

RADCOP: Manipulation and Visualization of SAMMY Covariances

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RADCOP : Manipulation and Visualization of SAMMY Covariances

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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 (eV)	Tag	Value	Abs. Unc.	Rel. Unc.	Group	Max_OffDiag Correlation	param #	Exclude
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)

```

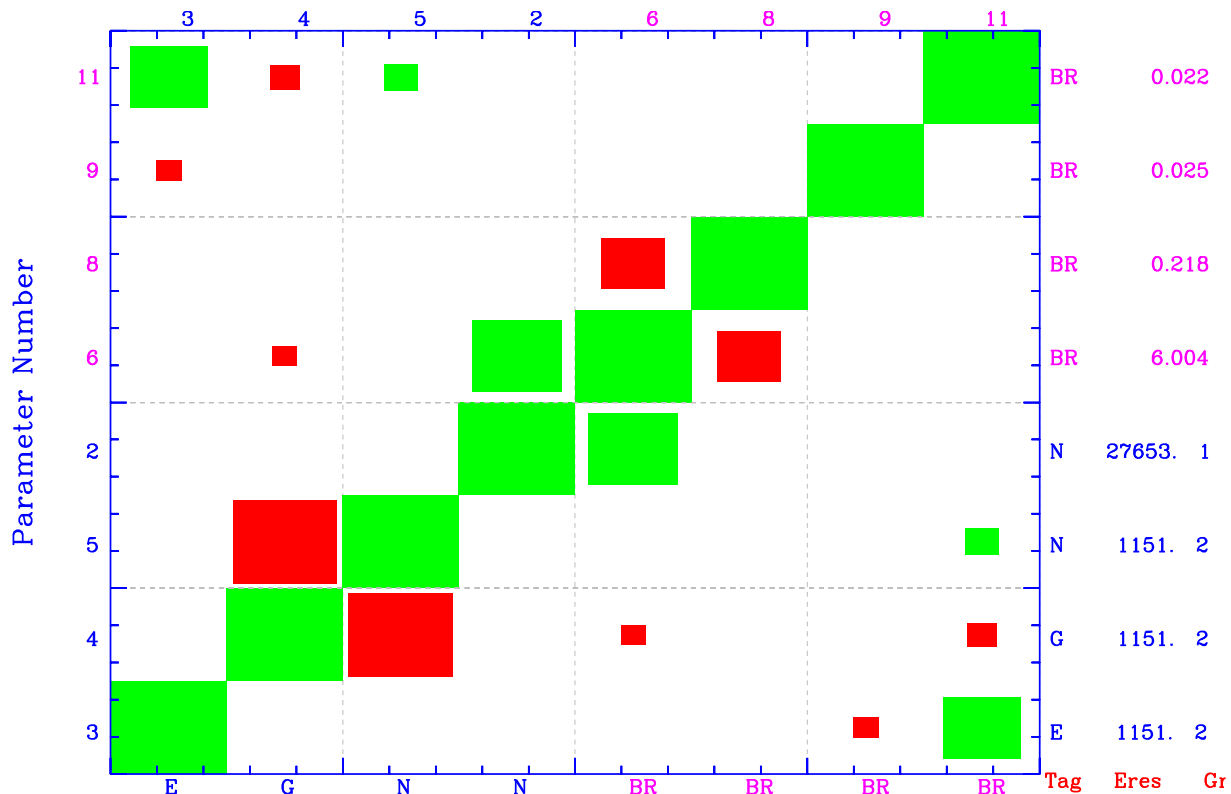
3. Plot Options

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

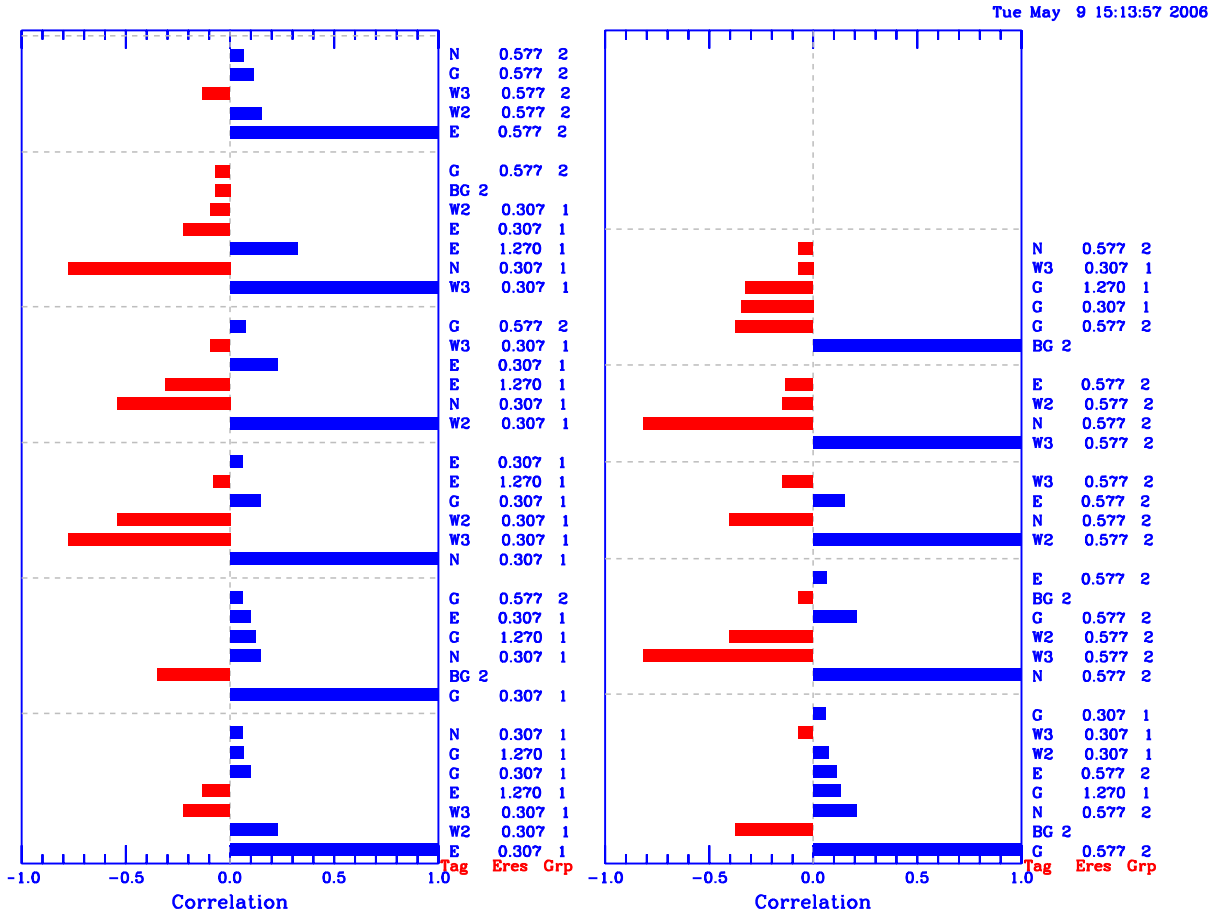
A 2D plot of parameter correlations may be produced for a user-specified energy range. Fig. 1 is an example of such a 2D plot with symbols of size proportional to the correlation. A parameter type tag (e.g., E, G, N), the associated resonance energy, spin group number, and parameter number are written 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 RAD COP 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 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.



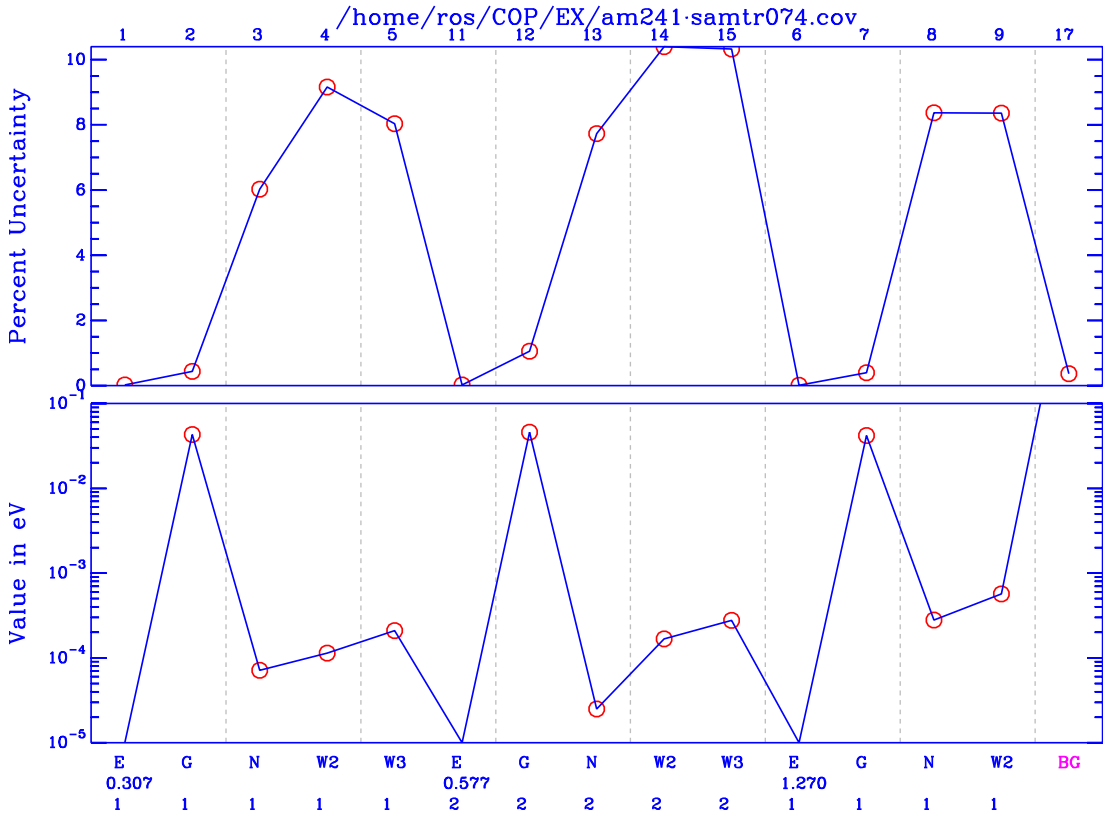
***** Flagged Resonance Parameters :

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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- 4) N. M. Larson, "Updated users' guide for multilevel R-matrix fits to neutron cross section data using Bayes' equations," ORNL/TM-9179/R6, Oak Ridge National Laboratory (2003).
- 5) R. O. Sayer, "RSAP - a code for display of neutron cross section data and SAMMY fit results," ORNL/TM-2003/133, Oak Ridge National Laboratory (2003).
- 6) M. J. LeBrun, G. Furnish, and T. Richardson, "The PLPLOT plotting library," (1994). <http://sourceforge.net/projects/plplot>.

Appendix A. Auxiliary File 32 example for MPAR = 5

***** Flagged Resonance Parameters :

Index	param #	Eres (eV)	Tag	Value	Abs. Unc.	Rel. Unc.	Group	Max_OffDiag Correlation	param #	Exclude
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	7.1418D-02	4.306D-03	0.060	1	-77.8	5	0
4	4	0.31	W	1.1400D-01	1.045D-02	0.092	1	-54.3	3	0
5	5	0.31	W	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	2.4973D-02	1.930D-03	0.077	2	-81.7	15	0
9	14	0.58	W	1.6804D-01	1.747D-02	0.104	2	-40.1	13	0
10	15	0.58	W	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	2.7901D-01	2.334D-02	0.084	1	-99.8	9	0
14	9	1.27	W	5.6702D-01	4.739D-02	0.084	1	-99.8	8	0
15	10	1.27	W	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-4	4954332151	7		
	.57652179	3.0	2.49734E-5	4.59400E-2	1.68040E-4	2.76970E-4	4954332151	8		
	1.2695578	2.0	2.79009E-4	4.20386E-2	5.67023E-4	1.01074E-4	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 (eV)	Tag	Value	Abs. Unc.	Rel. Unc.	Group	Max_OffDiag Correlation	param #	Exclude
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