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Abstract

Resonance parameter representations of nuclear data are used by processor codes to compute quantities needed for criticality safety and other nuclear applications. Usually these calculations also require the associated parameter covariance matrices (PCMs) that contain both the variances of resonance parameters and the correlations between parameters. The SAMMY code is widely used to fit neutron cross section data to obtain both resonance parameter representations and the corresponding PCMs, which are output to binary files. We have written a code, RADCOP, that facilitates the manipulation and visualization of information from SAMMY PCMs. RADCOP produces both one- and two-dimensional correlation plots that permit one to quickly trace the important off-diagonal correlations. ENDF File 2 and File 32 files for the Reich-Moore representation may be output.

KEYWORDS: Nuclear data, visualization, resonance parameter covariance matrices

1. Introduction

Nuclear data evaluations typically yield resonance parameter representations that can be used by processor codes (e.g., AMPX [1], NJOY [2], etc.) to compute cross sections and integral quantities needed for criticality safety and other nuclear applications. An important part of the evaluation process involves the generation of parameter covariance matrices (PCMs) that contain both the variances of resonance parameters and the correlations between parameters. The ENDF format [3] now incorporates PCMs in File 32, reaction type number MT=151, that correspond to resonances in File 2, MT=151. The SAMMY [4] code is widely used to fit neutron cross-section data to obtain both resonance parameter representations and the corresponding PCMs, which are output to binary files.

Because a typical evaluation produces a representation with hundreds or thousands of parameters, one needs to examine and display subsets of the diagonal and off-diagonal matrix elements. We have written a code, RADCOP, that facilitates the manipulation and visualization of information from SAMMY PCMs. RADCOP can produce both one- and two-dimensional (1D and 2D) plots of the parameter correlations for user-specified neutron energy ranges; the display formats permit the user to quickly trace the important off-diagonal correlations. RADCOP also outputs ENDF File 2 and File 32 files for the Reich-Moore representation

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(LRF=3, LCOMP=1). The ENDF flag LCOMP specifies the format for covariance information; for LCOMP=2 the PCM is written in a compact format whereas for LCOMP=1 the upper triangular part of the PCM is written in an expanded format.

SAMMY also writes an ASCII file that lists the resonance parameter uncertainties. This "PUB" file can be edited, either manually or with the RSAP code [5], to modify the uncertainties. This procedure is generally utilized when analyzing data sets for which nonstatistical uncertainties in quantities such as normalization or background are poorly known. We have written another code, PUB2COV, that reads the modified PUB file and replaces the uncertainties (diagonal elements) in the PCM file while preserving the off-diagonal correlations. PUB2COV may be run from a RADCOP script file.

In the following sections we discuss program input and output, plot options, and ENDF output.

2. Program Input and Output

The RADCOP code is written in Fortran 90 and currently runs on the Linux platform. The code uses the PLPLOT [6] graphics package.

Most input consists of commands followed by one numerical argument. An exception is the "cov" command, which is followed by the PCM file name. Other exceptions are the "ndf" commands used to request ENDF File 32 output.

For quantities in the PCM file, we distinguish between resonance parameters (resonance energy E, gamma width G, neutron width N) and nonresonance parameters (radii, isotopic abundance, broadening parameters, etc). For each resonance parameter, the PCM file also contains several associated quantities such as the type of parameter (gamma width, particle width, etc.), the resonance energy, spin group, parameter value, etc. The parameters are ordered by spin group, not resonance energy.

RADCOP reads a user-specified PCM file and a user-specified energy range, indexes the parameters in order of increasing resonance energy, and outputs an energy-ordered list that includes the parameter type, value, absolute and relative uncertainty, spin group, and extreme off-diagonal correlation. Part of the list output is given below for a simple example. Note that the PCM contains only parameters that were varied (flagged) in the SAMMY run.

```
11 parameters  (5 resonance,   6 non-resonance)
min,max E =  0,      3.00000D+05 eV               correlation threshold =   0.200

************ Flagged Resonance Parameters :
 Index  param       Eres  Tag       Value      Abs.   Rel. Group Max_OffDiag param  Exclude
            #       (eV)                      Unc.   Unc.       Correlation     #
 -----  -----  ---------  ---  ----------  --------  ----- ----- ----------- -----  -------
     1      3    1151.12  E    1.1511D+03 5.820D-02  0.000     2        +.67    11     0
     2      4    1151.12  G    5.8274D+02 1.295D+02  0.222     2        -.90     5     0
     3      5    1151.12  N    5.8820D+01 6.812D+00  0.116     2        -.90     4     0
     4      1   27652.55  E    2.7653D+04 3.998D+02  0.014     1        -.16     6     1
     5      2   27652.55  N    1.4780D+06 1.146D+05  0.078     1        +.77     6     0

   3 parameters excluded from plot (Extreme off diag. correlation below threshold)
```

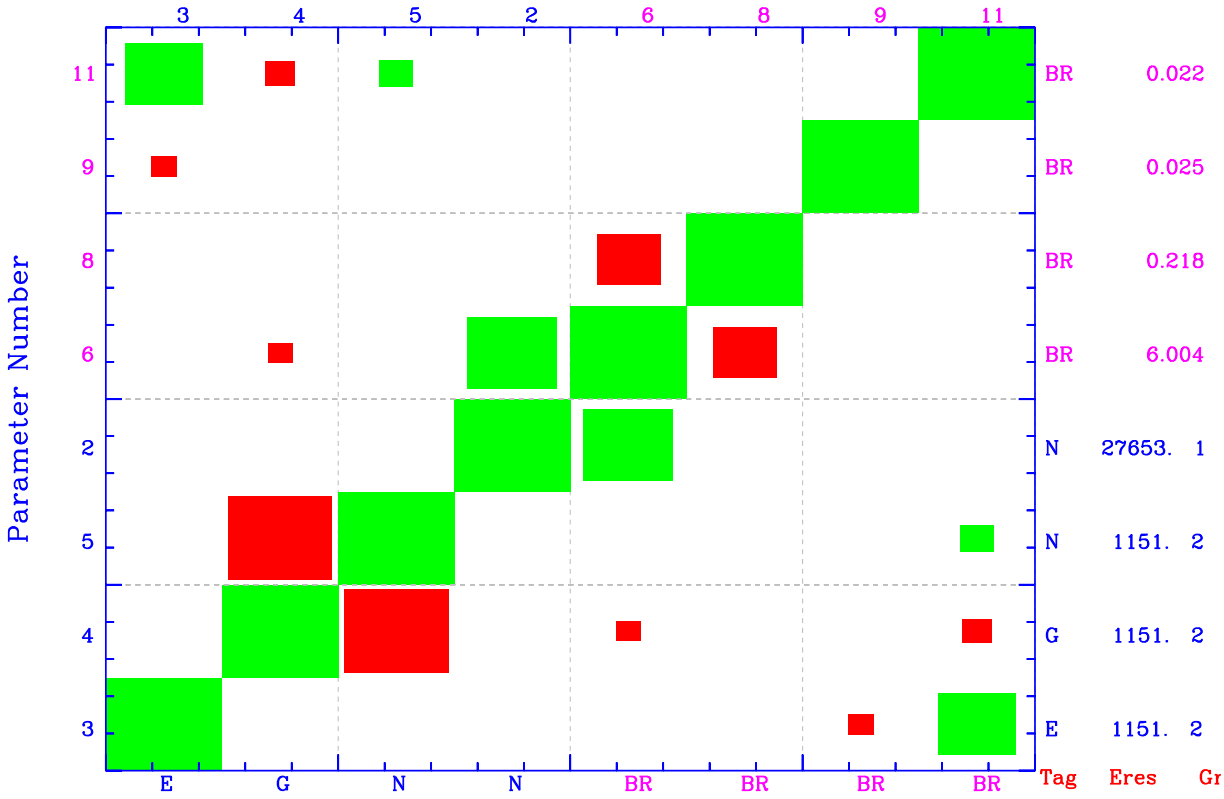
3. Plot Options

Several types of 1D and 2D plots are supported in the code. Plots are output to both the user's X window and to color postscript files.

3.1 2D Plots

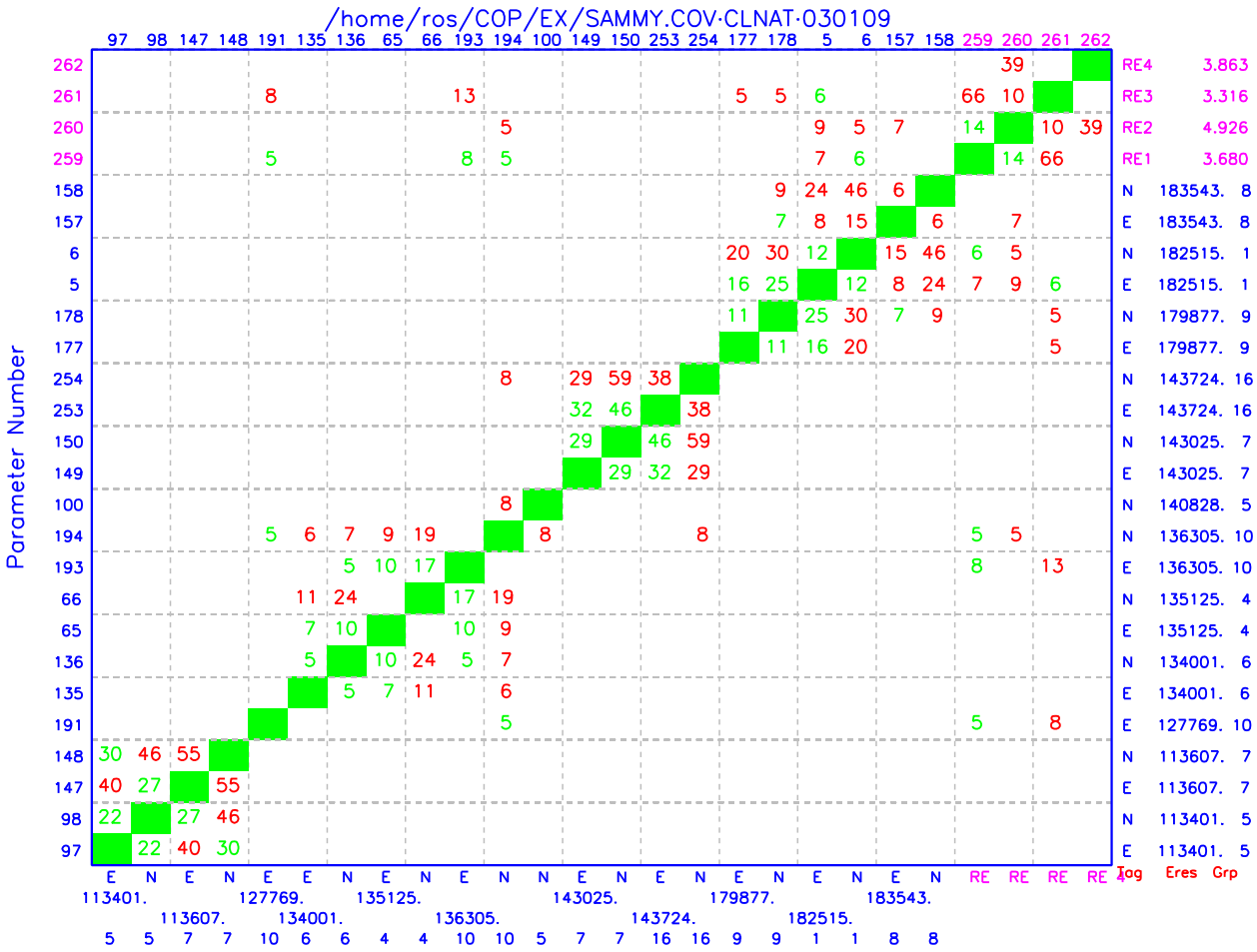
A 2D plot of parameter correlations may be produced for a user-specified energy range. Fig. 1 is an example of such a 2D plot with symbols of size proportional to the correlation. A parameter type tag (e.g., E, G, N), the associated resonance energy, spin group number, and parameter number are written along the plot axes. Up to 50 parameters may be plotted. Non-resonance parameters are also plotted; in Fig. 1 four broadening parameters are denoted by the "BR" tag.

Figure 1: Example RADCOP 2D correlation plot (three parameters excluded). Positive (negative) correlations are shown in green (red). The label BR denotes broadening parameters.



The 2D plot in Fig. 2 illustrates the option to plot off-diagonal correlations as two-digit numbers; positive (negative) correlations are shown in green (red). Values for parameter tags, resonance energies in eV, and SAMMY spin group numbers are written below the x axis and to the right of the plot. The tags E, G, and N indicate resonance energy, gamma width, and neutron width, respectively. The tag RE denotes effective radii; radius values in fm are written to the right of the plot. An alternative option is to plot signed two-digit numbers for correlation values.

Figure 2: Example RADCOP 2D plot with numerical off-diagonal correlations. Positive (negative) correlations are shown in green (red). The label RE denotes radius parameters.

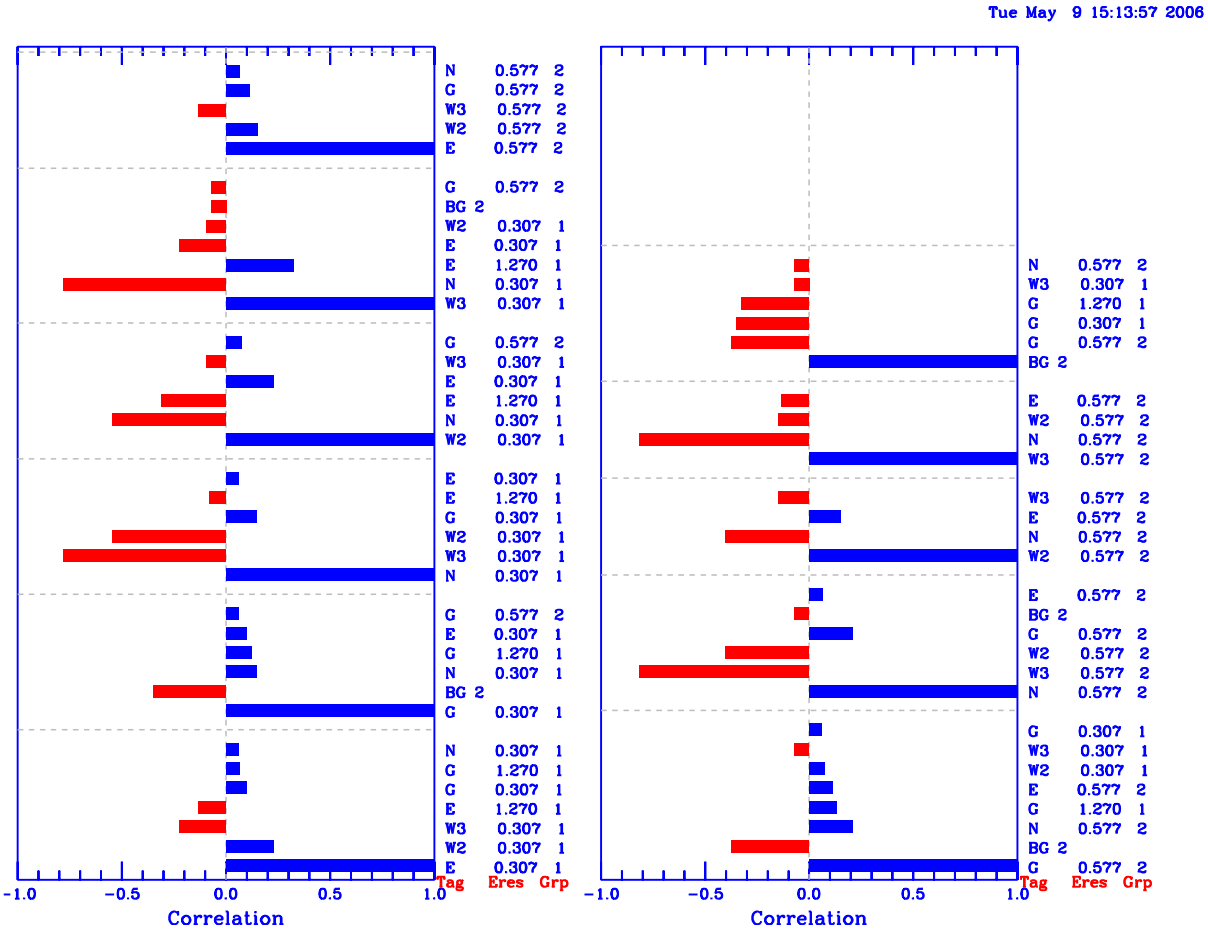


3.2 Bar Plots

A bar plot consists of horizontal bars that show all correlations that exceed the threshold, not just those in the specified energy range. The example given in Fig. 3 illustrates the use of the optional horizontal axis range -1 to +1. Positive (negative) correlations are shown in blue (red). If the user selects the axis range 0 to 1, negative correlation bars are shown hatched to distinguish them from positive correlation bars on a monochrome hard copy.

For a given parameter, the horizontal bars indicate the magnitudes of all correlations (up to a maximum of 10) that exceed the threshold, not just those in the specified energy range. For each flagged parameter in the specified energy range, the percent correlation values, tags, associated resonance energy, parameter value, spin group number, and SAMMY parameter number are written to an output file. Part of this list output is illustrated on the following page.

Figure 3: RADCOP 1D Bar Plot. Parameter tags E, G, N, and BG denote energy, gamma width, neutron width, and background parameters, respectively. Tags W2 and W3 denote fission widths.



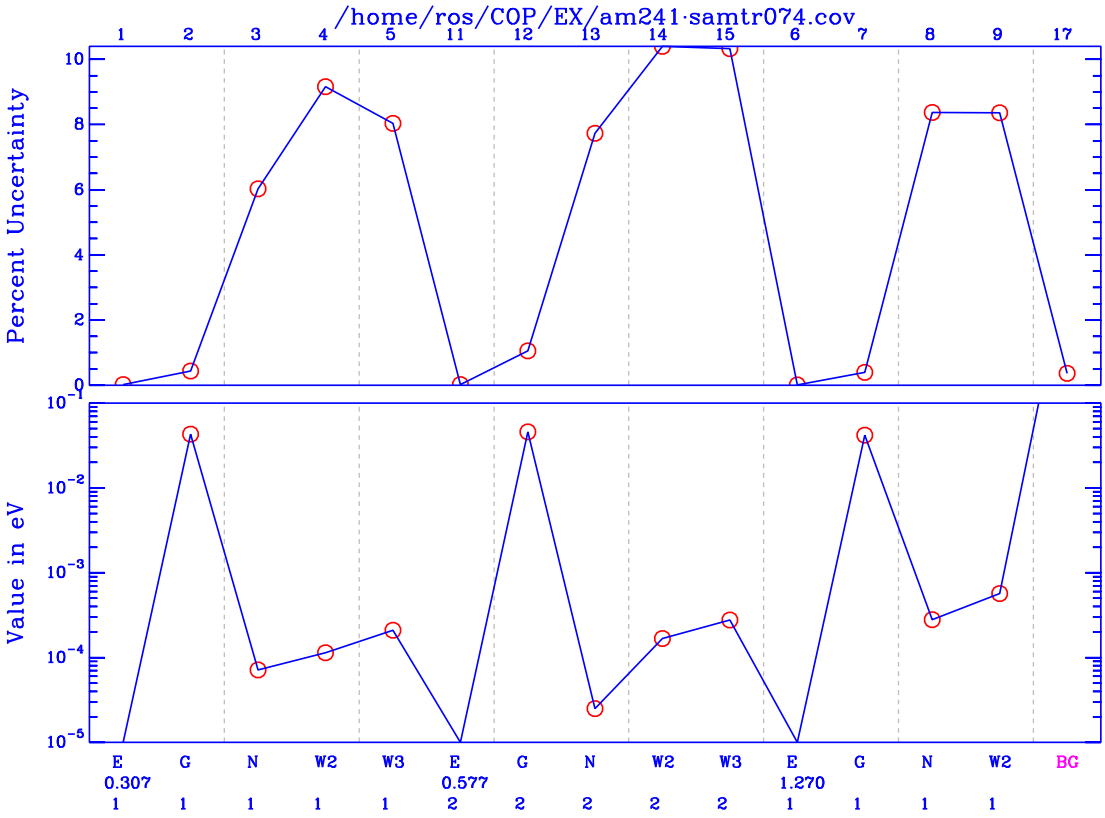
********** Flagged Resonance Parameters :

Correl.	Tag	Eres (eV)	Value	Grp	param #
100.0	E	0.31	3.073D-01	1	1
22.6	W 2	0.31	1.140D-01	1	4
-22.3	W 3	0.31	2.094D-01	1	5
-13.1	E	1.27	1.270D+00	1	6
9.8	G	0.31	4.317D+01	1	2
6.5	G	1.27	4.204D+01	1	7
5.9	N 1	0.31	7.142D-02	1	3
100.0	G	0.31	4.317D+01	1	2
-34.8	BG 2		4.471D+00		17
14.5	N 1	0.31	7.142D-02	1	3
12.3	G	1.27	4.204D+01	1	7
9.8	E	0.31	3.073D-01	1	1
5.9	G	0.58	4.594D+01	2	12

3.3 Parameter Value-Uncertainty Plots

Often during the analysis of nuclear data it is desirable to examine visually a set of parameter values and corresponding uncertainties. A stacked plot of parameter values and uncertainties for a specified energy range may be obtained with one simple RADCOP command. An example is given in Fig. 4.

Figure 4: RADCOP Parameter Value-Uncertainty Plot for ^{241}Am. Tags E, G, N, and BG denote energy, gamma width, neutron width, and background parameters, respectively. Tags W2 and W3 denote fission widths. Energy values are set to the minimum y-axis value.



4. ENDF Output

ENDF File 2 and File 32 output for the LCOMP=1 option may be produced for the Reich-Moore representation. Required input parameters are MAT, MPAR, LRF, Z, A, AWR, ABN, SPI, AP, and APL. In addition to the ENDF output files, auxiliary output files that include documentary text are written.

An example auxiliary output file is given in Appendix A for the test case of ^{241}Am, which has ground state spin $5/2^+$. In this simple example, only s waves are considered, and only 3 resonances are included. The flagged parameters for each resonance are E, Γ_n, Γ_γ, and the two fission widths. Because MPAR was set to 5, File 32 contains 15 diagonal covariance elements and the 105 upper off-diagonal elements. Even if nonresonance parameters (background, etc.) are flagged, only the resonance parameter covariances are written to File 32.

For non-fissioning nuclei such as ^{37}Cl, MPAR may be set to 3 to give a File 32 with only 40% as many elements as a file with MPAR = 5. See Appendix B for an example with MPAR = 3.

5. Conclusion

We have written a code, RADCOP, that facilitates the manipulation and visualization of information from SAMMY PCMs. RADCOP produces both 1D and 2D correlation plots that permit one to quickly trace the important off-diagonal correlations. ENDF File 2 and File 32 files for the Reich-Moore representation (LRF=3) may be output. We expect that RADCOP will be a valuable tool for nuclear data evaluators and others who need to examine and display subsets of diagonal and off-diagonal PCM elements.

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References

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Appendix A. Auxiliary File 32 example for MPAR = 5

```
************ Flagged Resonance Parameters :
 Index  param       Eres  Tag       Value      Abs.   Rel. Group Max_OffDiag param  Exclude
           #        (eV)                        Unc.   Unc.       Correlation     #
 -----  -----  ---------  ---  ----------  --------  -----  ----- ----------- -----  -------
     1      1       0.31  E    3.0725D-01 6.494D-05  0.000     1        22.6     4     0
     2      2       0.31  G    4.3174D+01 1.896D-01  0.004     1       -34.8    17     0
     3      3       0.31  N  1 7.1418D-02 4.306D-03  0.060     1       -77.8     5     0
     4      4       0.31  W  2 1.1400D-01 1.045D-02  0.092     1       -54.3     3     0
     5      5       0.31  W  3 2.0943D-01 1.683D-02  0.080     1       -77.8     3     0
     6     11       0.58  E    5.7652D-01 1.462D-04  0.000     2        15.2    14     0
     7     12       0.58  G    4.5940D+01 4.841D-01  0.011     2       -37.6    17     0
     8     13       0.58  N  1 2.4973D-02 1.930D-03  0.077     2       -81.7    15     0
     9     14       0.58  W  2 1.6804D-01 1.747D-02  0.104     2       -40.1    13     0
    10     15       0.58  W  3 2.7697D-01 2.859D-02  0.103     2       -81.7    13     0
    11      6       1.27  E    1.2696D+00 6.984D-05  0.000     1        32.3     5     0
    12      7       1.27  G    4.2039D+01 1.662D-01  0.004     1       -32.6    17     0
    13      8       1.27  N  1 2.7901D-01 2.334D-02  0.084     1       -99.8     9     0
    14      9       1.27  W  2 5.6702D-01 4.739D-02  0.084     1       -99.8     8     0
    15     10       1.27  W  3 1.0107D-04 1.005D-05  0.099     1         1.3     1     1

## Covariance File :/home/ros/COP/EX/am241_samtr074.cov

##       ZA        AWR                              NIS
    95241.0 2.38986E+2          0          0          1          0954332151    1

##      ZAI        ABN                    LFW        NER
    95241.0 1.00000E+0          0          1          1          0954332151    2

##     Emin       Emax        LRU        LRF        NRO       NAPS
 1.00000E-1 2.00000E+0          1          3          0          0954332151    3

##     SPIN     Radius                 LCOMP        NLS
        2.5 9.03600E-1          0          1          1          1954332151    4

##     AWRI                                        NSRS       NLRS
 2.38986E+2 0.00000E+0          0          0          1          0954332151    5

##                           MPAR             NVS+6*NRB        NRB
                               5          0        138          3954332151    6
##       ER         AJ  G_neutron    G_gamma        GFA        GFB
##     (eV)                 (eV)       (eV)       (eV)       (eV)
.30725147          2.0 7.14181E-5 4.31740E-2 1.14005E-4 2.09428E-4954332151    7
.57652179          3.0 2.49734E-5 4.59400E-2 1.68040E-4 2.76970E-4954332151    8
1.2695578          2.0 2.79009E-4 4.20386E-2 5.67023E-4 1.01074E-7954332151    9

   3 Resonances and     120 Covariance elements written to radcop.n32
```

Appendix B. Auxiliary File 32 example for MPAR = 3

```
************ Flagged Resonance Parameters :
 Index  param       Eres  Tag       Value      Abs.   Rel. Group Max_OffDiag param  Exclude
           #       (eV)                        Unc.   Unc.       Correlation     #
 -----  -----  ---------  ---  ----------  --------  ----- ----- ----------- -----  -------
     1      1   -1000.00  G    2.2459D+02 0.000D+00  0.000     9         0.0   151     1
     2      2   -1000.00  N  1 9.5557D+03 0.000D+00  0.000     9         0.0   151     1
     3     41    8320.82  E    8.3208D+03 3.012D+00  0.000    10        15.8    43     0
     4     42    8320.82  G    1.9634D+02 2.314D+01  0.118    10         4.1    43     1
     5     43    8320.82  N  1 7.8704D+04 4.758D+03  0.060    10        15.8    41     0
     6      3   25579.30  E    2.5579D+04 1.415D+01  0.001     9         7.1     5     0
     7      4   25579.30  G    5.1278D+02 1.228D+02  0.240     9         1.9     5     1
     8      5   25579.30  N  1 6.5222D+05 6.788D+04  0.104     9         7.1     3     0
 ...
    66    339  143721.36  E    1.4372D+05 2.130D+01  0.000    16       -20.8   151     0
    67    340  143721.36  G    1.7061D+02 9.961D+01  0.584    16        -2.3   150     1
    68    341  143721.36  N  1 6.5297D+05 1.074D+05  0.164    16       -36.8   151     0
    69    149  144342.04  E    1.4434D+05 4.956D+01  0.000    12        10.0   339     0
    70    150  144342.04  G    1.5444D+02 8.952D+01  0.580    12        -2.3   340     1
    71    151  144342.04  N  1 6.4086D+04 3.222D+04  0.503    12       -36.8   341     0

## Covariance File :/home/ros/covMatrix.1/cl37out.cov

##       ZA        AWR                              NIS
    17037.0 3.66483E+1          0          0          1          0172532151    1

##      ZAI        ABN                   LFW        NER
    17037.0 1.00000E+0          0          1          1          0172532151    2

##     Emin       Emax        LRU        LRF        NRO       NAPS
-1.00000E+9 1.50000E+5          1          3          0          0172532151    3

##     SPIN     Radius                 LCOMP        NLS
        1.5 3.36510E-1          0          1          2          2172532151    4

##     AWRI                                       NSRS       NLRS
 3.66483E+1 0.00000E+0          0          0          1          0172532151    5

##                           MPAR             NVS+6*NRB        NRB
                                3          0       2772        24172532151    6
##       ER         AJ  G_neutron    G_gamma        GFA        GFB
##     (eV)                 (eV)       (eV)       (eV)       (eV)
-1000.000         -1.0 9.55569E+0 2.24585E-1                      172532151    7
8320.8168          2.0 7.87043E+1 1.96340E-1                      172532151    8
25579.301         -1.0 6.52216E+2 5.12780E-1                      172532151    9
27824.080         -2.0 5.53672E+0 7.88080E-2                      172532151   10
32187.017         -1.0 1.05349E+1 8.22790E-2                      172532151   11
42357.528         -1.0 2.78949E-1 2.60250E-1                      172532151   12
46653.155          2.0 3.90486E+2 2.65280E-1                      172532151   13
...
135433.59          0.0 1.63916E+2 2.37990E-1                      172532151   27
136284.67          2.0 1.39180E+3 2.62000E-1                      172532151   28
143721.36          3.0 6.52968E+2 1.70610E-1                      172532151   29
144342.04         -1.0 6.40858E+1 1.54440E-1                      172532151   30

  24 Resonances and    2628 Covariance elements written to radcop.n32
```