5 of this report). See also the SAMMY manual [Ref. 1]. In conventional R-matrix theory, the penetrabilities are zero for negative energies. The theory uses the "theoretical" definition of a reduced width, $\Gamma(E) = 2P_l(E)\gamma^2$, where E is a channel energy (center-of-mass), and it suffices to say that $P_l(E) = 0$ if $E < 0$.

In ENDF, the "experimental" definition is used, $\Gamma(E) = \Gamma(|E_r|)P_l(E)/P_l(|E_r|)$, and it is necessary to make the convention that a penetrability for a negative **resonance** energy is evaluated at its absolute value. A negative kinetic energy can occur in an exit channel if the reaction is exothermic, and in this case $P_l(E < 0)$ is zero.

ϕ_l is the (negative of a) hard-sphere phase shift,

$$\phi_0 = \hat{\rho}, \qquad\qquad \phi_2 = \hat{\rho} - \tan^{-1}\left\{\frac{3\hat{\rho}}{3 - \hat{\rho}^2}\right\},$$

$$\phi_1 = \hat{\rho} - \tan^{-1}\hat{\rho}, \qquad \phi_3 = \hat{\rho} - \tan^{-1}\left\{\frac{\hat{\rho}(15 - \hat{\rho})^2}{15 - 6\hat{\rho}^2}\right\}. \qquad (D.1.1\text{-}13)$$

For higher *l*-values, the ϕ_l are defined by Equation 2.12 in Reference 1 [Ref. 5]. It is not necessary to evaluate a phase shift at negative energies.

ρ and $\hat{\rho}$ are defined as k × RADIUS, where RADIUS is defined as follows:

Let *a* = channel radius in units of 10^{-12} cm

   = 0.123 AWRI$^{1/3}$ + 0.08, but see footnote[2]

AP = energy-independent scattering radius, which determines the low-energy scattering cross section. It is given in File 2 following SPI.

AP(E) = energy-dependent scattering radius, given as a TAB1 card preceding the "SPI AP.... NLS..." card.

If   NRO = 0 (AP energy-independent)
NAPS = 0 then $\rho = ka$; $\hat{\rho} = k\,\text{AP}$
NAPS = 1 then $\rho = \hat{\rho} = k\,\text{AP}$

If   NRO = 1 (AP energy-dependent)
NAPS = 0 then $\rho = ka$; $\hat{\rho} = k\,\text{AP}(E)$
NAPS = 1 then $\rho = \hat{\rho} = k\,\text{AP}(E)$
NAPS = 2 then $\rho = k\,\text{AP}$; $\hat{\rho} = k\,\text{AP}(E)$

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[2] The channel radius, strictly speaking, involves A$^{1/3}$ (the target mass in amu), and not (AWRI)$^{1/3}$, but as long as the mass of the incident particle is approximately unity, as it is for neutrons, the difference is not important. AWRI = A/m_n, where m_n is the neutron mass (see Appendix H of ENDF-102, which is not reproduced in this report).

D.1.2. **Multilevel Breit-Wigner (MLBW):** LRU = 1, LRF = 2

The equations are the same as **SLBW**,[3] except that a resonance-resonance interference term is included in the equation for elastic scattering of *l*-wave neutrons, $\sigma_{n,n}^{l}(E)$:

$$\frac{\pi}{k^2}\sum_J g_J \sum_{r=2}^{NR_J} \sum_{s=1}^{r-1} \frac{2\Gamma_{nr}\Gamma_{ns}\left((E-E'_r)(E-E'_s)+\frac{1}{4}\Gamma_r\Gamma_s\right)}{\left((E-E'_r)^2+(\Gamma_r/2)^2\right)\left((E-E'_s)^2+(\Gamma_s/2)^2\right)} \quad . \tag{D.1.2-1}$$

This form, which has $\sim NR_J^2$ energy-dependent terms and can involve a great deal of computer time, may be written in the following form with only NR$_J$ terms (see Section 2.4.14 of ENDF-102, not included in this report)

$$\frac{\pi}{k^2}\sum_J g_J \sum_{r=1}^{NR_J} \frac{G_r\Gamma_r+2H_r(E-E'_r)}{(E-E'_r)^2+(\Gamma_r/2)^2} \quad , \tag{D.1.2-2}$$

where

$$G_r = \frac{1}{2}\sum_{\substack{s=1;\\(s\neq r)}}^{NR_J} \frac{\Gamma_{nr}\Gamma_{ns}(\Gamma_r+\Gamma_s)}{(E'_r-E'_s)^2+\frac{1}{4}(\Gamma_r+\Gamma_s)^2} \quad , \tag{D.1.2-3}$$

and

$$H_r = \sum_{\substack{s=1;\\(s\neq r)}}^{NR_J} \frac{\Gamma_{nr}\Gamma_{ns}(E'_r-E'_s)}{(E'_r-E'_s)^2+\frac{1}{4}(\Gamma_r+\Gamma_s)^2} \quad . \tag{D.1.2-4}$$

For the user who does not require ψ- and χ-broadening, the following equations, which are mathematically identical to the MLBW equations, require less computing time (See Section 2.4.19 of ENDF-102, not included in this report):

$$\sigma_{n,n}(E) = \sum_{l=0}^{NLS-1} \sigma_{n,n}^{l}(E) \tag{D.1.2-5}$$

$$\sigma_{n,n}^{l}(E) = \frac{\pi}{k^2} \sum_{s=|I-1/2|}^{I+1/2} \sum_{J=|l-s|}^{l+s} g_J \left|1-U_{nn}^{lsJ}(E)\right|^2 \tag{D.1.2-6}$$

$$U_{nn}^{lsJ}(E) = e^{-2i\phi_l}\left(1+\sum_{r=1}^{NR_{sJ}} \frac{i\Gamma_{nr}^{lsJ}}{E'_r-E-i\Gamma_r/2}\right) \tag{D.1.2-7}$$

CAUTION: Use of this formalism is NOT recommended. Computation time is no longer a valid issue for modern computers. All new evaluations should be done with the Reich-Moore formalism (LRF = 3 format for very simple cases, LRF = 7 for most cases), or with the full R-matrix

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[3] Including footnote on page D.1 (page 53 of this report).

formalism (LRF = 7 with KRM = 4, an option not yet implemented in SAMMY or in any of the processor codes).

It is important to note that ENDF's version of the multilevel Breit Wigner formalism does not correspond exactly to the "usual" multilevel formalism. Instead, ENDF's MLBW format allows multilevel computations only for elastic scattering; for other types of partial cross sections, the formalism is single level.

D.1.3 Reich-Moore (R-M): LRU = 1, LRF = 3

Evaluators should be aware that the actual Reich-Moore formalism is far more general than the so-called Reich-Moore format would suggest; the LRF = 3 format permits only a severely limited subset of Reich-Moore capabilities. For a more general treatment of the Reich-Moore formalism, use the LRF = 7 format.

This description of the ENDF Reich-Moore formalism differs from previous versions by using notation in closer agreement with References 1 and 5 of ENDF-102 ([Ref. 5] and [Ref. 6], respectively, in this report). The dependence of all quantities on channel spin has been made explicit, to support a format extension which permits specifying the individual channel-spin components of the neutron width.

Partial cross sections may be obtained from a collision matrix U_{ab}, which connects entrance channels a with exit channels b. In ENDF, the formalism is applied to neutron reactions, $a = n$:

$$\sigma_{nb} = \frac{\pi}{k^2} g_n \left| \delta_{nb} - U_{nb} \right|^2 \quad . \tag{D.1.3-1}$$

These partial cross sections are not observable, but must be summed over the appropriate entrance and exit channels to yield observable cross sections. The statistical factor g_n is a result of prior averaging over channels with different magnetic sub-states, since the ENDF formulae apply to unpolarized particles.

In the Reich-Moore formalism as implemented in LRF = 3, the only reactions requiring explicit channel definitions are elastic scattering and fission; capture is obtained by subtraction (although it is possible to obtain it directly from the collision matrix elements). Neutron channels are labeled by three quantum numbers, l, s, and J. In the ENDF format, l runs from zero to NLS−1, the highest l-value that contributes to the cross section in the energy range of interest. The channel spin s is the vector sum of the target spin I and the neutron spin i (1/2), and takes on the range of values $|I - 1/2|$ to $I + 1/2$. The total angular momentum J is the vector sum of l and s, and runs from $| l - s |$ to $l + s$. The fission channels do not correspond to individual two-body fission product breakup but to Bohr-channels in deformation space, which is why two are adequate for describing many neutron-induced fission cross sections. It is not necessary to specify the quantum numbers associated with the two "ENDF-allowed" fission channels, and they can simply be labeled f_1 and f_2.

If one sums over all incident channels n and exit channels b, and invokes unitarity, the resulting total cross section can be expressed in terms of the diagonal matrix elements as

$$\sigma_T(E) \;=\; \frac{2\pi}{k^2} \sum_{l=0}^{\text{NLS}} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=\left||l-s|\right|}^{l+s} g_J \, \text{Re}\left(1 - U_{lsJ\,lsJ}\right) \quad . \tag{D.1.3-2}$$

The elastic cross section is obtained by summing the incident neutron channels over all possible lsJ values and the exit neutron channels over those quantities $l's'J'$ that have the same ranges as lsJ. Conservation of total angular momentum requires that $J' = J$; the ENDF format imposes additional "conservation rules" $l' = l$ and $s' = s$ which are actually just simplifying assumptions, with some basis in theory and experiment. (Modern evaluation practices do NOT use

these assumptions; hence, the newer LRF = 7 ENDF format is often required.) The sixfold summation then reduces to the familiar form

$$\sigma_{nn}(E) \;=\; \frac{2\pi}{k^2} \sum_{l=0}^{NLS} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=\left|l-s\right|}^{l+s} g_J \left|1-U_{lsJ\,lsJ}\right|^2 \quad . \tag{D.1.3-3}$$

The absorption (non-elastic) cross section is obtained by subtraction:

$$\sigma_{abs}\left(E\right) = \sigma_T\left(E\right) - \sigma_{nn}\left(E\right) \quad . \tag{D.1.3-4}$$

Fission is obtained from the collision matrix by summing Eq. (D.8) over all incident lsJ values and over the two exit fission channels, $b = f1$ and $b = f2$:

$$\sigma_f(E) \;=\; \frac{2\pi}{k^2} \sum_{l=0}^{NLS} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=\left|l-s\right|}^{l+s} g_J \left[\left|U_{nf_1}^{lsJ}\right|^2 + \left|U_{nf_2}^{lsJ}\right|^2 \right]. \tag{D.1.3-5}$$

The Reich-Moore formalism is described in Reference 2 of ENDF-102 [Ref. 7 of this report]. Here we repeat the level-matrix form of the collision matrix as given in the earlier versions of this manual:

$$U_{nb}^J = e^{-i\left(\phi_n+\phi_b\right)} \left[2\left(\left(I-K\right)^{-1}\right)_{nb} - \delta_{nb} \right] \quad , \tag{D.1.3-6}$$

where

$$\left(I-K\right)_{nb} = \delta_{nb} - \frac{i}{2} \sum_r \frac{\Gamma_{nr}^{1/2} \, \Gamma_{br}^{1/2}}{E_r - E - i\,\Gamma_{\gamma r}/2} \quad . \tag{D.1.3-7}$$

Here ϕ_b is zero for fission, $\phi_n = \phi_l$ (defined previously), and the summation is over those resonances r which have partial widths in both of the channels n and b; E_r is the resonance energy; $\Gamma_{\gamma r}$ is the "eliminated" radiation width; Γ_{nr} and Γ_{br} are the partial widths for the rth resonance in channels n and b.

Caution: While the following equations are correct, they can lead to serious numerical problems if programmed in this form. For a computationally more stable form, the reader is referred to Section II of the SAMMY manual [Ref. 1].

If we define a matrix ρ by the equation

$$\rho_{nb} = \delta_{nb} - \left(\left(1-K\right)^{-1}\right)_{nb} \quad , \tag{D.1.3-8}$$

then the various cross sections take the following forms:

Total:

$$\sigma_T\left(E\right) = \frac{2\pi}{k^2} \sum_{lsJ} g_J \left[\left(1-\cos 2\phi_l\right) + 2\,\mathrm{Re}\left(\rho_{nn} e^{-2i\phi_l}\right)\right] \quad . \tag{D.1.3-9}$$

Elastic:

$$\sigma_{nn}(E) = \frac{\pi}{k^2} \sum_{lsJ} g_J \left[2 - 2\cos 2\phi_l + 4\,\mathrm{Re}\left(\rho_{nn} e^{-2i\phi_l}\right) - 4\,\mathrm{Re}\left(\rho_{nn}\right) + 4\left|\rho_{nn}\right|^2 \right] \quad . \text{(D.1.3-10)}$$

Absorption (fission plus capture):

$$\sigma_{nabs}(E) = \frac{4\pi}{k^2} \sum_{lsJ} g_J \left[\mathrm{Re}\left(\rho_{nn}\right) - \left|\rho_{nn}\right|^2 \right] \quad . \tag{D.1.3-11}$$

Fission:

$$\sigma_{nf}(E) = \frac{4\pi}{k^2} \sum_{lsJ} g_J \left[\left|\rho_{nf_1}\right|^2 + \left|\rho_{nf_2}\right|^2 \right] \quad . \tag{D.1.3-12}$$

The phase shifts and penetrabilities are evaluated in terms of a and AP as described earlier. The shift factor has been set equal to zero in the above equations $(E'_r \rightarrow E_r)$; hence, they are strictly correct only for s-wave resonances. Originally, the ENDF Reich-Moore format was used for low-energy resonances in fissile materials, which **are** s-waves. However, it is believed that the "no-shift" formulae can be safely applied to higher l-values also, since the difference in shape between a shifted resonance and one that is not shifted at the same energy has no practical significance. Evaluations using the correct shift factors can be reported in the newer LRF = 7 format.

Footnote 1 (from the SLBW section, page 53 of this report) applies to the Reich-Moore formalism also. Until this revision (i.e., until a format modification approved by CSEWG in 1999), the format did not permit the specification of channel spin; therefore, if an evaluation includes $l > 0$ resonances for $I > 0$ nucleus, it was necessary for the processing codes to include the potential-scattering contributions from the "missing" channels. (It is adequate to arbitrarily assume that the supplied values are for the $s = I - 1/2$ channels, and to use the same potential-scattering radius in the missing $I + 1/2$ channels. See Sections 2.4.23 and 2.4.24 of ENDF-102, which is not repeated in this report.) Having the ability to specify which channel spin is intended does not solve this problem, unless the evaluator actually supplies resonances for both channels. In cases where the data can be fit with all the resonances in the same s-channel, the "other one" will still be absent from the ENDF file, since the format stipulates nothing about avoiding missing channels. This is why it is reasonable for the processing codes to run over the triple lsJ loop, inserting potential scattering in every channel, and resonances whenever they are supplied.

Note: When both positive and negative AJ values are given in the file, negative AJ implies $s = I - 1/2$ and positive AJ implies $s = I + 1/2$. When AJ = 0, one and only one of $I - 1/2$ or $I + 1/2$ is possible, so the possible ambiguity of ± 0 does not arise. In this case $s = l$, so parity conservation prevents the occurrence, for a given J, of two s-values differing by one unit.

D.1.4. Adler-Adler (AA): LRU = 1, LRF = 4   not included in this document

D.1.5. General R-Matrix (GRM): LRU = 1, LRF = 5   no longer available

D.1.6 Hybrid R-function (HRF): LRU = 1, LRF = 6   no longer available

D.1.7 R-Matrix Limited Format (RML) : LRU =1, LRF = 7

In R-Matrix theory, a channel may be defined by $c = (\alpha, l, s, J)$, where

- α represents the two particles making up channel; α includes mass (m_a and m_b with subscript a indicating the incident particle for an entrance channel), charge (Z_a and Z_b), spin (i_a and i_b), and parity (π_a and π_b) and all other quantum numbers for each of the two particles, plus the Q-value.

- l is the orbital angular momentum; the associated parity is $(-1)^l$.

- s represents the channel spin (including the associated parity); that is, s is the vector sum of the spins of the two particles of the pair.

- J is the total angular momentum (and associated parity); J is the vector sum of l and s.

Only J and its associated parity are conserved for any given interaction. The other quantum numbers may differ from channel to channel, so long as the sum rules for spin and parity are obeyed.

In the Reich-Moore approximation to R-matrix theory, the radiation width is treated separately and differently from widths for other channels (which are hereafter referred to as "particle channels"). In this LRF = 7 format, there is assumed to be an "eliminated channel" which, for the strict interpretation of the Reich-Moore approximation, contains all the radiation width; in this format, it is possible for some portion of the radiation width to be treated in the same fashion as the particle widths. In the equations below, the eliminated width appears only in the denominator of the R-matrix.

In all formulae given below, spin quantum numbers (e.g., J) are implicitly assumed to include the associated parity. Vector sum rules are implicitly assumed to be obeyed; readers unfamiliar with these sum rules are referred to Section D.1.7.4 for details.

Let the angle-integrated cross sections from entrance channel c to exit channel c' with total angular momentum J be represented by $\sigma_{cc'}$. This cross section is given in terms of the scattering matrix $U_{cc'}$ as

$$\sigma_{cc'} = \frac{\pi}{k_a^2} g_{J\alpha} \left| e^{i w_c} \delta_{cc'} - U_{cc'} \right|^2 \delta_{JJ'} \quad , \tag{D.1.7-1}$$

where (1) k_α is the center-of mass momentum associated with incident particle-pair α, (2) is $g_{J\alpha}$ is the spin statistical factor, and (3) w_c is zero for non-Coulomb channels. (Details for the charged-particle case are presented later.) The spin statistical factor is given by

$$g_{J\alpha} = \frac{2J+1}{(2i_a+1)(2i_b+1)} \quad , \tag{D.1.7-2}$$

and center-of mass momentum k_α by

$$k_\alpha^2 = \frac{2m_a m_b^2}{\left(m_a+m_b\right)^2} E \quad . \tag{D.1.7-3}$$

The scattering matrix U can be written in terms of the matrix W as

$$U_{cc'} = \Omega_c W_{cc'} \Omega_{c'} \quad , \tag{D.1.7-4}$$

where Ω is given by

$$\Omega_c = e^{i\left(w_c - \phi_c\right)} \quad . \tag{D.1.7-5}$$

Here again, w_c is zero for non-Coulomb channels, and the potential scattering phase shifts for non-Coulomb interactions φ_c are defined in many references (e.g., Ref. 1, which is [Ref. 5] of this report; see also [Ref. 1] of this report). The matrix W in Eq. (D.1.7-4) is related to the R-matrix (in matrix notation with indices suppressed) via

$$W = P^{1/2}(I - RL)^{-1}(I - RL^*)P^{-1/2} \quad . \tag{D.1.7-6}$$

The quantity I in this equation represents the identity matrix. The quantity L in Eq. (D.1.7-6) is given by

$$L = (S - B) + i P \quad , \tag{D.1.7-7}$$

with P the penetration factor, S the shift factor, and B the arbitrary boundary constant at the channel radius a_c. Formulae for P and S are likewise found in many references (see, e.g., Eq. (2.9) in Ref. 1 [Ref. 5 of this report]); for non-Coulomb interactions see Table D.1.7.1 for the appropriate formulae. For fission, the penetrability is unity. For non-eliminated capture channels, the penetrability is unity. For two charged particles, formulae for the penetrabilities are provided in Section II.C.4 of the SAMMY users' manual [Ref. 1] and will be added to this report as time permits.

In the eliminated-channel approximation, the R-matrix of Eq. (D.1.7-6) (for the spin group defined by total spin J and implicit parity π) has the form

$$R_{cc'} = \left[\sum_\lambda \frac{\gamma_{\lambda c} \, \gamma_{\lambda c'}}{E_\lambda - E - i\Gamma_{\lambda\gamma}/2} + R_c^{\text{bkg}} \, \delta_{cc'} \right] \delta_{JJ'} \quad , \tag{D.1.7-8}$$

where all levels (resonances) of that spin group are included in the sum. Subscripts λ designate the particular level; subscripts c and c' designate channels (including particle-pairs and all the relevant quantum numbers). Again, the width $\Gamma_{\lambda\gamma}$ occurring in the denominator corresponds to the "eliminated" non-interfering capture channels of the Reich-Moore approximation.

The "background R-matrix" R_c^{bkg} of Eq. (D.1.7-8) will be discussed in Section D.1.7.5.

The channel width $\Gamma_{\lambda c}$ is given in terms of the reduced width amplitude $\gamma_{\lambda c}$ by

$$\Gamma_{\lambda c} = 2 \, \gamma_{\lambda c}^2 \, P_c(E) \quad , \tag{D.1.7-9}$$

where P_c is the penetrability, whose value is a function of the type of particles in the channel, of the orbital angular momentum l, and of the energy E. Note that the reduced-width amplitude $\gamma_{\lambda c}$ is always independent of energy, but the width $\Gamma_{\lambda c}$ may depend on energy via the penetration factor.

Cross sections may be calculated by using the above expressions for R and L to calculate W, and from there calculating U and, ultimately, σ. However, while Eq. (D.1.7-6) for W is correct, an equivalent form which is computationally more stable is

$$W = I + 2iX \quad , \tag{D.1.7-10}$$

where X is given in matrix notation by

$$X = P^{1/2}L^{-1}\left(L^{-1} - R\right)^{-1}RP^{1/2} \quad . \tag{D.1.7-11}$$

When the suppressed indices and implied summations are inserted, the expression of X becomes

$$X_{cc'} = P_c^{1/2}L_c^{-1}\sum_{c''}\left[(L^{-1} - R)^{-1}\right]_{cc''}R_{c''c'}P_{c'}^{1/2}\delta_{JJ'} \quad . \tag{D.1.7-12}$$

The various cross sections are then written in terms of X.

Table D.1.7.1. Hard-sphere penetrability (penetration factor) P, level shift factor S, and potential scattering phase shift ϕ for orbital angular momentum l, center of mass momentum k, and channel radius a_c, with $\rho = ka_c$

l	P_l	S_l	ϕ_l
0	ρ	0	ρ
1	$\rho^3/(1 + \rho^2)$	$-1/(1 + \rho^2)$	$\rho - \tan^{-1}\rho$
2	$\rho^5/(9 + 3\rho^2 + \rho^4)$	$-(18 + 3\rho^2)/(9 + 3\rho^2 + \rho^4)$	$\rho - \tan^{-1}[3\rho/(3 - \rho^2)]$
3	$\rho^7/(225 + 45\rho^2 + 6\rho^4 + \rho^6)$	$-(675 + 90\rho^2 + 6\rho^4)/(225 + 45\rho^2 + 6\rho^4 + \rho^6)$	$\rho - \tan^{-1}[\rho(15 - \rho^2)/(15 - 6\rho^2)]$
4	$\rho^9/(11025 + 1575\rho^2 + 135\rho^4 + 10\rho^6 + \rho^8$	$-(44100 + 4725\rho^2 + 270\rho^4 + 10\rho^6)/(11025 + 1575\rho^2 + 135\rho^4 + 10\rho^6 + \rho^8)$	$\rho - \tan^{-1}[\rho(105 - 10\rho^2)/(105 - 45\rho^2 + \rho^4)]$
l	$\dfrac{\rho^2 P_{l-1}}{(l - S_{l-1})^2 + P_{l-1}^2}$	$\dfrac{\rho^2(l - S_{l-1})}{(l - S_{l-1})^2 + P_{l-1}^2} - l$	$\phi_{l-1} - \tan^{-1}\left((P_{l-1}/(l - S_{l-1}))\right)$ or $B_l = (B_{l-1} + X_l)/(1 - B_{l-1}X_l)$ with $B_l = \tan(\rho - \phi_l)$ and $X_l = (P_{l-1})/(l - S_{l-1})$

D.1.7.1 Energy-Differential (Angle-Integrated) Cross Sections (Non-Coulomb Channels)

The observable cross sections are found in terms of X by first substituting Eq. (D.1.7 - 4, -5, and -10) into Eq. (D.1.7-1), summing over spin groups (i.e., over J^π), and then summing over all channels corresponding to those particle pairs and spin groups. If X^r represents the real part and X^i the imaginary part of X, then the angle-integrated (but energy-differential) cross section for the interaction which leads from particle-pair α to particle-pair α' has the form

$$\sigma_{\alpha,\alpha'}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[\left(\sin^2\phi_c \left(1 - 2X_{cc}^i\right) - X_{cc}^i \sin(2\phi_c) \right) \delta_{\alpha,\alpha'} \right.$$
$$\left. + \sum_{c'} \left\{ X_{cc'}^{i\ 2} + X_{cc'}^{r\ 2} \right\} \right] \ . \tag{D.1.7.1-1}$$

[This formula is accurate only for cases in which one of particles in α is a neutron; however, both particles in α' may be charged.]

In Eq. (D.1.7.1-1) the summations are over those channels c and c' {of the spin group defined by J^π} for which the particle-pairs are respectively α and α'. More than one "incident channel" $c = (\alpha, l, s, J)$ can contribute to this cross section, for example, when both $l = 0$ and $l = 2$ are possible, or when, in the case of incident neutrons and non-zero spin target nuclei, both channel spins are allowed. Similarly, there may be several "exit channels" $c' = (\alpha', l', s', J')$, depending on the particular reaction being calculated (elastic, inelastic, fission, etc.).

The total cross section (for non-Coulomb initial states) is the sum of Eq. (D.1.7.1-1) over all possible final-state particle-pairs α', assuming the scattering matrix is unitary (i.e., assuming that the sum over c' of $\left| U_{cc'} \right|^2 = 1$). Written in terms of the X matrix, the total cross section has the form

$$\sigma_{\alpha,\,total}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[\frac{1}{2} \sin^2\phi_c + X_{cc}^i \cos(2\phi_c) - X_{cc}^r \sin(2\phi_c) \right] \ , \tag{D.1.7.1-2}$$

where again the sum over c includes only those channels of the J^π spin group for which the particle-pair is α.

The angle integrated elastic cross section is given by

$$\sigma_{\alpha,\alpha}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[\sin^2\phi_c \left(1 - 2X_{cc}^i\right) - X_{cc}^r \sin(2\phi_c) + \sum_{c'} \left\{ X_{cc'}^{i\ 2} + X_{cc'}^{r\ 2} \right\} \right] \ . \tag{D.1.7.1-3}$$

In this case, both c and c' are limited to those channels of the J^π spin group for which the particle-pair is α; again, there may be more than one such channel for a given spin group.

Similarly, the reaction cross section from particle-pair α to particle-pair α' (where α' is not equal to α) is

$$\sigma_{\alpha,\alpha'}(E) \;=\; \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \sum_{c'} \left[X_{cc'}^{i\ 2} + X_{cc'}^{r\ 2} \right] \ . \tag{D.1.7.1-4}$$

Here c is restricted to those channels of the J^π spin group from which the particle-pair is α, and c' to those channels for which the particle-pair is α'.

The absorption cross section has the form

$$\sigma_{\alpha\,\text{absorption}}(E) \;=\; \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[X_{cc}^i - \sum_{c'} \left\{ X_{cc'}^{i\ 2} + X_{cc'}^{r\ 2} \right\} \right] \ . \tag{D.1.7.1-5}$$

Here both the sum over c and the sum over c' include <u>all</u> <u>incident</u> particle channels (i.e., particle-pair α only) for the J^π spin group.

The capture cross section for the eliminated radiation channels can be calculated directly as

$$\sigma_{\alpha\gamma}(E) \;=\; \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_{\text{inc}\,c} \left[X_{cc}^i - \sum_{\text{all}\,c'} \left\{ X_{cc'}^{i\ 2} + X_{cc'}^{r\ 2} \right\} \right] \tag{D.1.7.1-6}$$

or may be found by subtracting the sum of all reaction cross sections from the absorption cross section. In Eq. (D.1.7.1-6), the sum over c includes all incident particle channels for the J^π spin group, and the sum over c' includes <u>all</u> particle channels, both incident and exit, for that spin group.

D.1.7.2 Angular Distributions

Angular distributions (elastic, inelastic, or other reaction) cross sections for incident neutrons can be calculated from Reich-Moore resonance parameters. Following Blatt and Biedenharn [Ref. 7] [Ref. 8 in this report] with some notational changes, the angular distribution cross section in the center-of-mass system may be written

$$\frac{d\sigma_{ss'}}{d\Omega_{CM}} = \sum_L C_{L\alpha\alpha'}(E) P_L(\cos\beta) \quad , \tag{D.1.7.2-1}$$

in which the subscript $\alpha\alpha'$ indicates which type of cross section is being considered, P_L is the Legendre polynomial of degree L, and β is the angle of the outgoing neutron (or other particle) relative to the incoming neutron in the center-of-mass system. The coefficients $C_{L\alpha\alpha'}(E)$ are given by

$$C_{L\alpha\alpha'}(E) = \frac{1}{4k_\alpha^2} \sum_{J_1} \sum_{J_2} \sum_{c_1=(\alpha\, l_1\, s_1\, J_1)} \sum_{c_1'=(\alpha'\, l_1'\, s_1'\, J_1)} \sum_{c_2=(\alpha\, l_2\, s_2\, J_2)} \sum_{c_2'=(\alpha'\, l_2'\, s_2'\, J_2)}$$

(D.1.7.2-2)

$$\times\, B_{\{l_1 s_1 l_1' s_1' J_1\}\{l_2 s_2 l_2' s_2' J_2\}L}\, \frac{1}{(2i_a+1)(2i_b+1)}\, \mathrm{Re}\left[(\delta_{c_1 c_1'}-U_{c_2 c_2'})(\delta_{c_1 c_1'}-U^*_{c_2 c_2'})\right] \quad ,$$

where the various summations are to be interpreted as follows:

(1) sum over all spin groups defined by spin J_1 and the implicit associated parity.
(2) sum over all spin groups defined by spin J_2 and implicit associated parity.
(3) sum over all those channels c_1 belonging to the J_1 spin group and having particle-pair α
$\qquad$ [$c_1 = (\alpha, l_1, s_1, J_1)$].
(4) sum over those channels c_1' J_1 spin group with particle-pair α' [$c_1' = (\alpha', l'_1, s'_1, J_1)$].
(5) sum over those channels c_2 J_2 spin group with particle-pair α [$c_2 = (\alpha, l_2, s_2, J_2)$].
(6) sum over those channels c_2' J_2 spin group with particle-pair α' [$c_2' = (\alpha', l'_2, s'_2, J_2)$].

Also note that i_a and i_b are spins of the two particles in particle-pair α.

The geometric factor B can be exactly evaluated as a product of terms

$$B_{\{l_1 s_1 l_1' s_1' J_1\}\{l_2 s_2 l_2' s_2' J_2\}L} = A_{l_1 s_1 l_1' s_1'; J_1}\, A_{l_2 s_2 l_2' s_2'; J_2}\, D_{l_1 s_1 l_1' s_1' l_2 s_2 l_2' s_2'; L J_1 J_2} \quad , \tag{D.1.7.2-3}$$

where the factor $A_{l_1 s_1 l_1' s_1'; J_1}$ is of the form

$$A_{l_1 s_1 l_1' s_1'; J_1} = \sqrt{(2l_1+1)(2l_1'+1)}\,(2J_1+1)\,\Delta(l_1 J_1 s_1)\,\Delta(l_1' J_1 s_1') \quad . \tag{D.1.7.2-4}$$

The expression for D is

$$
\begin{aligned}
D_{l_1 s_1 l_1' s_1' l_2 s_2 l_2' s_2'; L J_1 J_2} &= (2L+1)\ \Delta^2\left(J_1 J_2 L\right)\ \Delta^2\left(l_1 l_2 L\right)\ \Delta^2\left(l_1' l_2' L\right) \\
&\times w\left(l_1 J_1 l_2 J_2, s_1 L\right)\ w\left(l_1' J_1 l_2' J_2, s_1' L\right)\ \delta_{s_1 s_2}\ \delta_{s_1' s_2'}\ (-1)^{s_1 - s_1'} \qquad \text{(D.1.7.2-5)} \\
&\times \frac{n!\ (-1)^n}{(n-l_1)!\ (n-l_2)!\ (n-L)!}\ \frac{n'!\ (-1)^{n'}}{(n'-l_1')!\ (n'-l_2')!\ (n'-L)!}\quad,
\end{aligned}
$$

in which n is defined by

$$
2n = l_1 + l_2 + L\ ; \qquad\qquad\qquad \text{(D.1.7.2-6)}
$$

D is zero if $l_1 + l_2 + L$ is an odd number. A similar expression defines n'. The Δ^2 term is given by

$$
\Delta^2\left(abc\right) = \frac{(a+b-c)!\ (a+b+c)!\ (a+b+c)!}{(a+b+c+1)!}\quad, \qquad\qquad \text{(D.1.7.2-7)}
$$

for which the arguments a, b, and c are to be replaced by the appropriate values given in Eqs. (D.1.7.2-4) and (D.1.7.2-5). The expression for Δ^2 ($a\,b\,c$) implicitly includes a selection rule for the arguments; that is, the vector sum must hold:

$$
\vec{a} + \vec{b} = \vec{c}\quad. \qquad\qquad\qquad \text{(D.1.7.2-8)}
$$

The quantity w in Eq. (23) is defined as

$$
\begin{aligned}
w\left(l_1 J_1 l_2 J_2, s L\right) = \sum_{k=kmin}^{kmax} &\left[\frac{(-1)^{k+l_1+J_1+l_2+J_2}\ (k+1)!}{\left(k-(l_1+J_1+s)\right)!\ \left(k-(l_2+J_2+s)\right)!} \right. \\
&\times \frac{1}{\left(k-(l_1+l_2+L)\right)!\ \left(k-(J_1+J_2+L)\right)!} \qquad \text{(D.1.7.2-9)} \\
&\left. \times \frac{1}{\left(l_1+J_1+l_2+J_2-k\right)!\ \left(l_1+J_2+s+L-k\right)!\ \left(l_2+J_1+s+L-k\right)!} \right]
\end{aligned}
$$

(and similarly for the primed expression), where $kmin$ and $kmax$ are chosen such that none of the arguments of the factorials are negative. That is,

$$
\begin{aligned}
kmin &= \max\left\{ (l_1+J_1+s),\ (l_2+J_2+s),\ (l_1+l_2+L),\ (J_1+J_2+L) \right\} \\
kmax &= \min\left\{ (l_1+J_1+l_2+J_2),\ (l_1+J_2+s+L),\ (l_2+J_1+s+L) \right\}\quad.
\end{aligned} \qquad \text{(D.1.7.2-10)}
$$

Single-channel case

For the single-channel case, the coefficients $C_{L\alpha\alpha'}(E)$ reduce to

$$
\begin{aligned}
C_{L\alpha\alpha}(E) = \frac{1}{4k_\alpha^2} \sum_{J_1} \sum_{J_2} \sum_{c_1=(\alpha\,l_1\,s_1\,J_1)} & \left[\sum_{c_2=(\alpha\,l_2\,s_2\,J_2)} B_{\{l_1 s_1 l_1 s_1 J_1\}\{l_2 s_2 l_2 s_2 J_2\} L} \right. \\
& \left. \times \frac{1}{(2i_a+1)(2i_b+1)} \,\mathrm{Re}\left[\left(1-U_{c_1 c_1}\right)\left(1-U_{c_2 c_2}^*\right) \right] \right] ,
\end{aligned}
$$

(D.1.7.2-11)

where the existence of only one channel requires that the primed quantities of Eq. (D.1.7.2-2) be equal to the unprimed (e.g., $\alpha = \alpha'$). The geometric factor B becomes

$$
B_{\{l_1 s_1 l_1 s_1 J_1\}\{l_2 s_2 l_2 s_2 J_2\} L} = A_{l_1 s_1 l_1 s_1; J_1}\, A_{l_2 s_2 l_2 s_2; J_2}\, D_{l_1 s_1 l_1 s_1 l_2 s_2 l_2 s_2; L J_1 J_2}
$$

(D.1.7.2-12)

where the factor A reduces to the simple form

$$
A_{l_1 s_1 l_1 s_1; J_1} = (2l_1+1)(2J_1+1)\,\Delta^2(l_1\,J_1\,s_1) ,
$$

(D.1.7.2-13)

and the expression for D reduces to

$$
\begin{aligned}
D_{l_1 s_1 l_1 s_1 l_2 s_2 l_2 s_2; L J_1 J_2} = (2L+1)\,\Delta^2(J_1\,J_2\,L)\,\Delta^4(l_1\,l_2\,L)\,w^2(l_1\,J_1\,l_2\,J_2, s_1\,L) \\
\times \left[\frac{n!}{(n-l_1)!\,(n-l_2)!\,(n-L)!} \right]^2 \delta_{s_1 s_2}
\end{aligned}
$$

(D.1.7.2-14)

in which n is again defined as in Eq. (D.1.7.2-6).

D.1.7.3 Kinematics for Angular Distributions of Elastic Scattering

If E represents the laboratory kinetic energy of the incident neutron, E' the lab kinetic energy of the outgoing particle, θ the laboratory angle of the outgoing neutron, and Q the Q-value for the reaction, then E' may be expressed in terms of E, θ, and Q as

$$E' = E \left[\frac{m_a}{m_a + m_b} \cos\theta + \sqrt{\left(\frac{m_b}{m_a + m_b}\right)^2 - \sin^2\theta \left(\frac{m_a}{m_a + m_b}\right)^2} \right]^2 . \quad \text{(D.1.7.3-1)}$$

where m_a represents the mass of the incident particle (neutron) and m_b, the mass of the sample (target) nucleus. Similarly, the center-of-mass angle β between outgoing and incoming neutron is found from

$$\cos\beta = \pm \frac{m_a}{m_b} \left\{ \cos\theta \sqrt{\left(\frac{m_b^2}{m_a^2} - \sin^2\theta\right)} - \sin^2\theta \right\} , \quad \text{(D.1.7.3-2)}$$

and the Jacobian of transformation from center-of-mass to laboratory system is

$$\frac{d(\cos\beta)}{d(\cos\theta)} = 2\cos\theta \frac{m_a}{m_b} + \frac{1 + (2\cos^2\theta - 1) m_a^2/m_b^2}{\sqrt{1 - \sin^2\theta \; m_a^2/m_b^2}} . \quad \text{(D.1.7.3-3)}$$

The elastic angular distribution cross section in the laboratory system is then found by combining Eq. (D.1.7.2-1) with (D.1.7.3-3), using the relationship in Eq. (D.1.7.3-2), to give

$$\frac{d\sigma}{d\Omega_{lab}}(\theta) = \frac{d\sigma}{d\Omega_{CM}} \frac{d(\cos\beta)}{d(\cos\theta)} . \quad \text{(D.1.7.3-4)}$$

Note that the lowest energy into which a neutron may scatter (i.e., the energy of a neutron after 180-degree scattering) is

$$E'(\cos\theta = -1) = E \left[\frac{m_b - m_a}{m_b + m_a}\right]^2 , \quad \text{(D.1.7.3-5)}$$

and the energy of 90-degree scattering is

$$E'(\cos\theta = 0) = E \left[\frac{m_b - m_a}{m_b + m_a}\right] . \quad \text{(D.1.7.3-6)}$$

D.1.7.4 Spin and Angular Momentum Conventions

The spin and angular momentum conventions used in the R-Matrix Limited Format are described in Table D.1.7.4. Note that the word "channel" refers to the physical configuration as well as to the quantum numbers given here. For example, for an incident neutron (intrinsic spin $i = \frac{1}{2}$) impinging on a target (sample) whose spin is I, the channel spin is s, where $\vec{s} = \vec{i} + \vec{I}$. The relative orbital angular momentum of this channel (neutron + target) is l, and total spin is J, where $\vec{J} = \vec{s} + \vec{l}$. The exit channel might be the same as the entrance channel, or it might include, for example, two particles whose individual spins are i' and I' and whose channel spin is s', where $\vec{s}' = \vec{i}' + \vec{I}'$. The relative angular momentum of the two particles is l', and the total J must satisfy $\vec{J} = \vec{s}' + \vec{l}'$.

For readers unfamiliar with vector summation, the rules are as follows: All quantum numbers are either integer (0, 1, 2, …) or half-integer (1/2, 3/2, 5/2, …). If vectors of magnitude a and b are to be added, then the sum c has magnitude in the range $|a\text{-}b| \leq c \leq a + b$; c takes on only integer values if $a + b$ is integer, and half-integer values if $a + b$ is half-integer. The parity associated with c is the product of the parities associated with a and b. Note also that parity associated with orbital angular momentum l is rarely expressed explicitly, as it is always $(-1)^{l}$.

Table D.1.7.4 Spin and angular momentum conventions

Symbol	Meaning	Value or range of values
i or i'	Intrinsic spin of incident neutron or outgoing particle	½ for incident neutron
I or I'	Spin of target or residual nuclei	integer or half-integer
l or l'	Orbital angular momentum of incident or outgoing particle	non-negative integer
s or s'	Incident or outgoing channel spin, equal to target spin plus incident particle spin	$\vec{s} = \vec{I} + \vec{i}$ or $\vec{s}' = \vec{I}' + \vec{i}'$
J	(1) Spin of resonance (2) Spin of excited level in the compound nucleus (3) Total angular momentum quantum number	$\vec{J} = \vec{l} + \vec{s} = \vec{l}' + \vec{s}'$

D.1.7.5 Extensions to R-matrix Theory

As stated in Eq. (D.1.7-8), the R-matrix has the form

$$R_{cc'} = \left[\sum_\lambda \frac{\gamma_{\lambda c}\, \gamma_{\lambda c'}}{E_\lambda - E - i\Gamma_{\lambda\gamma}/2} + R_c^{\mathrm{bkg}}\, \delta_{cc'} \right] \delta_{JJ'} \quad . \tag{D.1.7.5-1}$$

The external or background R-matrix R_c^{bkg} can be written in many different ways; four options are available in the RML format:

Option 0. $R_c^{\mathrm{bkg}} = 0$ (in which case the background is described by "dummy" resonances whose energies lie outside the range of validity of this parameterization).

Option 1. R_c^{bkg} is a tabulated complex function of the energy.

Option 2. R_c^{bkg} is a real statistical parameterization of the form available in SAMMY [Ref. 11 of ENDF-102, Ref. 1 in this report],

$$R_c^{\mathrm{bkg}}(E) = \overline{R}_{\mathrm{con},c} + \overline{R}_{\mathrm{lin},c}E + \overline{R}_{\mathrm{q},c}\, E^2 - s_{\mathrm{lin},c}\left(E_c^{\mathrm{up}} - E_c^{\mathrm{down}} \right)$$
$$- \left(s_{\mathrm{con},c} - s_{\mathrm{lin},c}\, E \right)\ln\left[\frac{E_c^{\mathrm{up}} - E}{E - E_c^{\mathrm{down}}} \right] \quad . \tag{D.1.7.5-2}$$

Option 3. R_c^{bkg} is a complex statistical parameterization of the form described by Fröhner [Ref. 6 and 10 of ENDF-102, Refs. 8 and 9 in this document],

$$R_c^{\mathrm{bkg}}(E) = \overline{R}_c + 2s_c\left[\tanh^{-1}\left(\frac{E - \overline{E}}{\tilde{Q}/2} \right) + i\,\frac{\Gamma_\gamma/\tilde{Q}}{1 - \left(\dfrac{E - \overline{E}}{\tilde{Q}/2} \right)} \right] \quad , \tag{D.1.7.5-3}$$

with

$$\tilde{Q} = E_c^{\mathrm{up}} - E_c^{\mathrm{down}} \quad \text{and} \quad \overline{E} = \left(E_c^{\mathrm{up}} + E_c^{\mathrm{down}} \right)/2 \quad . \tag{D.1.7.5-4}$$

[This quantity $\tilde{Q}$ is not to be confused with the Q-value for channel c.]

D.1.7.6. Modifications for Charged Particles

The penetrabilities P_l, shift factors S_l, and potential-scattering phase shifts φ_l defined in Table D.1.7.1 apply only to non-Coulomb interactions such as those involving incident neutrons. However, it is possible for the two particles in a channel to both have a positive charge; examples are the exit channels for (n,α) or (n,p) interactions. In this case the expressions for penetrabilities, shift factors, and phase shifts must be modified to include the long-range interaction; see, for example, the discussion of Lane and Thomas [Ref. 6].

Expressions for P_l, S_l, and φ_l for particle pair α involve the parameter η_α, which is defined as

$$\eta_\alpha = \frac{z_\alpha Z_\alpha e^2 \mu_\alpha}{\hbar^2 k_\alpha} \quad , \tag{D.1.7.6-1}$$

where z and Z are the charge numbers for the two particles in the particle pair. The reduced mass μ_α is defined in the usual manner as

$$\mu_\alpha = \frac{m_\alpha M_\alpha}{m_\alpha + M_\alpha} \quad , \tag{D.1.7.6-2}$$

where m_α and M_α are the masses of the two particles in channel α. The center-of-mass (COM) momentum $\hbar k_\alpha$ is defined as

$$\hbar^2 k_\alpha^2 = \frac{2 m_\alpha M_\alpha}{\left(m_\alpha + M_\alpha\right)} \left(E \frac{M}{\left(m + M\right)} + Q \right) \quad , \tag{D.1.7.6-3}$$

where Q is the Q-value for the particle-pair.

If a_c is the channel radius for this channel, we again define ρ as
$$\rho = k_\alpha a_c \tag{D.1.7.6-4}$$
The penetrabilities $P_l(\eta, \rho)$, shift factors $S_l(\eta, \rho)$, and phase shifts $\varphi_l(\eta, \rho)$ are then calculated as functions of $F_l(\eta, \rho)$ and $G_l(\eta, \rho)$, the regular and irregular Coulomb wave functions, respectively. The equations are as follows:

$$P_l = \frac{\rho}{A_l^2}, \quad S_l = \frac{\rho}{A_l}\frac{\partial A_l}{\partial \rho}, \quad \text{and} \quad \cos \varphi_l = \frac{G_l}{A_l}, \quad \text{with } A_l^2 = F_l^2 + G_l^2 \quad . \tag{D.1.7.6-5}$$

In Eq. (D.1.7-5), the Coulomb phase-shift difference w_c is required for charged-particle interactions. From Lane and Thomas [Ref. 6], this quantity has the value

$$w_c = \begin{cases} 0 & l = 0 \\ \sum_{n=1}^{l} \tan^{-1}\left(\frac{\eta_\alpha}{n}\right) & l \neq 0 \end{cases} \quad . \tag{D.1.7.6-6}$$

VI. EXAMPLES

In this section, examples are given for most of the types of ENDF File 2 and File 32 that can be produced via the SAMMY code. In each case, the example is annotated. That is, interspersed with the actual ENDF lines are comment lines, beginning with ####, that describe the information appearing on the following ENDF line or lines. Inclusion of these annotations makes it significantly easier for a person to understand exactly what is in the ENDF file.

With the addition of a simple input command, SAMMY can produce the annotated version of File 2 or 32, in addition to the usual non-annotated version.

Examples shown on the following pages are described below. Most examples are abbreviated to fit on a single page. None of the examples given in this document correspond to actual ENDF evaluated files, and none should be used for any purposes other than to illustrate the format. Additional examples may be found in other SAMMY test cases; see the listing in Section XII.B of the SAMMY manual [Ref. 1].

Example number	Nuclide	Which file	LRF	LCOMP if File 32	SAMMY test case; Comments
1	^{242}Pu	2	1 (SLBW)		tr126 run d10
2	^{242}Pu	32	1 (SLBW)	0	tr126 run d10
3	^{242}Pu	32	1 (SLBW)	1	tr126 run d11
4	^{242}Pu	32	1 (SLBW)	2	tr126 run d12
5	^{242}Pu	2	7 (RML)		tr126 run d71 Same resonance parameters as in example number 1
6	^{242}Pu	32	7 (RML)	1	tr126 run d71
7	^{242}Pu	32	7 (RML)	2	tr126 run d72
8	^{23}Na	2	2 (MLBW)		tr126 run c20
9	^{23}Na	32	2 (MLBW)	0	tr126 run c20
10	^{23}Na	32	2 (MLBW)	1	tr126 run c21
11	^{23}Na	32	2 (MLBW)	2	tr126 run c22
12	^{27}Al	2	3 (RM)		tr126 run b31
13	^{27}Al	32	3 (RM)	1	tr126 run b31
14	^{27}Al	32	3 (RM)	2	tr126 run b32
15	^{27}Al	2	7 (RML)		tr147 run c Spin groups reorganized properly
16	^{19}Fl	2	7 (RML)		tr158 run a Includes inelastic channels
17	^{35}Cl	2	7 (RML)		New evaluation includes proton channel
18	^{35}Cl	32	7 (RML)	2	New evaluation

Example 1 (²⁴²Pu): File 2, LRF = 1 (SAMMY test case tr126 run d10)

```
   94242.0   2.399790+2          0          0          1      09446 2151    1
####
####  Z_A    Abundance           0        LFW        NER
   94242.0   1.000000+0          0          1          1      09446 2151    2
####
#### Emin     Emax          Lru=1 => Resolved Resonance Region
####                              Lrf=1 => SL Breit Wigner
####                                       NRO        NAPS
 1.000000-5 9.860000+2          1          1          0      19446 2151    3
####
#### Spin    Radius             Number of L-values = 1
     0.0   9.225000-1           0          0          1      09446 2151    4
####
#### Weight                 L=0        Number of resonances=    68
 2.399790+2                    0          0        408     689446 2151    5
####
#### E_res       +/-J    Gamma_Tot   Gamma_n   Gamma_gam
-69.9998579      0.5    1.743963-1 1.509889-1 2.340738-2 .0100000-99446 2151    6
2.669994986      0.5    2.435226-2 2.324757-3 2.202751-2 .0100000-99446 2151    7
14.59999486      0.5    2.345205-2 6.098099-5 2.339107-2 .0100000-99446 2151    8
22.56998002      0.5    2.329159-2 2.899690-4 2.300162-2 .0100000-99446 2151    9
40.94989196      0.5    2.749059-2 4.500253-4 2.704057-2 .0100000-99446 2151   10
53.45994779      0.5    7.391505-2 5.171570-2 2.215534-2 4.400399-59446 2151   11
67.60009754      0.5    2.739818-2 4.499818-3 2.282137-2 7.699799-59446 2151   12
88.45000553      0.5    2.407907-2 6.597934-4 2.338727-2 3.199998-59446 2151   13
107.3199928      0.5    3.806815-2 1.699672-2 2.102043-2 5.100012-59446 2151   14
131.3999765      0.5    3.217609-2 6.098045-3 2.602905-2 4.900010-59446 2151   15
141.4299735      0.5    2.349997-2 1.188056-4 2.338116-2 .0100000-99446 2151   16
149.6999724      0.5    3.713600-2 1.399309-2 2.309391-2 4.900043-59446 2151   17
163.4999864      0.5    2.391318-2 5.240091-4 2.338917-2 .0100000-99446 2151   18
204.7998221      0.5    7.489540-2 5.147833-2 2.292609-2 4.909839-49446 2151   19
210.0001221      0.5    2.369086-2 4.184880-4 2.327238-2 .0100000-99446 2151   20
215.3000663      0.5    2.851730-2 5.250955-3 2.326635-2 .0100000-99446 2151   21
219.3000369      0.5    2.364474-2 2.994013-4 2.334533-2 .0100000-99446 2151   22
232.6999666      0.5    2.839634-2 4.898817-3 2.342352-2 7.400024-59446 2151   23
264.4998802      0.5    2.378320-2 3.599751-4 2.342322-2 .0100000-99446 2151   24
271.9497308      0.5    2.394245-2 1.667106-4 2.368474-2 9.100427-59446 2151   25
273.5997584      0.5    3.947655-2 1.642313-2 2.305341-2 .0100000-99446 2151   26
274.7501252      0.5    2.316048-2 1.665146-4 2.299397-2 .0100000-99446 2151   27
281.0499164      0.5    2.340116-2 1.291200-4 2.327204-2 .0100000-99446 2151   28
298.6994604      0.5    3.518638-2 7.953436-3 2.723295-2 .0100000-99446 2151   29
303.5994186      0.5    4.324557-2 1.790109-2 2.523441-2 1.100601-49446 2151   30
319.8968637      0.5    2.466411-1 2.143735-1 3.203685-2 2.308282-49446 2151   31
327.6002547      0.5    2.328180-2 4.875570-4 2.279424-2 .0100000-99446 2151   32
332.4012021      0.5    8.703326-2 7.047611-2 1.645733-2 9.981178-59446 2151   33
374.2999704      0.5    2.983458-2 6.392793-3 2.344178-2 .0100000-99446 2151   34
379.6297849      0.5    2.351097-2 2.676846-4 2.324329-2 .0100000-99446 2151   35
382.2002379      0.5    6.790591-2 4.617891-2 2.164302-2 8.397476-59446 2151   36
396.1001173      0.5    2.582683-2 2.499819-3 2.332701-2 .0100000-99446 2151   37
399.9001084      0.5    2.515574-2 1.800332-3 2.335541-2 .0100000-99446 2151   38
...
949.1003969      0.5    3.661332-2 1.401404-2 2.259929-2 .0100000-99446 2151   72
977.9003123      0.5    3.722911-2 1.451083-2 2.271828-2 .0100000-99446 2151   73
```

Example 2 (^{242}Pu): File 32, LRF = 1, LCOMP = 0 (SAMMY test case tr126 run d10)

```
   94242.0   2.399790+2          0          0          1      0944632151    1
####
####  Z_A    Abundance          0         LFW        NER
   94242.0   1.000000+0          0          1          1      0944632151    2
####
#### Emin     Emax           Lru=1 => Resolved Resonance Region
####                             Lrf=1 => SL Breit Wigner
   1.000000-5 9.860000+2          1          1          0     1944632151    3
####
#### Spin    Radius              LCOMP = 0
      0.0   9.225000-1          0          0          1      0944632151    4
####
#### Weight                   L=0       Number of resonances=    68
  2.399790+2                    0          0       1224      68944632151    5
 -69.9998579        0.5   1.743963-1 1.509889-1 2.340738-2 .0100000-9944632151    6
  8.314354-3 1.147453-4          5.458204-6                   944632151    7
  1.00000-24                                                  944632151    8
 2.669994986        0.5   2.435226-2 2.324757-3 2.202751-2 .0100000-9944632151    9
  9.254801-8 1.345990-9          1.812478-7                   944632151   10
  1.00000-24                                                  944632151   11
 14.59999486        0.5   2.345205-2 6.098099-5 2.339107-2 .0100000-9944632151   12
  1.026582-7 .0013987-9          4.066726-7                   944632151   13
  1.00000-24                                                  944632151   14
 22.56998002        0.5   2.329159-2 2.899690-4 2.300162-2 .0100000-9944632151   15
  9.181883-8 .0271261-9          3.306715-7                   944632151   16
  1.00000-24                                                  944632151   17
 40.94989196        0.5   2.749059-2 4.500253-4 2.704057-2 .0100000-9944632151   18
  1.243403-7 .0641022-9          4.546858-7                   944632151   19
  1.00000-24                                                  944632151   20
...
 949.1003969        0.5   3.661332-2 1.401404-2 2.259929-2 .0100000-9944632151  204
  2.271531-7 6.597905-8          6.415409-7                   944632151  205
  1.00000-24                                                  944632151  206
 977.9003123        0.5   3.722911-2 1.451083-2 2.271828-2 .0100000-9944632151  207
  2.389999-7 7.193126-8          6.558754-7                   944632151  208
  1.00000-24                                                  944632151  209
```

Example 3 (^{242}Pu): File 32, LRF = 1, LCOMP = 1 (SAMMY test case tr126 run d11)

```
    94242.0   2.399790+2          0          0          1        0944632151     1
####
####  Z_A    Abundance           0         LFW         NER
    94242.0   1.000000+0          0          1          1        0944632151     2
####
#### Emin      Emax             Lru=1 => Resolved Resonance Region
####                                    Lrf=1 => SL Breit Wigner
  1.000000-5 9.860000+2          1          1          0        1944632151     3
####
#### Spin     Radius                LCOMP = 1
       0.0   9.225000-1          0          1          0        0944632151     4
####
#### Weight         Number of short-range sections =    1
   2.399790+2                     0          0          1        0944632151     5
                                  4          0      37536       68944632151     6
####
#### E_res       +/-J    Gamma_Tot   Gamma_n   Gamma_gam
 -69.9998579     0.5   1.743963-1 1.509889-1 2.340738-2 .0100000-9944632151     7
 2.669994986     0.5   2.435226-2 2.324757-3 2.202751-2 .0100000-9944632151     8
 14.59999486     0.5   2.345205-2 6.098099-5 2.339107-2 .0100000-9944632151     9
 22.56998002     0.5   2.329159-2 2.899690-4 2.300162-2 .0100000-9944632151    10
 40.94989196     0.5   2.749059-2 4.500253-4 2.704057-2 .0100000-9944632151    11
...
 949.1003969     0.5   3.661332-2 1.401404-2 2.259929-2 .0100000-9944632151    73
 977.9003123     0.5   3.722911-2 1.451083-2 2.271828-2 .0100000-9944632151    74
 8.314354-3-1.399189-5-2.617880-8-4.77983-27 .2911310-9-2.420094-9944632151    75
-6.302573-8-1.30083-26-.2088863-9-.0616098-9-3.050185-8-5.57360-27944632151    76
-.1967337-9-.1293111-9-1.690199-8-3.19521-27-.1222330-9-.1424239-9944632151    77
-1.427914-8-1.95600-27 .0571293-9 5.306716-8-1.045402-7-.0004314-9944632151    78
...
-8.93599-25 .1717002-9 .5908220-9-.2247201-9-4.25074-29 .0562223-9944632151  6254
 .1618799-9-.0278185-9-5.23406-30 1.00000-24 3.22170-29 1.10859-28944632151  6255
-4.21655-29-7.97591-48 1.05493-29 3.03744-29-5.21974-30-9.82097-49944632151  6256
 2.271531-7 1.951824-8 5.777406-8 1.09283-26-.0008382-9 .0030162-9944632151  6257
-.0760592-9-1.43105-29 6.597905-8-4.619432-8-8.73798-27-.0070418-9944632151  6258
-.0025099-9-.2471283-9-4.64972-29 6.415409-7-8.78955-25 .0875423-9944632151  6259
 .2470591-9 .0351968-9 6.62230-30 1.00000-24 1.65592-29 4.67330-29944632151  6260
 6.65774-30 1.25265-48 2.389999-7 2.427716-8 6.449781-8 1.21352-26944632151  6261
 7.193126-8-4.831065-8-9.08966-27 6.558754-7-8.76818-25 1.00000-24944632151  6262
       0.0        0.0          0          0          0        0944632  0 6263
```

Example 4 (^{242}Pu): File 32, LRF = 1, LCOMP = 2 (SAMMY test case tr126 run d12)

```
   94242.0   2.399790+2         0         0         1         0944632151    1
####
####  Z_A     Abundance         0        LFW       NER
   94242.0   1.000000+0         0         1         1         0944632151    2
####
#### Emin     Emax          Lru=1 => Resolved Resonance Region
####                           Lrf=1 => SL Breit Wigner
 1.000000-5 9.860000+2         1         1         0         1944632151    3
####
#### Spin     Radius            LCOMP = 2
     0.0     9.225000-1         0         2         1         0944632151    4
####
#### Weight                   L=0      Number of resonances=    68
 2.399790+2                     0         0       816         68944632151    5
####
#### E_res       +/-J    Gamma_Tot   Gamma_n   Gamma_gam
-69.9998579     0.5    1.743963-1 1.509889-1 2.340738-2 .0100000-9944632151    6
 9.118308-2                       1.071192-2 2.336280-3 .0010000-9944632151    7
2.669994986     0.5    2.435226-2 2.324757-3 2.202751-2 .0100000-9944632151    8
 3.042170-4                       3.668774-5 4.257321-4 .0010000-9944632151    9
14.59999486     0.5    2.345205-2 6.098099-5 2.339107-2 .0100000-9944632151   10
 3.204031-4                       1.182701-6 6.377089-4 .0010000-9944632151   11
22.56998002     0.5    2.329159-2 2.899690-4 2.300162-2 .0100000-9944632151   12
 3.030162-4                       5.208275-6 5.750405-4 .0010000-9944632151   13
40.94989196     0.5    2.749059-2 4.500253-4 2.704057-2 .0100000-9944632151   14
 3.526192-4                       8.006386-6 6.743039-4 .0010000-9944632151   15
...
949.1003969     0.5    3.661332-2 1.401404-2 2.259929-2 .0100000-9944632151  138
 4.766058-4                       2.568639-4 8.009625-4 .0010000-9944632151  139
977.9003123     0.5    3.722911-2 1.451083-2 2.271828-2 .0100000-9944632151  140
 4.888761-4                       2.682000-4 8.098613-4 .0010000-9944632151  141
       0.0         0.0         2       272       240         0944632151  142
#### Correlation matrix follows
     2     1   -1                                           944632151  143
     6     2   -5 -1                                        944632151  144
     7     2   -7 -4      1-55                              944632151  145
    10     2   -5               2                           944632151  146
    11     2   -5               2 12                        944632151  147
    14     2   -3                          2                944632151  148
    15     2   -3                          3                944632151  149
    18     2   -3                                  1        944632151  150
    19     2   -3                                  3 -2     944632151  151
    22     2    7                                    1  1 944632151  152
    22    21    4                                           944632151  153
    23     2  -13                                           944632151  154
    23    21    3-43                                        944632151  155
    26    22   -1  1      3                                 944632151  156
    27     2   -1                                           944632151  157
    27    22   -1         5-21                              944632151  158
...
   270   269   18                                           944632151  381
   271   269   16-22                                        944632151  382
       0.0         0.0         0         0         0         0944632  0  383
```

Example 5 (^{242}Pu): File 2, LRF = 7 (SAMMY test case tr126 run d71)

```
   94242.0   2.399790+2        0        0        1        09446 2151    1
####
####  Z_A    Abundance         0       LFW       NER
   94242.0   1.000000+0        0        1        1        09446 2151    2
####
#### Emin     Emax          Lru=1 => Resolved Resonance Region
####                              Lrf=7 => R-Matrix Limited
 1.000000-5 9.860000+2        1        7        0        19446 2151    3
####
####   Flag for Gamma not gamma  0
####              Flag for Reich-Moore =  3
####                     Number of J values =  1
     0.0             0        3        1        09446 2151    4
####
####  3 pairs of particles are defined next
#### First pair is gamma & compound nucleus
#### Others are particle pairs
     0.0       0.0       3        0       36        69446 2151    5
####
####   MA        MB        ZA        ZB        IA        IB
####   Q         PNT       SHF       MT        PA        PB
0.000000000 2.409790+2   0.0       0.0       1.0       0.0   9446 2151    6
0.000000000    0.0       0.0     102.0       0.0       0.0   9446 2151    7
1.000000000 2.399790+2   0.0       0.0       0.5       0.0   9446 2151    8
0.000000000    1.0       0.0       2.0       0.0       1.0   9446 2151    9
1.000000000 2.399790+2   0.0       0.0     999.0     999.0   9446 2151   10
0.000000000    0.0       0.0      18.0       0.0       0.0   9446 2151   11
####
####    Spin group is defined in the next lines
####    J     Parity                     Number of channels=  3
     0.5       0.0        0        0       18        39446 2151   12
####
#### First channel is gamma, second is neutron
####   IPP       L     Ch Spin                  APE       APT
     1.0       0.0       0.0       0.0                     9446 2151   13
     2.0       0.0       0.5       0.0   9.225000-1 9.225000-19446 2151   14
     3.0       0.0       0.5       0.0   9.225000-1 9.225000-19446 2151   15
####
####     Number of channels =   3, res=   68,      Lines/Res=   1
     0.0       0.0        0       68      408        19446 2151   16
####  E_res Gamma_gam  Gamma_n   Gamma_others
-69.9998579 2.340738-2 1.509889-1 .0100000-9               9446 2151   17
2.669994986 2.202751-2 2.324757-3 .0100000-9               9446 2151   18
14.59999486 2.339107-2 6.098099-5 .0100000-9               9446 2151   19
22.56998002 2.300162-2 2.899690-4 .0100000-9               9446 2151   20
40.94989196 2.704057-2 4.500253-4 .0100000-9               9446 2151   21
...
949.1003969 2.259929-2 1.401404-2 .0100000-9               9446 2151   83
977.9003123 2.271828-2 1.451083-2 .0100000-9               9446 2151   84
```

Example 6 (^{242}Pu): File 32, LRF = 7, LCOMP = 1 (SAMMY test case tr126 run d71)

```
   94242.0    2.399790+2           0           0           1      0944632151    1
####
####   Z_A    Abundance            0         LFW         NER
   94242.0    1.000000+0           0           1           1      0944632151    2
####
#### Emin     Emax           Lru=1 => Resolved Resonance Region
####                                Lrf=7 => R-Matrix Limited
 1.000000-5 9.860000+2           1           7           0      1944632151    3
####
####   Flag for Gamma not gamma   0
####                              Lcomp =   1
#### Number of J values for which resonances exist =   1
     0.0                         0           1           1      0944632151    4
####
#### Weight        Number of short-range sections =     1
                                 0           0           1      0944632151    5
####
####     Number of J-values =    1 in this short-range section
                                 1           0           0      0944632151    6
####
####      Number of channels =    3, res=   68,       Lines/Res=   1
     0.0        0.0             3          68         408      1944632151    7
####  E_res Gamma_gam  Gamma_n   Gamma_others
-69.9998579 2.340738-2 1.509889-1 .0100000-9                    944632151    8
2.669994986 2.202751-2 2.324757-3 .0100000-9                    944632151    9
14.59999486 2.339107-2 6.098099-5 .0100000-9                    944632151   10
22.56998002 2.300162-2 2.899690-4 .0100000-9                    944632151   11
40.94989196 2.704057-2 4.500253-4 .0100000-9                    944632151   12
...
949.1003969 2.259929-2 1.401404-2 .0100000-9                    944632151   74
977.9003123 2.271828-2 1.451083-2 .0100000-9                    944632151   75
####
####           number of cov matrix elements =     37128 npar=   272
     0.0        0.0             0           0       37128     272944632151   76
 8.314354-3-2.617880-8-1.399189-5-4.77983-27 .2911310-9-6.302573-8944632151   77
-2.420094-9-1.30083-26-.2088863-9-3.050185-8-.0616098-9-5.57360-27944632151   78
-.1967337-9-1.690199-8-.1293111-9-3.19521-27-.1222330-9-1.427914-8944632151   79
-.1424239-9-1.95600-27 .0571293-9-1.045402-7 5.306716-8-.0004314-9944632151   80
-.0560153-9-5.561526-9 .0191419-9-.0000628-9-.0761678-9-4.204162-9944632151   81
-.0744416-9-.0000078-9-.0061998-9-8.075000-9 2.440102-9-.0000475-9944632151   82
-.0288992-9-2.005735-9 .0838244-9-.0000071-9 .0112440-9-2.860412-9944632151   83
-.0151774-9-5.22878-28 .0529062-9-2.939658-9 1.133388-9-.0000132-9944632151   84
-.0022765-9-.6253506-9-.0095699-9-1.14265-28 .7362126-9-2.877007-9944632151   85
...
 .0030162-9-1.43105-29 6.415409-7-4.619432-8-8.78955-25 .0875423-9944632151 6260
 .0351968-9 .2470591-9 6.62230-30 6.597905-8-8.73798-27-.0070418-9944632151 6261
-.2471283-9-.0025099-9-4.64972-29 1.00000-24 1.65592-29 6.65774-30944632151 6262
 4.67330-29 1.25265-48 2.389999-7 6.449781-8 2.427716-8 1.21352-26944632151 6263
 6.558754-7-4.831065-8-8.76818-25 7.193126-8-9.08966-27 1.00000-24944632151 6264
     0.0        0.0             0           0           0      0944632  0 6265
```

Example 7 (^{242}Pu): File 32, LRF = 7, LCOMP = 2 (SAMMY test case tr126 run d72)

```
   94242.0    2.399790+2         0           0           1        0944632151    1
####
#### Z_A    Abundance           0          LFW         NER
   94242.0    1.000000+0         0           1           1        0944632151    2
####
#### Emin     Emax              Lru=1 => Resolved Resonance Region
####                                      Lrf=7 => R-Matrix Limited
 1.000000-5 9.860000+2          1           7           0        1944632151    3
####
####   Flag for Gamma not gamma  0
####                                   Lcomp =  2
#### Number of J values for which resonances exist =  1
     0.0                0           2           1        0944632151    4
####
####  3 pairs of particles are defined next
#### First pair is gamma & compound nucleus
#### Others are particle pairs
     0.0        0.0             3           0          36        6944632151    5
####
####   MA        MB          ZA          ZB          IA          IB
####   Q         PNT         SHF         MT          PA          PB
0.000000000 2.409790+2        0.0         0.0         1.0         0.0  944632151    6
0.000000000        0.0        0.0       102.0         0.0         0.0  944632151    7
1.000000000 2.399790+2        0.0         0.0         0.5         0.0  944632151    8
0.000000000        1.0        0.0         2.0         0.0         1.0  944632151    9
1.000000000 2.399790+2        0.0         0.0       999.0       999.0  944632151   10
0.000000000        0.0        0.0        18.0         0.0         0.0  944632151   11
####
####     Spin group is defined in the next lines
####    J     Parity                      Number of channels=  3
     0.5        0.0             0           0          18        3944632151   12
####
#### First channel is gamma, second is neutron
####   IPP       L       Ch Spin                   APE         APT
     1.0        0.0         0.0         0.0                          944632151   13
     2.0        0.0         0.5         0.0   9.225000-1 9.225000-1944632151   14
     3.0        0.0         0.5         0.0   9.225000-1 9.225000-1944632151   15
####
####      Number of channels =   3, res=   68,       Lines/Res=   1
     0.0        0.0             0          68         816        1944632151   16
####  E_res Gamma_gam  Gamma_n   Gamma_others
-69.9998579 2.340738-2 1.509889-1 .0100000-9                      944632151   17
 9.118308-2 2.336280-3 1.071192-2 .0010000-9                      944632151   18
2.669994986 2.202751-2 2.324757-3 .0100000-9                      944632151   19
 3.042170-4 4.257321-4 3.668774-5 .0010000-9                      944632151   20
...
977.9003123 2.271828-2 1.451083-2 .0100000-9                      944632151  151
 4.888761-4 8.098613-4 2.682000-4 .0010000-9                      944632151  152
#### Correlation matrix follows
       0.0        0.0             2         272         239        0944632151  153
     3      1   -1                                                 944632151  154
     6      2   -4  -7       1                                     944632151  155
     7      2   -1  -5          -55                                944632151  156
...
   267    265   15-22                                              944632151  390
   270    269   16                                                 944632151  391
   271    269   18-22                                              944632151  392
       0.0        0.0             0           0           0        0944632  0  393
```

Example 8 (^{23}Na): File 2, LRF = 2 (SAMMY test case tr126 run c20)

```
   11023.0   2.279200+1          0          0          1     01125 2151    1
####
####  Z_A    Abundance           0        LFW        NER
   11023.0   1.000000+0          0          0          1     01125 2151    2
####
#### Emin     Emax           Lru=1 => Resolved Resonance Region
####                              Lrf=2 => ML Breit Wigner
####                                       NRO      NAPS
 1.000000-5 5.000000+5          1          2          0     11125 2151    3
####
#### Spin    Radius             Number of L-values = 3
      1.5   5.410000-1          0          0          3     01125 2151    4
####
#### Weight                   L=0       Number of resonances=    4
 2.279200+1                     0          0         24     41125 2151    5
####
#### E_res       +/-J   Gamma_Tot    Gamma_n  Gamma_gam
2810.794885     -1.0   3.767281+2 3.763751+2 3.529968-1       1125 2151    6
242969.1586     -1.0   3.361620+2 3.346627+2 1.499230+0       1125 2151    7
298319.3838      2.0   2.036237+3 2.035217+3 1.020005+0       1125 2151    8
539188.7892     -1.0   6.230475+4 6.229461+4 1.014000+1       1125 2151    9
####
#### Weight                   L=1       Number of resonances=   12
 2.279200+1                     1          0         72    121125 2151   10
####
#### E_res       +/-J   Gamma_Tot    Gamma_n  Gamma_gam
7617.000003     -2.0   6.058086-1 5.798879-3 6.000097-1       1125 2151   11
35390.00253     -1.0   3.499837+0 1.599909+0 1.899928+0       1125 2151   12
53221.04922     -2.0   1.112909+3 1.112124+3 7.849998-1       1125 2151   13
117430.3589     -1.0   3.100990+1 2.677970+1 4.230197+0       1125 2151   14
143130.4654      0.0   2.351946+1 1.640453+1 7.114931+0       1125 2151   15
201235.2222     -1.0   4.932734+3 4.929794+3 2.939992+0       1125 2151   16
214270.6538      0.0   1.424561+4 1.424097+4 4.640000+0       1125 2151   17
239019.8687     -2.0   5.380853+3 5.379653+3 1.200013+0       1125 2151   18
299414.3668     -1.0   1.319195+2 1.293591+2 2.560432+0       1125 2151   19
392438.3777     -1.0   2.279061+4 2.278074+4 9.870012+0       1125 2151   20
597973.3723     -1.0   2.580224+4 2.580224+4 1.000000-3       1125 2151   21
726950.4752      3.0   4.501252+4 4.501251+4 1.000000-3       1125 2151   22
####
#### Weight                   L=2       Number of resonances=    7
 2.279200+1                     2          0         42     71125 2151   23
####
#### E_res       +/-J   Gamma_Tot    Gamma_n  Gamma_gam
190060.0114      0.0   2.749747+1 1.819726+1 9.300214+0       1125 2151   24
236710.1242     -2.0   6.672161+1 6.513158+1 1.590030+0       1125 2151   25
305200.2229      0.0   7.800650+1 6.830654+1 9.699952+0       1125 2151   26
430897.3099      0.0   4.006030+3 4.000740+3 5.289999+0       1125 2151   27
448816.3453     -2.0   7.022648+3 7.019128+3 3.520001+0       1125 2151   28
697096.6622      4.0   6.000314+4 6.000314+4 1.000000-3       1125 2151   29
780016.0085      4.0   4.399728+4 4.399728+4 1.000000-3       1125 2151   30
```

Example 9 (^{23}Na): File 32, LRF = 2, LCOMP = 0 (SAMMY test case tr126 run c20)

```
   11023.0   2.279200+1          0          0          1       0112532151   1
####
####  Z_A   Abundance           0         LFW        NER
   11023.0   1.000000+0          0          0          1       0112532151   2
####
#### Emin    Emax            Lru=1 => Resolved Resonance Region
####                             Lrf=2 => ML Breit Wigner
 1.000000-5 5.000000+5          1          2          0       1112532151   3
####
#### Spin    Radius              LCOMP = 0
      1.5   5.410000-1          0          0          3       0112532151   4
####
#### Weight                 L=0        Number of resonances=   4
 2.279200+1                 0          0         72       4112532151   5
2810.794885      -1.0   3.767281+2 3.763751+2 3.529968-1     112532151   6
 2.348437+1 2.616888+1            1.246061-3                  112532151   7
                                                             112532151   8
242969.1586      -1.0   3.361620+2 3.346627+2 1.499230+0     112532151   9
 1.800140+2 7.909686+2            2.248793-2                  112532151  10
                                                             112532151  11
298319.3838       2.0   2.036237+3 2.035217+3 1.020005+0     112532151  12
 7.031740+2 5.935011+3            1.040400-2                  112532151  13
                                                             112532151  14
539188.7892      -1.0   6.230475+4 6.229461+4 1.014000+1     112532151  15
 1.651040+8 2.660382+7            1.028196+0                  112532151  16
                                                             112532151  17
####
#### Weight                 L=1        Number of resonances=  12
 2.279200+1                 1          0        216      12112532151  18
7617.000003      -2.0   6.058086-1 5.798879-3 6.000097-1     112532151  19
 2.329590-3 1.988610-7            2.558230-3                  112532151  20
                                                             112532151  21
35390.00253      -1.0   3.499837+0 1.599909+0 1.899928+0     112532151  22
 5.667135-3 2.961028-3            1.401073-2                  112532151  23
                                                             112532151  24
...
597973.3723      -1.0   2.580224+4 2.580224+4 1.000000-3     112532151  49
 1.656556+8 6.960870+6            1.000000-8                  112532151  50
                                                             112532151  51
726950.4752       3.0   4.501252+4 4.501251+4 1.000000-3     112532151  52
 5.060806+8 2.224173+7            1.000000-8                  112532151  53
                                                             112532151  54
####
#### Weight                 L=2        Number of resonances=   7
 2.279200+1                 2          0        126       7112532151  55
190060.0114       0.0   2.749747+1 1.819726+1 9.300214+0     112532151  56
 5.512197+0 2.504657+0            8.167593-1                  112532151  57
                                                             112532151  58
...
780016.0085       4.0   4.399728+4 4.399728+4 1.000000-3     112532151  74
 4.839709+8 2.622167+7            1.000000-8                  112532151  75
                                                             112532151  76
```

Example 10 (^{23}Na): File 32, LRF = 2, LCOMP = 1   (SAMMY test case tr126 run c21)

```
   11023.0    2.279200+1          0          0          1    0112532151      1
####
####  Z_A     Abundance           0         LFW        NER
   11023.0    1.000000+0          0          0          1    0112532151      2
####
#### Emin     Emax             Lru=1 => Resolved Resonance Region
####                                Lrf=2 => ML Breit Wigner
  1.000000-5 5.000000+5          1          2          0    1112532151      3
####
#### Spin     Radius                 LCOMP = 1
     1.5     5.410000-1          0          1          0    0112532151      4
####
#### Weight        Number of short-range sections =    1
   2.279200+1                    0          0          1    0112532151      5
                                 3          0       2553  23112532151      6
####
#### E_res       +/-J    Gamma_Tot   Gamma_n   Gamma_gam
2810.794885    -1.0  3.767281+2 3.763751+2 3.529968-1     112532151      7
242969.1586    -1.0  3.361620+2 3.346627+2 1.499230+0     112532151      8
298319.3838     2.0  2.036237+3 2.035217+3 1.020005+0     112532151      9
539188.7892    -1.0  6.230475+4 6.229461+4 1.014000+1     112532151     10
7617.000003    -2.0  6.058086-1 5.798879-3 6.000097-1     112532151     11
35390.00253    -1.0  3.499837+0 1.599909+0 1.899928+0     112532151     12
53221.04922    -2.0  1.112909+3 1.112124+3 7.849998-1     112532151     13
117430.3589    -1.0  3.100990+1 2.677970+1 4.230197+0     112532151     14
143130.4654     0.0  2.351946+1 1.640453+1 7.114931+0     112532151     15
201235.2222    -1.0  4.932734+3 4.929794+3 2.939992+0     112532151     16
214270.6538     0.0  1.424561+4 1.424097+4 4.640000+0     112532151     17
239019.8687    -2.0  5.380853+3 5.379653+3 1.200013+0     112532151     18
299414.3668    -1.0  1.319195+2 1.293591+2 2.560432+0     112532151     19
392438.3777    -1.0  2.279061+4 2.278074+4 9.870012+0     112532151     20
597973.3723    -1.0  2.580224+4 2.580224+4 1.000000-3     112532151     21
726950.4752     3.0  4.501252+4 4.501251+4 1.000000-3     112532151     22
190060.0114     0.0  2.749747+1 1.819726+1 9.300214+0     112532151     23
236710.1242    -2.0  6.672161+1 6.513158+1 1.590030+0     112532151     24
305200.2229     0.0  7.800650+1 6.830654+1 9.699952+0     112532151     25
430897.3099     0.0  4.006030+3 4.000740+3 5.289999+0     112532151     26
448816.3453    -2.0  7.022648+3 7.019128+3 3.520001+0     112532151     27
697096.6622     4.0  6.000314+4 6.000314+4 1.000000-3     112532151     28
780016.0085     4.0  4.399728+4 4.399728+4 1.000000-3     112532151     29
#### Covariance matrix follows
 2.348437+1 6.605618+0 7.650431-5 2.417883-1 3.168851-1-1.931889-5112532151     30
-4.505616-1 2.300898+0 1.496991-5 1.307987+3 1.555360+3-1.717212-6112532151     31
 4.157308-5-8.121918-5 6.853850-4 3.708057-5 2.271354-4 1.397461-4112532151     32
 1.071462-2 4.135067-1-2.441513-7 2.463617-3 3.181778-2-7.234549-5112532151     33
 6.515879-3 3.764583-2-1.773687-3-4.829232-1 9.397897+0 2.021679-6112532151     34
...
 1.860834-3 2.619456-3 8.72283-19-1.177161-3 7.637100-4 3.20248-19112532151    424
 5.696439+4 3.031515+3 1.329838-4 7.592660+3 8.733830+2 .0001490-9112532151    425
 9.741069+2 2.213427+0 .0000835-9 1.988082+5-1.284160-2 4.626283+4112532151    426
-2.198017+3-.0017462-9 1.036346+4-2.372020+3-.0004465-9 1.239040-1112532151    427
-5.214766-3 2.854597-4 1.32179-19-1.225271-3 2.722756-4 2.12981-20112532151    428
 8.985021+8 1.667383+8 .0323540-9-2.503170+5 3.159003+4 .0076110-9112532151    429
 6.692702+7 .0010555-9-1.371904+4 1.376714+3 .0001228-9 1.000000-8112532151    430
 .0053795-9-.0009049-9-4.41538-28 4.839709+8 5.763893+7 .0013234-9112532151    431
 2.622167+7-.0002558-9 1.000000-8                          112532151    432
       0.0        0.0          0          0          0    0112532  0    433
```

Example 11 (^{23}Na): File 32, LRF = 2, LCOMP = 2   (SAMMY test case tr126 run c22)

```
   11023.0    2.279200+1          0          0          1        0112532151    1
####
#### Z_A    Abundance          0         LFW         NER
   11023.0    1.000000+0          0          0          1        0112532151    2
####
#### Emin     Emax           Lru=1 => Resolved Resonance Region
####                              Lrf=2 => ML Breit Wigner
 1.000000-5 5.000000+5          1          2          0        1112532151    3
####
#### Spin    Radius              LCOMP = 2
     1.5    5.410000-1          0          2          3        0112532151    4
####
#### Weight                   L=0         Number of resonances=   23
 2.279200+1                      0          0        276        23112532151    5
####
#### E_res       +/-J   Gamma_Tot   Gamma_n   Gamma_gam
2810.794885    -1.0   3.767281+2 3.763751+2 3.529968-1          112532151    6
 4.846067+0                       5.115552+0 3.529959-2          112532151    7
242969.1586    -1.0   3.361620+2 3.346627+2 1.499230+0          112532151    8
 1.341693+1                       2.812416+1 1.499597-1          112532151    9
298319.3838     2.0   2.036237+3 2.035217+3 1.020005+0          112532151   10
 2.651743+1                       7.703902+1 1.020000-1          112532151   11
539188.7892    -1.0   6.230475+4 6.229461+4 1.014000+1          112532151   12
 1.284928+4                       5.157889+3 1.014000+0          112532151   13
...
697096.6622     4.0   6.000314+4 6.000314+4 1.000000-3          112532151   48
 2.997502+4                       8.180894+3 1.000000-4          112532151   49
780016.0085     4.0   4.399728+4 4.399728+4 1.000000-3          112532151   50
 2.199934+4                       5.120709+3 1.000000-4          112532151   51
#### Correlation matrix follows
        0.0        0.0          2         69         67        0112532151   52
     2    1  26                                               112532151   53
     5    4   6                                               112532151   54
     8    2   1          36                                   112532151   55
    10    1   2  2               -3                           112532151   56
    11    1   6  9       4       -4  3       67               112532151   57
    14    1  -3-14                    2  5                     112532151   58
    15    2   1                                35             112532151   59
    17    2  -1                1      2  7              -1     112532151   60
    18   11   1               -1 22                           112532151   61
    20   10   1  6                      6                     112532151   62
    23    8   1       2  9                                    112532151   63
    25   11   1                                               112532151   64
    26    8   2       2  8                              1     112532151   65
    27   26   7                                               112532151   66
    28   10  -2 -1                                            112532151   67
    29    5   1      -1  3           8                 1    3 112532151   68
    29   23   1      -3  1      15                            112532151   69
    31    5   1                                          1 112532151   70
    31   25  -1          17 38                                112532151   71
    32    2   1           1       1  1      11        1    1  112532151   72
    32   20   1      -1  1       7          -7-33             112532151   73
    34    4  23-15                                     -3     112532151   74
    34   31   3  4                                            112532151   75
...
    68   10  -1                                               112532151  118
    68   67  51                                               112532151  119
        0.0        0.0          0          0          0        0112532  0  120
```

Example 12 (^{27}Al): File 2, LRF = 3   (SAMMY test case tr126 run b31)


```
   13027.0    2.674961+1          0          0          1      01300 2151    1
####
####  Z_A     Abundance          0         LFW        NER
   13027.0    1.000000+0          0          0          1      01300 2151    2
####
#### Emin      Emax              Lru=1 => Resolved Resonance Region
####                                  Lrf=3 => Reich-Moore format
####                                            NRO       NAPS
 1.000000-5 8.400000+5          1          3          0      11300 2151    3
####
#### Spin     Radius             Number of L-values = 3
      2.5    4.322580-1          1          0          3      41300 2151    4
####
#### Weight    Radius           L=0        Number of resonances=   24
 2.674961+1 4.322580-1          0          0        144     241300 2151    5
####
#### E_res      +/-J       Gamma_n  Gamma_gam  Gamma_others
-3799639.12     -2.0   3.074628+6 9.967501-1                 1300 2151    6
...
1320479.141      3.0   2.110464+5 2.000002+0                 1300 2151   27
1460153.027      3.0   3.846106+4 2.000000+0                 1300 2151   28
1630069.615     -2.0   3.716185+4 2.000000+0                 1300 2151   29
####
#### Weight    Radius           L=1        Number of resonances=   38
 2.674961+1 6.064000-1          1          0        228     381300 2151   30
####
#### E_res      +/-J       Gamma_n  Gamma_gam  Gamma_others
5904.691853     -1.0   1.576800+1 7.300000-1                 1300 2151   31
90716.30643     -1.0   5.560800+0 8.676000-2                 1300 2151   32
...
917701.2064     -3.0   1.412775+5 2.000005+0                 1300 2151   66
1100000.000     -2.0   3.400000+3 2.000000+0                 1300 2151   67
1301995.797     -1.0   8.039633+4 2.000000+0                 1300 2151   68
####
#### Weight    Radius           L=2        Number of resonances=   19
 2.674961+1 4.396000-1          2          0        114     191300 2151   69
####
#### E_res      +/-J       Gamma_n  Gamma_gam  Gamma_others
261301.6472      4.0   1.343650+2 6.218560-1                 1300 2151   70
268709.4074      4.0   2.061541+2 2.088908-1                 1300 2151   71
...
604259.9813      4.0   2.220882+1 2.116048+0                 1300 2151   78
656160.4315      5.0   3.185940+1 2.106474+0                 1300 2151   79
656479.5669      4.0   2.234544+2 1.057579+0                 1300 2151   80
707472.3731      5.0   1.309373+3 2.257103+0                 1300 2151   81
713793.6249      0.0   1.418283+4 2.396929+0                 1300 2151   82
759412.0154     -1.0   8.734286+3 2.003903+0                 1300 2151   83
768449.4683      4.0   2.115070+2 2.299934+0                 1300 2151   84
787490.7037      5.0   1.232400+4 2.003397+0                 1300 2151   85
822793.8215      4.0   2.012128+2 2.288267+0                 1300 2151   86
851450.6242      4.0   3.436535+3 1.999998+0                 1300 2151   87
865849.1875      4.0   8.301900+1 2.000000+0                 1300 2151   88
```

Example 13 (^{27}Al): File 32, LRF = 3, LCOMP = 1   (SAMMY test case tr126 run b31)

```
   13027.0   2.674961+1         0         0         1       0130032151    1
####
####  Z_A    Abundance          0        LFW       NER
   13027.0   1.000000+0         0         0         1       0130032151    2
####
#### Emin     Emax          Lru=1 => Resolved Resonance Region
####                              Lrf=3 => Reich-Moore format
 1.000000-5 8.400000+5         1         3         0      1130032151    3
####
#### Spin    Radius             LCOMP = 1
     2.5   4.322580-1          0         1         0       0130032151    4
####
#### Weight      Number of short-range sections =    1
 2.674961+1                     0         0         1       0130032151    5
####                         Mpar=3
                               3         0     30132    81130032151    6
####
#### E_res      +/-J      Gamma_n  Gamma_gam  Gamma_others
-3799639.12   -2.0   3.074628+6 9.967501-1                 130032151    7
-313004.100    3.0   1.464537+4 9.959502-1                 130032151    8
-199032.761    3.0   6.003580+4 9.473815-1                 130032151    9
-16628.0001   -2.0   3.531120+1 1.778000+0                 130032151   10
-3143.00000    3.0   4.535966+0 2.000000+0                 130032151   11
34730.89081   -2.0   3.028536+3 3.100003+0                 130032151   12
87436.57493    3.0   1.038512+4 2.100014+0                 130032151   13
144449.3048    3.0   1.960962+4 5.100332+0                 130032151   14
203410.1011   -2.0   1.207204+4 6.008260+0                 130032151   15
280550.5160    3.0   1.591614+4 2.721547+0                 130032151   16
...
759412.0154   -1.0   8.734286+3 2.003903+0                 130032151   82
768449.4683    4.0   2.115070+2 2.299934+0                 130032151   83
787490.7037    5.0   1.232400+4 2.003397+0                 130032151   84
822793.8215    4.0   2.012128+2 2.288267+0                 130032151   85
851450.6242    4.0   3.436535+3 1.999998+0                 130032151   86
865849.1875    4.0   8.301900+1 2.000000+0                 130032151   87
#### Covariance matrix follows
 1.53234+11-1.66064+11-1.928704-4-1.685669+6-2.581071+6-1.607310-3130032151   88
-2.158737+8-3.517308+7-1.059240-2-1.269171+1-3.169273+3-8.188330-5130032151   89
-1.255953-3-4.609667+0-8.926399-5-8.411458+6-2.117553+7-2.339600-2130032151   90
 1.892243+7-1.928622+6-8.395932-2-2.139290+7 1.655011+7-6.962277-1130032151   91
-9.921463+5-2.109538+6 1.197417+2 6.785851+5 2.021701+6-1.245619+1130032151   92
...
-2.342453-5 6.262151-5 1.354018-9 1.452494-3-8.395122-5-.0339487-9130032151 5020
                                6.292993+2 1.187137+1 3.409646-4130032151 5021
-8.888938+2 2.956809+2-1.893107-6                         130032151 5022
 3.370744+2-1.615264-5 1.943209+1-2.297480+1 4.933992-6   130032151 5023
                       5.222658-2 2.369307-3-1.203563-3-.0705157-9130032151 5024
                       2.877717+6 2.809259+4 2.608780-4130032151 5025
                       1.146245+5-2.440211-5             130032151 5026
            3.999996-2                               130032151 5027
 5.103234+3                       6.892177+1          4.000000-2130032151 5028
      0.0         0.0         0         0         0       0130032  0 5029
```

Example 14 (^{27}Al): File 32, LRF = 3, LCOMP = 2   (SAMMY test case tr126 run b32)

```
   13027.0    2.674961+1            0           0           1         0130032151    1
####
#### Z_A    Abundance              0          LFW         NER
   13027.0    1.000000+0            0           0           1         0130032151    2
####
#### Emin      Emax            Lru=1 => Resolved Resonance Region
####                                Lrf=3 => Reich-Moore format
 1.000000-5 8.400000+5            1           3           0         1130032151    3
####
#### Spin     Radius              LCOMP = 2
     2.5    4.322580-1            1           2           1         0130032151    4
####
#### Weight                     Mpar=3        Number of resonances=   81
 2.674961+1                          3           0         972       81130032151    5
####
#### E_res        +/-J      Gamma_n   Gamma_gam   Gamma_others
-3799639.12     -2.0    3.074628+6 9.967501-1                        130032151    6
 3.914519+5             4.419370+5 9.967501-2                        130032151    7
-313004.100      3.0    1.464537+4 9.959502-1                        130032151    8
 7.353688+3             1.471813+3 9.959501-2                        130032151    9
-199032.761      3.0    6.003580+4 9.473815-1                        130032151   10
 2.921839+4             7.407974+3 9.473807-2                        130032151   11
-16628.0001     -2.0    3.531120+1 1.778000+0                        130032151   12
 1.855350+1             3.532059+0 1.778000-1                        130032151   13
...
851450.6242      4.0    3.436535+3 1.999998+0                        130032151  164
 1.696384+3             3.385623+2 1.999999-1                        130032151  165
865849.1875      4.0    8.301900+1 2.000000+0                        130032151  166
 7.143692+1             8.301914+0 2.000000-1                        130032151  167
#### Correlation matrix follows
         0.0          0.0            2         243         436       0130032151  168
     2     1 -95                                                      130032151  169
     5     4 -11                                                      130032151  170
     7     1  -1            -2                                        130032151  171
     8     1  -1            -2    -73                                 130032151  172
    16     1  -1                                                      130032151  173
    17     1 -17  6                                            21     130032151  174
    19     7  -2  1                                                   130032151  175
    20     5  -2   -13 -4                                      26     130032151  176
    22     1  -3   1         4    24  8                        -1     130032151  177
    22    20  20                                                      130032151  178
    23     1   3 -1        -4    -32 -4                               130032151  179
    23    19 -23-50    -84                                            130032151  180
    25     1 -10  5               1                            -6     130032151  181
    25    20   1   -6  4                                              130032151  182
    26     1  -5  2             -3  4                          -2     130032151  183
    26    19  -4 -8    47-24      4                                   130032151  184
    28     1   5 -1        -1    -7 -5                         -1     130032151  185
...
   236   227  -2             -1 -1     2                              130032151  597
   238    53  -1      3  2     1                                      130032151  598
   238   158  -1                                                     130032151  599
   238   178  -3 -1                                                   130032151  600
   238   235  -2                                                     130032151  601
   239    55  -3 -1                                                   130032151  602
   239   178   2  1                                                   130032151  603
   239   235   3       4                                              130032151  604
         0.0          0.0            0           0           0       0130032  0  605
```

Example 15 (^{27}Al): File 2, LRF = 7 (SAMMY test case tr147 run c; entire file is given here)

```
   13027.0    2.676806+1          0          0          1          0 987 2151    1
####
####  Z_A    Abundance           0          LFW        NER
   13027.0    1.000000+0          0          0          1          0 987 2151    2
####
#### Emin     Emax          Lru=1 => Resolved Resonance Region
####                              Lrf=7 => R-Matrix Limited
 1.000000+4 8.400000+5          1          7          0          1 987 2151    3
####
####   Flag for Gamma not gamma   0
####             Flag for Reich-Moore =   3
####                       Number of J values = 10
       0.0                  0          3         10          0 987 2151    4
####
####   2 pairs of particles are defined next
#### First pair is gamma & compound nucleus
#### Others are particle pairs
       0.0        0.0          2          0         24          4 987 2151    5
####
####   MA         MB         ZA         ZB         IA         IB
####   Q          PNT        SHF        MT         PA         PB
0.000000000 2.776806+1        0.0        0.0        1.0        0.0  987 2151    6
0.000000000        0.0        0.0      102.0        0.0        0.0  987 2151    7
1.000000000 2.676806+1        0.0        0.0        0.5        2.5  987 2151    8
0.000000000        1.0        0.0        2.0        0.0        0.0  987 2151    9
####
####     Spin group is defined in the next lines
####    J      Parity                     Number of channels=  4
       2.0        0.0          0          0         24          4 987 2151   10
####
#### First channel is gamma, second is neutron
####   IPP        L      Ch Spin                    APE        APT
       1.0        0.0        0.0        0.0                        987 2151   11
       2.0        0.0        2.0        0.0   4.322580-1 4.322580-1 987 2151   12
       2.0        2.0        2.0        0.0   4.396000-1 4.396000-1 987 2151   13
       2.0        2.0        3.0        0.0   4.396000-1 4.396000-1 987 2151   14
####
####       Number of channels =   4, res=   14,      Lines/Res=   1
       0.0        0.0          0         14         84          1 987 2151   15
####  E_res Gamma_gam  Gamma_n  Gamma_others
-4585600.00 9.967500-1 3.291200+6                                  987 2151   16
-16628.0000 1.596400+0 2.391700+1                                  987 2151   17
34827.50898 2.679000+0 3.347600+3                                  987 2151   18
203556.0484 3.416400+0 1.340600+4                                  987 2151   19
260781.8750 2.748000+0            9.926000+1                       987 2151   20
268535.1563 8.735000-1                       1.589000+2            987 2151   21
429510.1151 5.070300-1 5.199100+4                                  987 2151   22
490416.2952 4.909000-1 2.885600+3                                  987 2151   23
654609.3750 1.964000-1                       1.615000+2            987 2151   24
714903.3521 2.210000+0 1.452400+3                                  987 2151   25
759351.2965 1.090000+0                       6.600900+3            987 2151   26
822131.2787 2.210000+0 8.502600+3                                  987 2151   27
1120000.000 2.000000+0 1.147000+5                                  987 2151   28
1630000.000 2.000000+0 3.726200+4                                  987 2151   29
####
####     Spin group is defined in the next lines
####    J      Parity                     Number of channels=  4
       3.0        0.0          0          0         24          4 987 2151   30
####
```

```
#### First channel is gamma, second is neutron
####  IPP         L         Ch Spin                          APE         APT
      1.0         0.0         0.0         0.0                                  987 2151   31
      2.0         0.0         3.0         0.0     4.322580-1 4.322580-1 987 2151   32
      2.0         2.0         2.0         0.0     4.396000-1 4.396000-1 987 2151   33
      2.0         2.0         3.0         0.0     4.396000-1 4.396000-1 987 2151   34
####
####       Number of channels =    4, res=   19,        Lines/Res=   1
      0.0         0.0         0         19         114         1 987 2151   35
####   E_res Gamma_gam  Gamma_n  Gamma_others
-312910.000 9.959500-1 1.470500+4                              987 2151   36
-185070.000 9.473800-1 5.608500+4                              987 2151   37
-3143.00000 1.111100+0 1.801000+1                              987 2151   38
86267.71729 2.061700+0 1.093800+4                              987 2151   39
142925.5704 3.342600+0 1.869500+4                              987 2151   40
280288.8337 2.274500+0 1.417400+4                              987 2151   41
386353.5337 6.113000-1 2.303300+3                              987 2151   42
420255.2813 8.110000-1            4.008900+2                   987 2151   43
526195.7350 9.788000-1 5.141200+3                              987 2151   44
586240.0091 1.376000+0 4.596000+3                              987 2151   45
586285.6250 3.599000-1            1.055000+2                   987 2151   46
614569.4112 7.095900-1 1.364600+4                              987 2151   47
655086.0625 1.734000-1                      2.569000+2         987 2151   48
766337.3125 1.402000+0            3.189000+2                   987 2151   49
786709.4701 2.210000+0 2.424100+4                              987 2151   50
820722.9375 1.713000+0            2.590600+2                   987 2151   51
873858.3125 2.210000+0 1.040000+4                              987 2151   52
1290000.000 2.000000+0 2.142400+5                              987 2151   53
1460000.000 2.000000+0 3.861500+4                              987 2151   54
####
####     Spin group is defined in the next lines
####    J       Parity                         Number of channels=   2
     -1.0         0.0         0         0         12         2 987 2151   55
####
#### First channel is gamma, second is neutron
####  IPP         L         Ch Spin                          APE         APT
      1.0         0.0         0.0         0.0                                  987 2151   56
      2.0         1.0         2.0         0.0     6.064000-1 6.064000-1 987 2151   57
####
####       Number of channels =    2, res=   10,        Lines/Res=   1
      0.0         0.0         0         10         60         1 987 2151   58
####   E_res Gamma_gam  Gamma_n  Gamma_others
5904.676793 6.087600-1 1.669500+1                              987 2151   59
24306.05860 1.160000-2 1.539000+0                              987 2151   60
99731.67970 1.793000+0 4.390000+0                              987 2151   61
103837.5703 6.174000-1 3.756000+0                              987 2151   62
220294.4375 5.760000-1 1.000000+1                              987 2151   63
494375.4162 5.038000-1 9.998900+2                              987 2151   64
707707.6479 1.130000+0 1.001000+4                              987 2151   65
725166.4375 1.130000+0 8.907000+2                              987 2151   66
782103.5543 1.130000+0 4.577700+3                              987 2151   67
1300000.000 2.000000+0 8.130500+4                              987 2151   68
####
####     Spin group is defined in the next lines
####    J       Parity                         Number of channels=   3
     -2.0         0.0         0         0         18         3 987 2151   69
####
#### First channel is gamma, second is neutron
####  IPP         L         Ch Spin                          APE         APT
      1.0         0.0         0.0         0.0                                  987 2151   70
      2.0         1.0         2.0         0.0     6.064000-1 6.064000-1 987 2151   71
```

```
         2.0          1.0          3.0          0.0    6.064000-1 6.064000-1 987 2151   72
####
####      Number of channels =   3, res=   12,        Lines/Res=   1
         0.0          0.0          0           12          72          1 987 2151   73
####  E_res Gamma_gam  Gamma_n  Gamma_others
91248.51560 3.670000-1 2.018000+2                                      987 2151   74
146205.2969 1.986000-1 1.146000+2                                      987 2151   75
224054.9831 1.170000+0 4.712600+2                                      987 2151   76
367949.3223 1.539000+0            4.398300+3                           987 2151   77
376071.9029 6.540000-1 2.909200+3                                      987 2151   78
415747.6805 5.055100+0 2.110100+4                                      987 2151   79
490117.0968 3.760000-1 2.335000+3                                      987 2151   80
523432.8324 1.659000+0            7.200300+3                           987 2151   81
651967.6492 4.506000-1 3.583800+3                                      987 2151   82
762720.7055 1.130000+0 8.492800+4                                      987 2151   83
774592.0573 1.130000+0            6.725600+3                           987 2151   84
1100000.000 2.000000+0 3.400000+3                                      987 2151   85
####
####    Spin group is defined in the next lines
####    J      Parity                         Number of channels=  3
        -3.0         0.0          0            0          18          3 987 2151   86
####
#### First channel is gamma, second is neutron
####  IPP         L       Ch Spin                     APE         APT
         1.0          0.0          0.0          0.0                    987 2151   87
         2.0          1.0          2.0          0.0    6.064000-1 6.064000-1 987 2151   88
         2.0          1.0          3.0          0.0    6.064000-1 6.064000-1 987 2151   89
####
####      Number of channels =   3, res=    8,        Lines/Res=   1
         0.0          0.0          0            8          48          1 987 2151   90
####  E_res Gamma_gam  Gamma_n  Gamma_others
120007.2079 2.160500+0 2.815200+3                                      987 2151   91
158732.5501 8.442000-1 3.427700+3                                      987 2151   92
203758.4688 9.469000-1 4.522000+0                                      987 2151   93
257355.8339 5.869000-1 7.996400+2                                      987 2151   94
477351.9216 6.811000-1 1.273400+3                                      987 2151   95
569534.7123 1.642600+0 1.725500+4                                      987 2151   96
647302.8490 2.625200+0 1.032800+4                                      987 2151   97
948366.1875 1.130000+0 1.492700+5                                      987 2151   98
####
####    Spin group is defined in the next lines
####    J      Parity                         Number of channels=  2
        -4.0         0.0          0            0          12          2 987 2151   99
####
#### First channel is gamma, second is neutron
####  IPP         L       Ch Spin                     APE         APT
         1.0          0.0          0.0          0.0                    987 2151  100
         2.0          1.0          3.0          0.0    6.064000-1 6.064000-1 987 2151  101
####
####      Number of channels =   2, res=    3,        Lines/Res=   1
         0.0          0.0          0            3          18          1 987 2151  102
####  E_res Gamma_gam  Gamma_n  Gamma_others
366848.2087 1.518000+0 4.619000+3                                      987 2151  103
598238.8044 2.900000-1 1.547700+3                                      987 2151  104
858106.8750 1.130000+0 4.380000+3                                      987 2151  105
####
####    Spin group is defined in the next lines
####    J      Parity                         Number of channels=  2
         0.0         1.0          0            0          12          2 987 2151  106
####
#### First channel is gamma, second is neutron
```

```
####   IPP         L        Ch Spin                        APE         APT
       1.0        0.0        0.0        0.0                              987 2151  107
       2.0        2.0        2.0        0.0    4.396000-1 4.396000-1 987 2151  108
####
####       Number of channels =    2, res=    2,        Lines/Res=    1
       0.0        0.0        0          2         12          1 987 2151  109
####   E_res Gamma_gam   Gamma_n  Gamma_others
360344.4375 8.371000+0 2.668000+2                              987 2151  110
521237.4310 3.348000+0 3.591300+4                              987 2151  111
####
####     Spin group is defined in the next lines
####    J        Parity                        Number of channels=   3
       1.0        0.0        0          0         18          3 987 2151  112
####
#### First channel is gamma, second is neutron
####   IPP         L        Ch Spin                        APE         APT
       1.0        0.0        0.0        0.0                              987 2151  113
       2.0        2.0        2.0        0.0    4.396000-1 4.396000-1 987 2151  114
       2.0        2.0        3.0        0.0    4.396000-1 4.396000-1 987 2151  115
####
####       Number of channels =    3, res=    5,        Lines/Res=    1
       0.0        0.0        0          5         30          1 987 2151  116
####   E_res Gamma_gam   Gamma_n  Gamma_others
315049.2344 2.435400+0 8.154200+3                              987 2151  117
345111.8750 2.389000+0             1.155000+2                   987 2151  118
545874.5000 6.724000-1             1.480000+2                   987 2151  119
546264.3125 7.350000-1 9.545000+1                              987 2151  120
698920.9375 1.090000+0 5.355000+1                              987 2151  121
####
####     Spin group is defined in the next lines
####    J        Parity                        Number of channels=   3
       4.0        0.0        0          0         18          3 987 2151  122
####
#### First channel is gamma, second is neutron
####   IPP         L        Ch Spin                        APE         APT
       1.0        0.0        0.0        0.0                              987 2151  123
       2.0        2.0        2.0        0.0    4.396000-1 4.396000-1 987 2151  124
       2.0        2.0        3.0        0.0    4.396000-1 4.396000-1 987 2151  125
####
####       Number of channels =    3, res=    4,        Lines/Res=    1
       0.0        0.0        0          4         24          1 987 2151  126
####   E_res Gamma_gam   Gamma_n  Gamma_others
592722.1250 3.500000-1             4.400000+0                   987 2151  127
602909.5625 2.114000-1             4.737000+1                   987 2151  128
849584.1250 1.090000+0             3.701000+3                   987 2151  129
863506.4375 1.090000+0             8.302000+1                   987 2151  130
####
####     Spin group is defined in the next lines
####    J        Parity                        Number of channels=   2
       5.0        0.0        0          0         12          2 987 2151  131
####
#### First channel is gamma, second is neutron
####   IPP         L        Ch Spin                        APE         APT
       1.0        0.0        0.0        0.0                              987 2151  132
       2.0        2.0        3.0        0.0    4.396000-1 4.396000-1 987 2151  133
####
####       Number of channels =    2, res=    2,        Lines/Res=    1
       0.0        0.0        0          2         12          1 987 2151  134
####   E_res Gamma_gam   Gamma_n  Gamma_others
706342.4028 1.090000+0 1.295800+3                              987 2151  135
786106.2326 1.090000+0 1.113700+4                              987 2151  136
```

Example 16 (^{19}Fl): File 2, LRF = 7   (SAMMY test case tr158 run a; entire file is given here)

```
    9019.0    1.883519+1          0          0          1        0 925 2151    1
####
####  Z_A    Abundance           0          LFW        NER
    9019.0    1.000000+0          0          0          1        0 925 2151    2
####
#### Emin     Emax            Lru=1 => Resolved Resonance Region
####                             Lrf=7 => R-Matrix Limited
 1.000000-2 1.000000+6          1          7          0        1 925 2151    3
####
####   Flag for Gamma not gamma  0
####             Flag for Reich-Moore =  3
####                      Number of J values =  9
       0.0                 0          3          9        0 925 2151    4
####
####   4 pairs of particles are defined next
#### First pair is gamma & compound nucleus
#### Others are particle pairs
       0.0        0.0          4          0         48        8 925 2151    5
####
####   MA         MB         ZA         ZB         IA         IB
####   Q          PNT        SHF        MT         PA         PB
0.000000000 1.967320+1     0.0        9.0        1.0        0.0      925 2151    6
0.000000000     0.0        0.0      102.0        0.0        0.0      925 2151    7
1.000000000 1.867320+1     0.0        9.0        0.5        0.5      925 2151    8
0.000000000     1.0        0.0        2.0        0.0        0.0      925 2151    9
1.000000000 1.867320+1     0.0        9.0        0.5       -0.5      925 2151   10
-104308.024     1.0        0.0       51.0        0.0        0.0      925 2151   11
1.000000000 1.867320+1     0.0        9.0        0.5        2.5      925 2151   12
-187122.107     1.0        0.0       52.0        0.0        0.0      925 2151   13
####
####     Spin group is defined in the next lines
####    J      Parity                  Number of channels=  4
       0.0       -1.0          0          0         24        4 925 2151   14
####
#### First channel is gamma, second is neutron
####   IPP        L      Ch Spin                   APE        APT
       1.0        0.0        0.0        0.0                           925 2151   15
       2.0        1.0        1.0        0.0   5.360000-1 5.360000-1 925 2151   16
       3.0        0.0        0.0        0.0   5.360000-1 5.360000-1 925 2151   17
       4.0        3.0        3.0        0.0   5.360000-1 5.360000-1 925 2151   18
####
####     Number of channels =   4, res=   0,       Lines/Res=   1
       0.0        0.0          0          0          6        1 925 2151   19
####   E_res Gamma_gam  Gamma_n   Gamma_others
                                                         925 2151   20
####
####     Spin group is defined in the next lines
####    J      Parity                  Number of channels=  4
       0.0        1.0          0          0         24        4 925 2151   21
####
#### First channel is gamma, second is neutron
####   IPP        L      Ch Spin                   APE        APT
       1.0        0.0        0.0        0.0                           925 2151   22
       2.0        0.0        0.0        0.0   5.360000-1 5.360000-1 925 2151   23
       3.0        1.0       -1.0        0.0   5.360000-1 5.360000-1 925 2151   24
       4.0        2.0        2.0        0.0   5.360000-1 5.360000-1 925 2151   25
####
####     Number of channels =   4, res=   1,       Lines/Res=   1
```

```
      0.0          0.0            0            1            6          1 925 2151   26
#### E_res Gamma_gam  Gamma_n  Gamma_others
-338314.102 2.052563+0 1.907296+5                                      925 2151   27
####
####     Spin group is defined in the next lines
#### J       Parity                          Number of channels=  8
    -1.0         0.0            0            0           48          8 925 2151   28
####
#### First channel is gamma, second is neutron
#### IPP         L       Ch Spin                      APE         APT
    1.0         0.0          0.0          0.0                           925 2151   29
    2.0         1.0          0.0          0.0    5.360000-1 5.360000-1 925 2151   30
    2.0         1.0          1.0          0.0    5.360000-1 5.360000-1 925 2151   31
    3.0         0.0         -1.0          0.0    5.360000-1 5.360000-1 925 2151   32
    3.0         2.0         -1.0          0.0    5.360000-1 5.360000-1 925 2151   33
    4.0         1.0          2.0          0.0    5.360000-1 5.360000-1 925 2151   34
    4.0         3.0          2.0          0.0    5.360000-1 5.360000-1 925 2151   35
    4.0         3.0          3.0          0.0    5.360000-1 5.360000-1 925 2151   36
####
####     Number of channels =   8, res=    5,       Lines/Res=   2
      0.0          0.0            0            5           60          2 925 2151   37
#### E_res Gamma_gam  Gamma_n  Gamma_others
48931.02889 8.740337-1 1.716010+3 1.135764-1                           925 2151   38
                                                                       925 2151   39
97944.56930 2.745850+0 1.392614+4 1.631873-1                           925 2151   40
                                                                       925 2151   41
142255.9168 1.222463-1            4.170088+0 8.490063+0 1.314047+2 925 2151   42
                                                                       925 2151   43
257029.4263 2.508937-1 1.999330-1            1.704316+3            925 2151   44
 5.326507+4                                                            925 2151   45
499900.2874 4.089489+0 7.807878+1 3.320021+3 6.785874-1 6.775050-1 925 2151   46
-8.679718+1-1.010052+4 3.854020+1                                      925 2151   47
####
####     Spin group is defined in the next lines
#### J       Parity                          Number of channels=  7
    1.0         0.0            0            0           42          7 925 2151   48
####
#### First channel is gamma, second is neutron
#### IPP         L       Ch Spin                      APE         APT
    1.0         0.0          0.0          0.0                           925 2151   49
    2.0         0.0          1.0          0.0    5.360000-1 5.360000-1 925 2151   50
    2.0         2.0          1.0          0.0    5.360000-1 5.360000-1 925 2151   51
    3.0         1.0          0.0          0.0    5.360000-1 5.360000-1 925 2151   52
    3.0         1.0         -1.0          0.0    5.360000-1 5.360000-1 925 2151   53
    4.0         2.0          2.0          0.0    5.360000-1 5.360000-1 925 2151   54
    4.0         2.0          3.0          0.0    5.360000-1 5.360000-1 925 2151   55
####
####     Number of channels =   7, res=    4,       Lines/Res=   2
      0.0          0.0            0            4           48          2 925 2151   56
#### E_res Gamma_gam  Gamma_n  Gamma_others
268109.3783 3.048400+0 8.115107+3            2.201184+3            925 2151   57
 7.013273+0                                                            925 2151   58
308739.0765 4.003522-1 1.040526+1 1.439294+1 4.934973-1 6.343137+0 925 2151   59
 2.762858+0                                                            925 2151   60
924708.9783 2.674594+0            3.434312+4 4.036286+4            925 2151   61
 1.505126+3                                                            925 2151   62
1086723.031 5.000339-1 4.091653+5            7.980831+0            925 2151   63
 6.277813+1                                                            925 2151   64
####
####     Spin group is defined in the next lines
#### J       Parity                          Number of channels=  9
```

```
      -2.0         0.0            0           0         54         9 925 2151   65
####
#### First channel is gamma, second is neutron
####   IPP        L       Ch Spin                   APE       APT
       1.0         0.0         0.0         0.0                          925 2151   66
       2.0         1.0         1.0         0.0    5.360000-1 5.360000-1 925 2151   67
       2.0         3.0         1.0         0.0    5.360000-1 5.360000-1 925 2151   68
       3.0         2.0         0.0         0.0    5.360000-1 5.360000-1 925 2151   69
       3.0         2.0        -1.0         0.0    5.360000-1 5.360000-1 925 2151   70
       4.0         1.0         2.0         0.0    5.360000-1 5.360000-1 925 2151   71
       4.0         1.0         3.0         0.0    5.360000-1 5.360000-1 925 2151   72
       4.0         3.0         2.0         0.0    5.360000-1 5.360000-1 925 2151   73
       4.0         3.0         3.0         0.0    5.360000-1 5.360000-1 925 2151   74
####
####      Number of channels =   9, res=    5,         Lines/Res=   2
       0.0         0.0           0           5         60         2 925 2151   75
####   E_res Gamma_gam  Gamma_n  Gamma_others
27013.36468 1.180838+0 3.571340+2 1.318737-1                          925 2151   76
                                                                      925 2151   77
261219.8416 2.088477-2 3.190403+4            6.038645+4               925 2151   78
-5.878642+2                                                           925 2151   79
282455.3714 3.136277-2 8.287436+1           -5.131240+1               925 2151   80
 9.380974+1                                                           925 2151   81
406237.9402 1.437289+1 3.462385+4 3.170895+4-1.869180+5 1.087456+2 925 2151   82
 1.272494+5 2.403460+2 1.137275+1-1.286078+4                          925 2151   83
500000.8476 2.304022-1 5.299827+2 2.794795+1 4.433569+4-2.557080+1 925 2151   84
-1.242596+3 1.662113+1 8.832734+0 1.063319+1                          925 2151   85
####
####    Spin group is defined in the next lines
####    J      Parity                     Number of channels=  8
       2.0         0.0           0           0         48         8 925 2151   86
####
#### First channel is gamma, second is neutron
####   IPP        L       Ch Spin                   APE       APT
       1.0         0.0         0.0         0.0                          925 2151   87
       2.0         2.0         0.0         0.0    5.360000-1 5.360000-1 925 2151   88
       2.0         2.0         1.0         0.0    5.360000-1 5.360000-1 925 2151   89
       3.0         1.0        -1.0         0.0    5.360000-1 5.360000-1 925 2151   90
       3.0         3.0        -1.0         0.0    5.360000-1 5.360000-1 925 2151   91
       4.0         0.0         2.0         0.0    5.360000-1 5.360000-1 925 2151   92
       4.0         2.0         2.0         0.0    5.360000-1 5.360000-1 925 2151   93
       4.0         2.0         3.0         0.0    5.360000-1 5.360000-1 925 2151   94
####
####      Number of channels =   8, res=    8,         Lines/Res=   2
       0.0         0.0           0           8         96         2 925 2151   95
####   E_res Gamma_gam  Gamma_n  Gamma_others
120390.7616 2.715753+0 1.611880-1 9.317343-2 9.351649+0 9.193093+0 925 2151   96
                                                                      925 2151   97
421833.2568 3.629571-1 6.765020+3 9.630758+1-2.215552+0 4.279661+0 925 2151   98
-2.043338+3-4.265281-1 6.409055+1                                     925 2151   99
598371.3232 4.479380+0 5.484083+3 1.239144+1 3.623047+1 1.013699+0 925 2151  100
                                                                      925 2151  101
655088.8482 1.175513+1 3.712973-1            4.176071+2               925 2151  102
 1.225063+2                                                           925 2151  103
752171.3717 2.366799+1 8.228987+3           -4.197128+2               925 2151  104
 2.335137+4                                                           925 2151  105
792797.2467 2.598882+0 1.548307+4            3.795058+4               925 2151  106
-2.118429+1                                                           925 2151  107
846287.5857 7.274603-1 3.277450+1            1.671766+4               925 2151  108
 1.989256+3                                                           925 2151  109
856548.3236 5.196694-1 2.137031+3 3.256351+3-9.173437+2               925 2151  110
```

```
  4.037398+3                                                         925 2151  111
####
####     Spin group is defined in the next lines
####    J      Parity                          Number of channels=  8
     -3.0        0.0           0           0        48         8 925 2151  112
####
#### First channel is gamma, second is neutron
####   IPP        L       Ch Spin                      APE       APT
      1.0        0.0         0.0          0.0                       925 2151  113
      2.0        3.0         0.0          0.0   5.360000-1 5.360000-1 925 2151  114
      2.0        3.0         1.0          0.0   5.360000-1 5.360000-1 925 2151  115
      3.0        2.0        -1.0          0.0   5.360000-1 5.360000-1 925 2151  116
      4.0        1.0         2.0          0.0   5.360000-1 5.360000-1 925 2151  117
      4.0        1.0         3.0          0.0   5.360000-1 5.360000-1 925 2151  118
      4.0        3.0         2.0          0.0   5.360000-1 5.360000-1 925 2151  119
      4.0        3.0         3.0          0.0   5.360000-1 5.360000-1 925 2151  120
####
####      Number of channels =    8, res=    6,       Lines/Res=    2
      0.0        0.0           0           6        72         2 925 2151  121
####   E_res Gamma_gam  Gamma_n  Gamma_others
43572.28944 1.013099+0 2.535128-2 3.110732-2                       925 2151  122
                                                                   925 2151  123
385358.9216 5.971985+0 1.101529+3          2.470091+1 2.678417+3 925 2151  124
                                                                   925 2151  125
623498.3906 2.291738+0 1.939907+2 5.291103+2 2.979935+4 7.365453+0 925 2151  126
 6.737591+1 1.010839+1 1.119861+2                                  925 2151  127
663159.3684 2.678239+0 2.163960+0 3.169148+0 2.673549+3           925 2151  128
 1.018272+6                                                        925 2151  129
1113162.179 4.827504-1          4.735747+2 5.377886+4             925 2151  130
-1.245690+5                                                        925 2151  131
1383534.169 5.000000-1 1.214946+3          -2.394341+1            925 2151  132
 2.337540+6                                                        925 2151  133
####
####     Spin group is defined in the next lines
####    J      Parity                          Number of channels=  7
      3.0        0.0           0           0        42         7 925 2151  134
####
#### First channel is gamma, second is neutron
####   IPP        L       Ch Spin                      APE       APT
      1.0        0.0         0.0          0.0                       925 2151  135
      2.0        2.0         1.0          0.0   5.360000-1 5.360000-1 925 2151  136
      3.0        3.0         0.0          0.0   5.360000-1 5.360000-1 925 2151  137
      3.0        3.0        -1.0          0.0   5.360000-1 5.360000-1 925 2151  138
      4.0        0.0         3.0          0.0   5.360000-1 5.360000-1 925 2151  139
      4.0        2.0         2.0          0.0   5.360000-1 5.360000-1 925 2151  140
      4.0        2.0         3.0          0.0   5.360000-1 5.360000-1 925 2151  141
####
####      Number of channels =    7, res=    2,       Lines/Res=    2
      0.0        0.0           0           2        24         2 925 2151  142
####   E_res Gamma_gam  Gamma_n  Gamma_others
173599.3155 5.096430+0 2.099567-1 9.261048-2 5.206644-2           925 2151  143
                                                                   925 2151  144
945180.5782 7.792306-1 5.151561+3          1.064145+3             925 2151  145
 3.529486+4                                                        925 2151  146
####
####     Spin group is defined in the next lines
####    J      Parity                          Number of channels=  5
     -4.0        0.0           0           0        30         5 925 2151  147
####
#### First channel is gamma, second is neutron
####   IPP        L       Ch Spin                      APE       APT
```

```
      1.0          0.0          0.0          0.0                                      925 2151  148
      2.0          3.0          1.0          0.0    5.360000-1 5.360000-1 925 2151  149
      4.0          1.0          3.0          0.0    5.360000-1 5.360000-1 925 2151  150
      4.0          3.0          2.0          0.0    5.360000-1 5.360000-1 925 2151  151
      4.0          3.0          3.0          0.0    5.360000-1 5.360000-1 925 2151  152
####
####     Number of channels =   5, res=    0,        Lines/Res=   1
      0.0          0.0          0            0            6          1 925 2151  153
####  E_res Gamma_gam   Gamma_n   Gamma_others
                                                                     925 2151  154
```

Example 17 (^{35}Cl): File 2, LRF = 7   (Thanks to Royce Sayer for providing this file.)

```
    17035.0 3.46685E+1          0          0          1       01725 2151    1
####
####   Z_A    Abundance         0         LFW         NER
    17035.0 1.00000E+0          0          1          1       01725 2151    2
####
#### Emin     Emax          Lru=1 => Resolved Resonance Region
####                             Lrf=7 => R-Matrix Limited
 1.00000E-5 1.20000E+6          1          7          0       01725 2151    3
####
####   Flag for Gamma not gamma   0
####              Flag for Reich-Moore =   3
####                      Number of J values =   8
       0.0        0.0          0          3          8       01725 2151    4
####
####   3 pairs of particles are defined next
#### First pair is gamma & compound nucleus
#### Others are particle pairs
       0.0        0.0          3          0         36       61725 2151    5
####
####   MA         MB         ZA         ZB         IA         IB
####   Q          PNT        SHF        MT         PA         PB
 0.00000E+0 3.56685E+1        0.0        0.0        1.0        0.01725 2151    6
 0.00000E+0        0.0       -1.0      102.0        0.0        0.01725 2151    7
 1.00000E+0 3.46685E+1        0.0        0.0        0.5        1.51725 2151    8
 0.00000E+0        1.0       -1.0        2.0        0.0        0.01725 2151    9
 9.98624E-1 3.46685E+1        1.0       16.0        0.5        1.51725 2151   10
 6.15220E+5        1.0       -1.0      103.0        0.0        0.01725 2151   11
####
####     Spin group is defined in the next lines
####     J      Parity                   Number of channels=   3
       1.0        0.0          0          0         18       31725 2151   12
####
#### First channel is gamma, second is neutron
####   IPP        L        Ch Spin                  APE        APT
       1.0        0.0        0.0        0.0                   1725 2151   13
       2.0        0.0        1.0        0.0 3.66798E-1 4.82222E-11725 2151   14
       3.0        0.0        1.0        0.0 3.66798E-1 4.82222E-11725 2151   15
####
####     Number of channels =    4, res=   23,       Lines/Res=   1
       0.0        0.0          0         23        138      231725 2151   16
####   E_res Gamma_gam  Gamma_n   Gamma_others
 54931.9958 3.67260E-1 4.64424E+1                           1725 2151   17
 68236.1571 3.93360E-1 2.17904E+2 1.00000E-5                1725 2151   18
 115098.000 7.39000E-1 4.30778E+0                           1725 2151   19
...
 1109187.77 6.06000E-1 2.74235E+3                           1725 2151   38
 1205687.36 6.06000E-1 6.42584E+2                           1725 2151   39
####
####     Spin group is defined in the next lines
####     J      Parity                   Number of channels=   3
       2.0        0.0          0          0         18       31725 2151   40
####
#### First channel is gamma, second is neutron
####   IPP        L        Ch Spin                  APE        APT
       1.0        0.0        0.0        0.0                   1725 2151   41
       2.0        0.0        2.0        0.0 3.66798E-1 4.82222E-11725 2151   42
       3.0        0.0        2.0        0.0 3.66798E-1 4.82222E-11725 2151   43
####
```

```
####      Number of channels =   3, res=   32,        Lines/Res=   1
       0.0         0.0         0          32         192        321725 2151   44
####  E_res Gamma_gam  Gamma_n  Gamma_others
-180.650000 5.30150E-1 1.32770E+1 5.99230E-3                     1725 2151   45
 14801.9519 3.45680E-1 3.25995E+1 2.80002E-2                     1725 2151   46
...
 1257679.87 6.06000E-1 1.74983E+3                                1725 2151   75
 7563145.25 3.83980E-1 6.21905E+5 1.00000E+3                     1725 2151   76
####
####    Spin group is defined in the next lines
####    J       Parity                       Number of channels=  3
       0.0        -1.0         0          0          18         31725 2151   77
####
#### First channel is gamma, second is neutron
####   IPP        L        Ch Spin                   APE        APT
       1.0        1.0         0.0        0.0                     1725 2151   78
       2.0        1.0         1.0        0.0 4.88875E-1 4.82222E-11725 2151   79
       3.0        1.0         1.0        0.0 4.88875E-1 4.82222E-11725 2151   80
####
####      Number of channels =   3, res=    9,        Lines/Res=   1
       0.0         0.0         0          9          54         91725 2151   81
####  E_res Gamma_gam  Gamma_n  Gamma_others
 22396.3985 1.72480E+0 9.66367E-1                                1725 2151   82
 96604.1512 1.56500E+0 2.76138E+0                                1725 2151   83
...
 547854.482 8.60000E-1 7.64013E+2                                1725 2151   90
####
####    Spin group is defined in the next lines
####    J       Parity                       Number of channels=  3
      -1.0        0.0         0          0          18         31725 2151   91
####
#### First channel is gamma, second is neutron
####   IPP        L        Ch Spin                   APE        APT
       1.0        1.0         0.0        0.0                     1725 2151   92
       2.0        1.0         1.0        0.0 4.88875E-1 4.82222E-11725 2151   93
       3.0        1.0         1.0        0.0 4.88875E-1 4.82222E-11725 2151   94
####
####      Number of channels =   3, res=   38,        Lines/Res=   1
       0.0         0.0         0          38         228        381725 2151   95
####  E_res Gamma_gam  Gamma_n  Gamma_others
 4250.76249 4.72000E-1 6.28000E-1 2.30000E-1                     1725 2151   96
 5491.02019 9.70210E-1 3.86354E-3                                1725 2151   97
 37767.9176 1.91200E-1 4.40797E-1                                1725 2151   98
...
 1435502.40 8.60000E-1 5.36563E+3                                1725 2151  133
####
####    Spin group is defined in the next lines
####    J       Parity                       Number of channels=  3
      -2.0        0.0         0          0          18         31725 2151  134
####
#### First channel is gamma, second is neutron
####   IPP        L        Ch Spin                   APE        APT
       1.0        1.0         0.0        0.0                     1725 2151  135
       2.0        1.0         1.0        0.0 4.88875E-1 4.82222E-11725 2151  136
       3.0        1.0         1.0        0.0 4.88875E-1 4.82222E-11725 2151  137
####
####      Number of channels =   3, res=   67,        Lines/Res=   1
       0.0         0.0         0          67         402        671725 2151  138
####  E_res Gamma_gam  Gamma_n  Gamma_others
-336933.383 5.34010E-1 3.82018E+4                                1725 2151  139
 27346.3592 4.57921E-1 6.02780E+0 1.47221E-1                     1725 2151  140
```

```
 52974.1218 5.62410E-1 8.15947E-1                                        1725 2151  141
 57811.5946 5.38065E-1 1.07389E+2 9.98047E-1                             1725 2151  142
...
 1434335.85 8.60000E-1 5.42294E+3                                        1725 2151  205
####
####    Spin group is defined in the next lines
####    J      Parity                        Number of channels=  3
     -1.0        0.0          0         0        18        31725 2151  206
####
#### First channel is gamma, second is neutron
####  IPP        L       Ch Spin                      APE        APT
      1.0        1.0         0.0        0.0                          1725 2151  207
      2.0        1.0         2.0        0.0 4.88875E-1 4.82222E-11725 2151  208
      3.0        1.0         2.0        0.0 4.88875E-1 4.82222E-11725 2151  209
####
####     Number of channels =   3, res=   18,        Lines/Res=  1
      0.0        0.0          0        18       108       181725 2151  210
####  E_res Gamma_gam  Gamma_n  Gamma_others
 133988.409 2.31420E+0 6.60097E+2 1.00000E-5                            1725 2151  211
 225141.625 1.34620E+0 5.68527E+2 1.00000E-5                            1725 2151  212
 372899.675 2.10790E+0 1.79636E+3 1.00000E-5                            1725 2151  213
...
 1225253.78 8.60000E-1 1.80719E+3                                       1725 2151  228
####
####    Spin group is defined in the next lines
####    J      Parity                        Number of channels=  3
     -2.0        0.0          0         0        18        31725 2151  229
####
#### First channel is gamma, second is neutron
####  IPP        L       Ch Spin                      APE        APT
      1.0        1.0         0.0        0.0                          1725 2151  230
      2.0        1.0         2.0        0.0 4.88875E-1 4.82222E-11725 2151  231
      3.0        1.0         2.0        0.0 4.88875E-1 4.82222E-11725 2151  232
####
####     Number of channels =   3, res=   28,        Lines/Res=  1
      0.0        0.0          0        28       168       281725 2151  233
####  E_res Gamma_gam  Gamma_n  Gamma_others
 397.815407 6.65000E-1 5.05000E-2 3.22000E-1                            1725 2151  234
 113606.420 2.94770E-1 3.97203E+2                                       1725 2151  235
...
 1403884.92 8.60000E-1 8.06707E+3                                       1725 2151  260
 1441365.22 8.60000E-1 1.60874E+3                                       1725 2151  261
####
####    Spin group is defined in the next lines
####    J      Parity                        Number of channels=  3
     -3.0        0.0          0         0        18        31725 2151  262
####
#### First channel is gamma, second is neutron
####  IPP        L       Ch Spin                      APE        APT
      1.0        1.0         0.0        0.0                          1725 2151  263
      2.0        1.0         2.0        0.0 4.88875E-1 4.82222E-11725 2151  264
      3.0        1.0         2.0        0.0 4.88875E-1 4.82222E-11725 2151  265
####
####     Number of channels =   3, res=   57,        Lines/Res=  1
      0.0        0.0          0        57       342       571725 2151  266
####  E_res Gamma_gam  Gamma_n  Gamma_others
 16356.1239 3.86500E-1 5.98180E+0 1.64019E-1                            1725 2151  267
 17133.8671 8.02280E-1 1.40959E+1 3.19999E-2                            1725 2151  268
 40270.2759 5.77490E-1 1.77346E-1                                       1725 2151  269
...
 1485128.14 8.60000E-1 1.05409E+4                                       1725 2151  323
```

Example 18 (^{35}Cl): File 32, LRF = 7, LCOMP = 2

```
    17035.0 3.46685E+1         0          0          1        0172532151    1
####
#### Z_A   Abundance          0         LFW         NER
    17035.0 1.00000E+0         0          1          1        0172532151    2
####
#### Emin    Emax          Lru=1 => Resolved Resonance Region
####                            Lrf=7 => R-Matrix Limited
 1.00000E-5 1.20000E+6         1          7          0        0172532151    3
####
####  Flag for Gamma not gamma  0
####                            Lcomp =  2
#### Number of J values for which resonances exist =  8
         0.0        0.0         0          2          8        0172532151    4
####
####  3 pairs of particles are defined next
#### First pair is gamma & compound nucleus
#### Others are particle pairs
         0.0        0.0         3          7         36        6172532151    5
####
####   MA         MB          ZA         ZB         IA         IB
####   Q          PNT         SHF        MT         PA         PB
 0.00000E+0 3.56685E+1        0.0        0.0        1.0        0.0172532151    6
 0.00000E+0        0.0       -1.0      102.0        0.0        0.0172532151    7
 1.00000E+0 3.46685E+1        0.0        0.0        0.5        1.5172532151    8
 0.00000E+0        1.0       -1.0        2.0        0.0        0.0172532151    9
 9.98624E-1 3.46685E+1        1.0       16.0        0.5        1.5172532151   10
 6.15220E+5        1.0       -1.0      103.0        0.0        0.0172532151   11
####
####    Spin group is defined in the next lines
####    J      Parity                  Number of channels=  3
         1.0        0.0         0          0         18        3172532151   12
####
#### First channel is gamma, second is neutron
####   IPP       L       Ch Spin                 APE        APT
         1.0        0.0        0.0        0.0                 172532151   13
         2.0        0.0        1.0        0.0 3.66798E-1 4.82222E-1172532151   14
         3.0        0.0        1.0        0.0 3.66798E-1 4.82222E-1172532151   15
####
####     Number of channels =  3, res=  23,      Lines/Res=  1
         0.0        0.0         0         23        276       23172532151   16
####  E_res Gamma_gam  Gamma_n  Gamma_others
54931.9958 3.67260E-1 4.64424E+1                            172532151   17
     2.5801  1.8000E-1  6.1036E+0                            172532151   18
 68236.1571 3.93360E-1 2.17904E+2 1.00000E-5                172532151   19
     5.0382  2.0000E-1  2.2760E+1  1.5000E-2                172532151   20
 115098.000 7.39000E-1 4.30778E+0                            172532151   21
     14.768  1.3461E-1  1.6786E+0                            172532151   22
182522.969 7.45150E-1 1.75974E+3 1.00000E-5                172532151   23
     39.919  3.6707E-1  1.6980E+2  1.0000E-3                172532151   24
...
 882977.616 6.06000E-1 9.78061E+2                            172532151   57
    150.069  1.2120E-1  3.9103E+2                            172532151   58
1109187.77 6.06000E-1 2.74235E+3                            172532151   59
    361.02  1.2120E-1  1.0332E+3                            172532151   60
1205687.36 6.06000E-1 6.42584E+2                            172532151   61
    300.00  1.2120E-1  2.5703E+2                            172532151   62
####
####     Spin group is defined in the next lines
```

```
####    J       Parity                          Number of channels=  3
        2.0        0.0          0          0        18         3172532151  63
####
#### First channel is gamma, second is neutron
####   IPP        L       Ch Spin                      APE        APT
        1.0        0.0        0.0        0.0                      172532151  64
        2.0        0.0        2.0        0.0 3.66798E-1 4.82222E-1172532151  65
        3.0        0.0        2.0        0.0 3.66798E-1 4.82222E-1172532151  66
####
####      Number of channels =   3, res=   32,        Lines/Res=   1
        0.0        0.0          0         32       384       32172532151  67
####   E_res Gamma_gam   Gamma_n   Gamma_others
-180.650000 5.30150E-1 1.32770E+1 5.99230E-3                    172532151  68
   0.000010  5.3000E-3 1.3277E-1  1.8000E-4                     172532151  69
 14801.9519 3.45680E-1 3.25995E+1 2.80002E-2                    172532151  70
     0.7861 2.3701E-2  2.3014E+0  1.0000E-1                     172532151  71
...
 1257679.87 6.06000E-1 1.74983E+3                               172532151 128
     300.00 1.2120E-1  6.9993E+2                                172532151 129
 7563145.25 3.83980E-1 6.21905E+5 1.00000E+3                    172532151 130
 4000000.00 7.6796E-2  3.1095E+5  5.0000E+4                     172532151 131
####
####     Spin group is defined in the next lines
####    J       Parity                          Number of channels=  3
        0.0       -1.0          0          0        18         3172532151 132
####
#### First channel is gamma, second is neutron
####   IPP        L       Ch Spin                      APE        APT
        1.0        1.0        0.0        0.0                      172532151 133
        2.0        1.0        1.0        0.0 4.88875E-1 4.82222E-1172532151 134
        3.0        1.0        1.0        0.0 4.88875E-1 4.82222E-1172532151 135
####
####      Number of channels =   3, res=    9,        Lines/Res=   1
        0.0        0.0          0          9       108        9172532151 136
####   E_res Gamma_gam   Gamma_n   Gamma_others
22396.3985 1.72480E+0 9.66367E-1                                172532151 137
     0.8434 3.0260E-1  1.0923E-1                                172532151 138
 96604.1512 1.56500E+0 2.76138E+0                               172532151 139
    16.4577 4.0593E-1  1.0621E+0                                172532151 140
 230073.973 3.24010E-1 8.11818E+2                               172532151 141
    42.563  2.4923E-1  1.3641E+2                                172532151 142
 243215.280 7.03200E-1 2.17430E+2                               172532151 143
    46.867  5.1499E-1  6.4296E+1                                172532151 144
 245478.478 8.31970E-1 6.55642E+0                               172532151 145
    94.714  6.4526E-1  5.1654E+0                                172532151 146
 341338.932 6.54970E-1 5.72032E+3                               172532151 147
    733.010 6.1285E-1  2.8166E+3                                172532151 148
 481280.888 7.82130E-1 1.77427E+3                               172532151 149
    349.781 7.3518E-1  1.4399E+3                                172532151 150
 504856.656 8.60000E-1 6.79094E+2                               172532151 151
    152.887 1.7600E-1  4.5647E+2                                172532151 152
 547854.482 8.60000E-1 7.64013E+2                               172532151 153
    164.801 1.7600E-1  3.6524E+2                                172532151 154
####
####     Spin group is defined in the next lines
####    J       Parity                          Number of channels=  3
       -1.0        0.0          0          0        18         3172532151 155
####
#### First channel is gamma, second is neutron
####   IPP        L       Ch Spin                      APE        APT
        1.0        1.0        0.0        0.0                      172532151 156
```

```
        2.0          1.0          1.0          0.0 4.88875E-1 4.82222E-1172532151  157
        3.0          1.0          1.0          0.0 4.88875E-1 4.82222E-1172532151  158
####
####      Number of channels =   3, res=    38,          Lines/Res=   1
        0.0          0.0          0           38          456         38172532151  159
####  E_res Gamma_gam  Gamma_n  Gamma_others
 4250.76249 4.72000E-1 6.28000E-1 2.30000E-1                        172532151  160
    0.11990  2.5425E-2  4.3275E-2  2.2099E-2                        172532151  161
 5491.02019 9.70210E-1 3.86354E-3                                   172532151  162
    0.76725  2.9026E-1  5.3206E-4                                   172532151  163
 37767.9176 1.91200E-1 4.40797E-1                                   172532151  164
    3.8335  4.2536E-2  1.6606E-1                                    172532151  165
...
 1435502.40 8.60000E-1 5.36563E+3                                   172532151  234
    300.00  1.7600E-1  2.1463E+3                                    172532151  235
####
####    Spin group is defined in the next lines
####    J       Parity                    Number of channels=   3
       -2.0         0.0          0           0           18          3172532151  236
####
#### First channel is gamma, second is neutron
####   IPP          L       Ch Spin                    APE          APT
        1.0          1.0          0.0          0.0                   172532151  237
        2.0          1.0          1.0          0.0 4.88875E-1 4.82222E-1172532151  238
        3.0          1.0          1.0          0.0 4.88875E-1 4.82222E-1172532151  239
####
####      Number of channels =   3, res=    32,          Lines/Res=   1
        0.0          0.0          0           67          804         67172532151  240
####  E_res Gamma_gam  Gamma_n  Gamma_others
-336933.383 5.34010E-1 3.82018E+4                                   172532151  241
    0.000  1.0000E-1  1.0000E-1                                     172532151  242
 27346.3592 4.57921E-1 6.02780E+0 1.47221E-1                        172532151  243
    1.0736  2.6315E-2  1.1293E+0  1.4722E-1                         172532151  244
 52974.1218 5.62410E-1 8.15947E-1                                   172532151  245
    2.6391  5.3890E-2  1.6543E-1                                    172532151  246
...
 1434335.85 8.60000E-1 5.42294E+3                                   172532151  373
    300.00  1.7600E-1  2.1692E+3                                    172532151  374
####
####    Spin group is defined in the next lines
####    J       Parity                    Number of channels=   3
       -1.0         0.0          0           0           18          3172532151  375
####
#### First channel is gamma, second is neutron
####   IPP          L       Ch Spin                    APE          APT
        1.0          1.0          0.0          0.0                   172532151  376
        2.0          1.0          2.0          0.0 4.88875E-1 4.82222E-1172532151  377
        3.0          1.0          2.0          0.0 4.88875E-1 4.82222E-1172532151  378
####
####      Number of channels =   3, res=    18,          Lines/Res=   1
        0.0          0.0          0           18          216         18172532151  379
####  E_res Gamma_gam  Gamma_n  Gamma_others
 133988.409 2.31420E+0 6.60097E+2 2.00000E-6                        172532151  380
   16.602  5.0285E-1  8.0848E+1  1.0000E-3                          172532151  381
 225141.625 1.34620E+0 5.68527E+2 1.00000E-5                        172532151  382
   19.852  4.4907E-1  5.1848E+1  2.0000E-3                          172532151  383
...
 1225253.78 8.60000E-1 1.80719E+3                                   172532151  414
    300.00  1.7600E-1  7.2288E+2                                    172532151  415
####
####    Spin group is defined in the next lines
```

```
####    J      Parity                          Number of channels=  3
     -2.0          0.0           0          0        18        3172532151  416
####
#### First channel is gamma, second is neutron
####   IPP         L        Ch Spin                    APE         APT
      1.0          1.0          0.0          0.0                     172532151  417
      2.0          1.0          2.0          0.0 4.88875E-1 4.82222E-1172532151  418
      3.0          1.0          2.0          0.0 4.88875E-1 4.82222E-1172532151  419
####
####       Number of channels =   3, res=   28,      Lines/Res=   1
      0.0          0.0           0         28       336      28172532151  420
####   E_res Gamma_gam  Gamma_n  Gamma_others
 397.815407 6.65000E-1 5.05000E-2 3.22000E-1                   172532151  421
   0.010000  4.6000E-2  2.0000E-3  2.2000E-2                   172532151  422
 113606.420 2.94770E-1 3.97203E+2                              172532151  423
     12.665  1.0973E-1  5.1804E+1                              172532151  424
 143024.214 4.92180E-1 3.14743E+2                              172532151  425
      9.469  1.4492E-1  2.9918E+1                              172532151  426
...
 1441365.22 8.60000E-1 1.60874E+3                              172532151  475
    300.00  1.7600E-1  6.4350E+2                               172532151  476
####
####     Spin group is defined in the next lines
####    J      Parity                          Number of channels=  3
     -3.0          0.0           0          0        18        3172532151  477
####
#### First channel is gamma, second is neutron
####   IPP         L        Ch Spin                    APE         APT
      1.0          1.0          0.0          0.0                     172532151  478
      2.0          1.0          2.0          0.0 4.88875E-1 4.82222E-1172532151  479
      3.0          1.0          2.0          0.0 4.88875E-1 4.82222E-1172532151  480
####
####       Number of channels =   3, res=   57,      Lines/Res=   1
      0.0          0.0           0         57       684      57172532151  481
####   E_res Gamma_gam  Gamma_n  Gamma_others
 16356.1239 3.86500E-1 5.98180E+0 1.64019E-1                   172532151  482
     0.5920  1.5418E-2  7.4312E-1  1.6400E-1                   172532151  483
 17133.8671 8.02280E-1 1.40959E+1 3.19999E-2                   172532151  484
     0.6693  3.3580E-2  1.2626E+0  3.2000E-2                   172532151  485
...
 1485128.14 8.60000E-1 1.05409E+4                              172532151  594
    300.00  1.7600E-1  4.2164E+3                               172532151  595
#### Correlation matrix follows
                                        1088       3093       172532151  596
    2    1    2                                               172532151  597
    3    1    3  8                                            172532151  598
    7    5    8  5                                            172532151  599
   10    9    8                                               172532151  600
   11    9    3-55                                            172532151  601
   15   13   26  1                                            172532151  602
   17   15   -1                                               172532151  603
   19   17    2  2                                            172532151  604
   21   13    1  0  1  0  1                                   172532151  605
   23    5    1  0  0  0  0  0  0  4  0  5  0  3  0  3  0 41   172532151  606
   25   23   -3                                               172532151  607
   26   25    1                                               172532151  608
   27   13    1  0  1  0  0  0  0  0  2  0 -3  0 19  5         172532151  609
   29   21   -1  0 -2  0 -1  0 -5                             172532151  610
   31   23   -6  0  0  0-12  0  6                             172532151  611
   33   23   -1  0  0  0 -1  0  0  0 -1                       172532151  612
   35   23   -1  0  0  0  0  0  1  0  1  0 -1                 172532151  613
```

```
   39    15   -1   0   0   0   0   0  -2   0  -9   0   0   0  -5   0   0   0  -2     172532151   614
   39    35   -3   0 -35                                                             172532151   615
   41    23   -2   0   0   0  -1   0   0   0   0   0   0   0  -1                      172532151   616
   43    23   -4   0   0   0  -2   0   0   0   0   0   0   0  -1   0   0   0   6     172532151   617
   43    41   24                                                                     172532151   618
   47    23   -1   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   1     172532151   619
   47    45   -2                                                                     172532151   620
   51    39    1   0   0   0   0   0   1   0   4   0   1                              172532151   621
   53    47   -1   0   0   0  -1                                                     172532151   622
   55    23   -1   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   2     172532151   623
   55    45    2   0   5   0   2   0  -2   0   4                                      172532151   624
   59    23   -1   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   1     172532151   625
   59    45    1   0   2   0   0   0   0   0   5   0   2   0  -3                      172532151   626
   61    55    1   0   0   0   1                                                     172532151   627
   63    31    1   0   0   0   0   0   0   0   4   0   1   0   2   0   2   0   6     172532151   628
   63    51    2   0   5   0  11   0   0   0  13   0  16                              172532151   629
   65    63    1                                                                     172532151   630
   67    63   -5   0   1                                                             172532151   631
...
 1053   209    1   0   1                                                             172532151  3670
 1053   639   -1                                                                     172532151  3671
 1053   643    2   0   0   0  -1   0   2   0   8   0  38   0 -10                      172532151  3672
 1053   741    9                                                                     172532151  3673
 1053   831    2   0   0   0   5   0   5                                              172532151  3674
 1053   839    2                                                                     172532151  3675
 1053  1047   -2   0   0   0  -4                                                     172532151  3676
 1055    85   -1   0  -1   0   0   0   0   0   0   0  -1                              172532151  3677
 1055   207   -1   0  -4                                                             172532151  3678
 1055   211   -9                                                                     172532151  3679
 1055   397    1   0   3                                                             172532151  3680
 1055   621    1   0  -1                                                             172532151  3681
 1055   627   -1   0   0   0   4   0   2   0   0   0  -1   0   2   0   1              172532151  3682
 1055   643    3   0  -2   0   7   0  -9   0   0   0  62   0  23                      172532151  3683
 1055   737    1   0   3   0 -23   0  -5                                              172532151  3684
 1055   813   -1   0   0   0  -1   0  -2   0   1                                      172532151  3685
 1055   823   -3   0  -1   0   0   0  -1   0   1   0  -6   0 -13   0 -13   0 -19     172532151  3686
 1055  1013    1   0   3   0   0   0   3                                              172532151  3687
 1055  1021    1   0   0   0   2   0   4   0   0   0   0   0   2   0   3   0   1     172532151  3688
 1055  1039    1   0   0   0   6   0   5   0  15   0   2   0  14   0  20              172532151  3689
                                                                                    172532   099999
                                                                                    1725  0   0      0
```

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