Proceedings of the Korean Nuclear Society Spring Meeting
Gyeongju, Korea, May 2003

Natural Ag Transmission Data Analysis Using the SAMMY Code (0 eV - 100 eV)

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Abstract

Ag Transmission data measured at the Time-Of-Flight facility in the Pohang Accelerator Laboratory in 2002 was analyzed in the energy range from 0 eV to 100 eV by the SAMMY-M2a code. Resonance parameters within the above energy range are evaluated and external parameters below zero are also evaluated. Those values within the energy range from 0 eV to 100 eV are compared with ENDF/B-VI release 8 values.

1. Introduction

Natural silver material has been used as an absorbing material in reactor. And the Time-Of-Flight facility was installed at the Pohang Accelerator Laboratory (PAL) and transmission measurements were made using the facility in 2002. In this study the transmission data of natural Ag measured at the PAL Time-Of-Flight facility[1] were fitted in the energy range from 0 eV to 100 eV by the SAMMY-M2a[2] Code (Code System for Multilevel R-Matrix Fits to Neutron Data Using Bayes' Equations) and the results of SAMMY analysis were plotted using RSAP-Version 3[3]. The SAMMY methodologies are introduced in the next section, SAMMY analysis follows, and the results and discussions are in the final section.

2. Methodology Used in SAMMY Code

SAMMY code is used for analyses of neutron-induced cross section data in the resolved resonance region. In the resolved region, theoretical cross sections are generated using the Reich-Moore approximation to R-matrix theory. In the SAMMY

code, Bayes' theorem (generalized least squares) is used to find the "best fit" values of the parameters and the associated covariance matrix. In applying Bayes' theorem, the following three basic assumptions are introduced:

(a) the prior joint pdf is a joint normal
(b) the likelihood function is a joint normal
(c) the true value is a linear function of the parameters

The expression of the implicit data covariance matrix V used in this calculation is as follows:

$$V^{ij} = n^{i} d_{ij} + \sum_{k} X^{i}_{k} w_{k} X^{j}_{k} ,$$

where V is the data covariance, n represents the statistical uncertainties, X is the sensitivity matrix (partial derivative of data with respect to data-reduction parameters) and w is the covariance matrix for the data-reduction parameters.

Resolution function used in this calculation is the convolution of Gaussian and the exponential function and its mathematical expression is as follows:
The broadened cross section $f_{GE}(E)$ is given as

$$f_{GE}(E,E') = \frac{1}{\Delta_E \Delta_G \sqrt{p}} \int_{E-\Delta E_S}^{\infty} dE^0 \exp\left\{ -\frac{\left(E^0 - (E - \Delta E_S)\right)}{\Delta_E} \right\} \int_{-\infty}^{\infty} dE' \exp\left\{ -\frac{\left(E' - E^0\right)^2}{\Delta_G^2} \right\} f(E')$$

$$= \frac{1}{2\Delta_E} \int_{-\infty}^{\infty} dE'\, f(E') \exp\left\{ \left[\frac{\Delta_G}{2\Delta_E} \right]^2 - \left[\frac{E' - E + \Delta E_S}{\Delta_E} \right] \right\} erfc\left\{ \frac{\Delta_G}{2\Delta_E} - \frac{E' - E + \Delta E_S}{\Delta_G} \right\} ,$$

where m represents the mass of the neutron, M is the target mass, k is Boltzmann's constant, T is the effective temperature of the sample material, $f(E')$ represents the unbroadened cross section, the energy shift ΔE_S is introduced in order that the maximum of the broadening function is located at $E' = E$. Also Δ values are defined as follows:

$$\Delta_E = \frac{2E^{3/2}}{L\left(m/2\right)^{1/2}} \Delta t_E = \left(0.02766 \frac{\Delta t_E}{L} \right) E^{3/2}$$

$$\Delta_G^2 = \frac{2}{3} E^2 \left[\left(\frac{\Delta t_c}{t} \right)^2 + \left(\frac{\Delta L}{L} \right)^2 \right] + \frac{E^3}{\frac{m}{2} \ln 2} \left(\frac{\Delta t_G}{L} \right)^2$$

$$= \frac{2}{m} E^3 \left[\frac{1}{\ln 2} \left(\frac{\Delta t_G}{L} \right)^2 + \frac{2}{3} \left(\frac{\Delta t_c}{L} \right)^2 \right] + \frac{2}{3} E^2 \left(\frac{\Delta L}{L} \right)^2$$

$$\Delta_G = E[aE+b]^{1/2} \quad ,$$
$$= E\left[\left\{\left(0.01661\frac{\Delta t_G}{L}\right)^2 + \left(0.011293\frac{\Delta t_c}{L}\right)^2\right\}E + \left(0.81650\frac{\Delta L}{L}\right)^2\right]$$

where m is the neutron mass, Δt_E is the exponential folding width in ìsec, ΔL is the broadening in the flight path length L in meters, Δt_c is the finite channel width in ìsec and Δt_G is the neutron burst width the full width at half max in ìsec.

3. SAMMY Analysis

3.1 Experimental Conditions

Measurement was made at room temperature, flight path length of the Time-of-Flight was 10.81m with a full width of the square distribution of 0.04 m. Thermalization time constant was 0.25 μs in terms of the e-folding width of the exponential resolution function, burst width was 0.68 μs in terms of the FWHM of the Gaussian resolution function which corresponds to the linac pulse duration of 1μs in terms of a full width of the square distribution function, and the minimum channel width was 0.5 μs in terms of a full width of the square distribution function. Sample thickness is 0.002929 atoms/barn which corresponds to a thickness of 0.5mm.

3.2 SAMMY Input

Most of the atomic properties of silver such as atomic weight, natural abundance, and spin are obtained from reference 4 and the atomic density of silver is obtained from reference 5.

Initial parameter file up to the energy of 100 eV is prepared based on the resonance data such as resonance energy, gamma widths and neutron widths given in the ENDF/B-VI release 8 file and then p-wave resonance data from reference 6 is added in the parameter file. External resonance parameters from 100 eV to 200 eV are included in the file from the ENDF/B-VI release 8 file, where only s-wave resonances are considered because the p-wave resonances' effect is much smaller than the s-wave resonances'.

In this analysis, we used the transmission data measured at the Time-Of-Flight facility of The Pohang Accelerator Laboratory, at the Pohang University of Science and Technology and treated by Dr. V.R. Skoy, Frank Laboratory of Neutron Physics,

Joint Institute for Nuclear Research, Dubna, Moscow, Russia.

In SAMMY, there are two kinds of options for a covariance matrix. One is an explicit covariance matrix and the other is an implicit covariance matrix. In this study, the implicit covariance matrix option is used which is recommended in SAMMY.

3.3 Procedure of the SAMMY analysis and plotting the SAMMY output

SAMMY analysis is carried out according to the following four steps as shown in Fig.1 :

Step 1: Non-Bayes' analysis for adjusting resonance parameters manually
Step 2: Bayes' analysis
Step 3: Bayes' analysis for generating a covariance matrix
Step 4: Confirmatory Non-Bayes' analysis with a covariance matrix

In particular, in step 2, resonance parameters within the region to be analyzed are adjusted first, and then external resonance parameters outside the region to be analyzed are adjusted, and resonance parameters within the region to be analyzed are finally adjusted using the newly obtained external parameters. Also, When adjusting the external resonance parameters, only the resonance below zero eV is considered. In other words, external parameters above 100 eV were not adjusted because their effects did not improve the fitting results very much.

4. Results and Discussion

Figures 2 and 3 show final fitting results of the total cross section and transmission data obtained from the non-Bayes' analysis with a covariance matrix as given in Table 1. As shown in the above figures, the transmission data fitted well and $\div^2$/N was 1.41. However, we believe more studies using the capture cross section of natural Ag is needed in order to get better values of resonance parameters because only transmission data was considered in this study.

Finally, resonance parameters obtained in this study are compared with the ENDF/B-VI release 8 data and LANDOLT-BOERNSTEIN Data[6] as shown in Table 2.

Acknowledgement

This work is carried out under auspices of Korean Ministry of Science and Technology as a Mid- and Long-Term Nuclear R&D Program.

References

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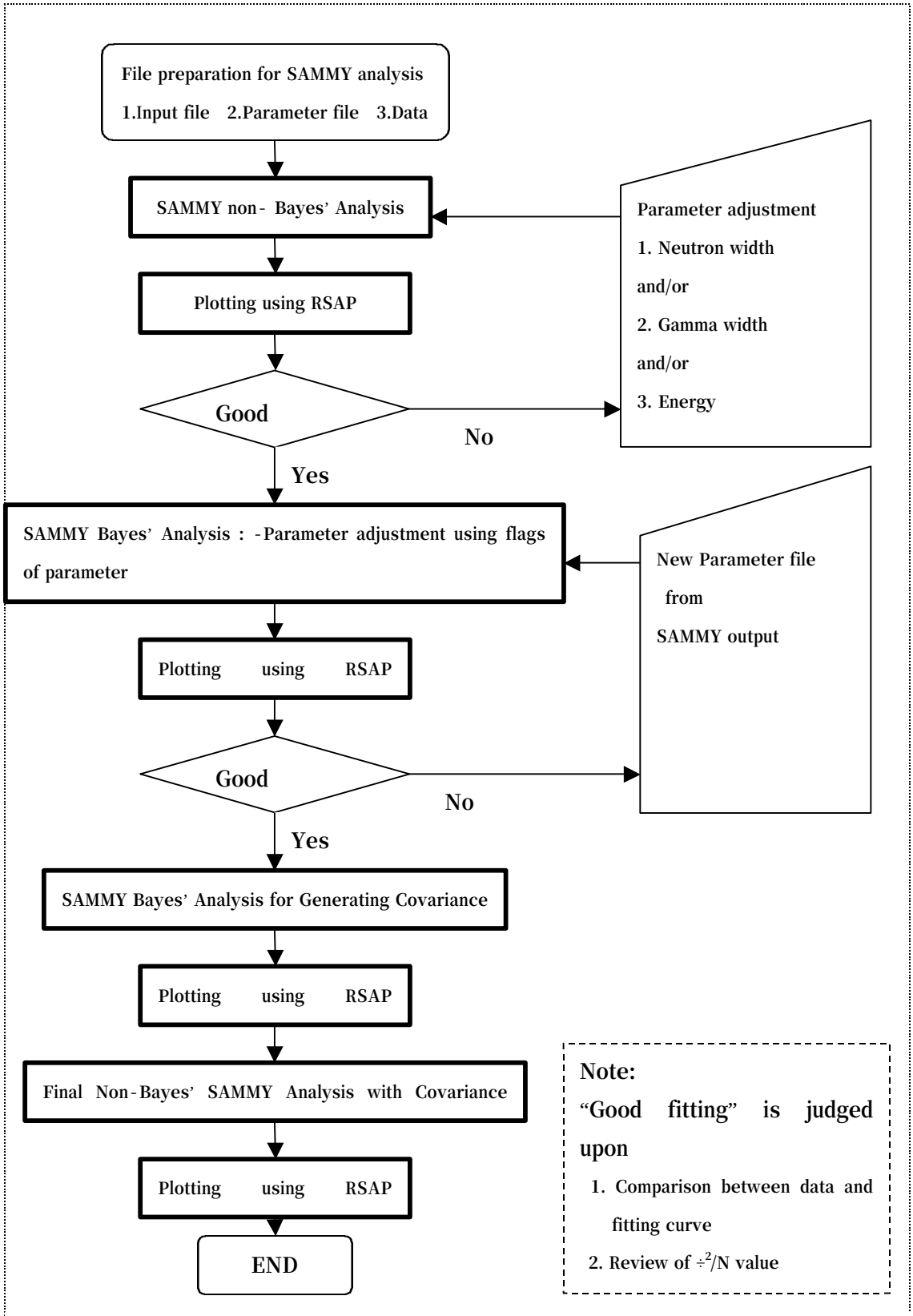

Fig.1 Procedure for the analysis of natural Ag transmission data using SAMMY and RSAP codes

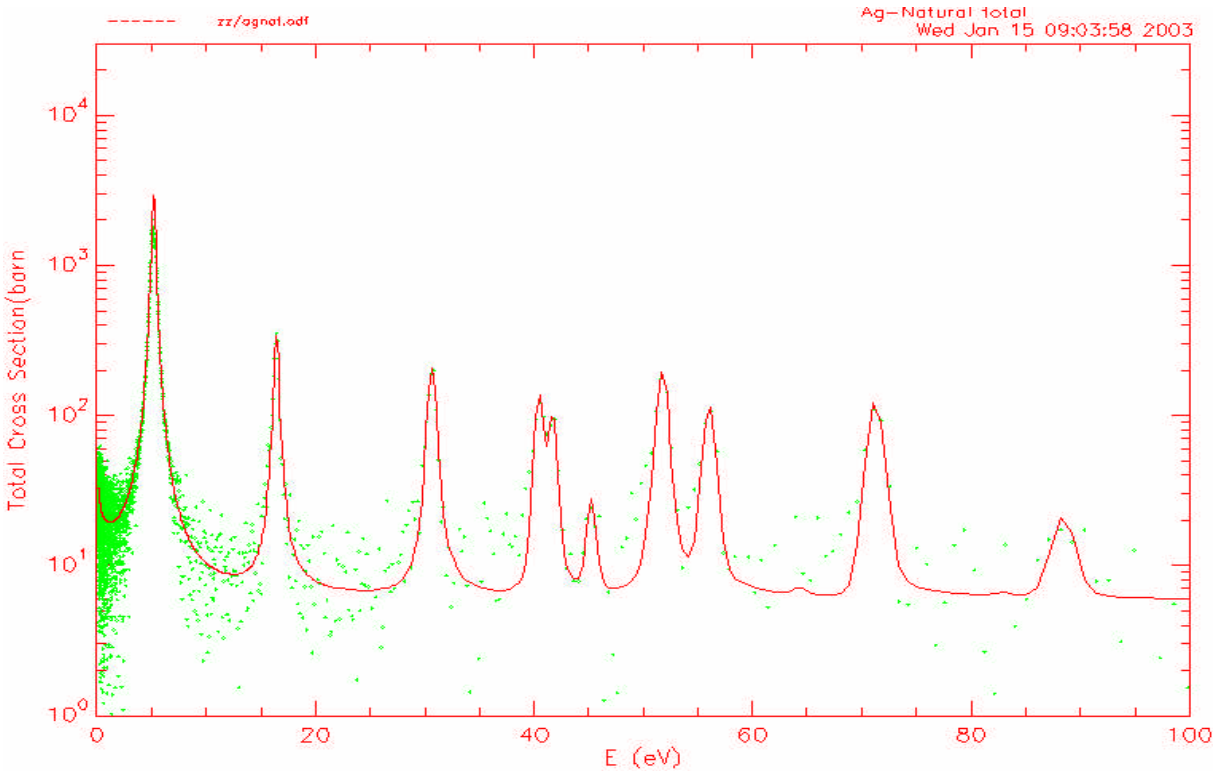

Fig. 2 . Measured data (green dot) and SAMMY prediction (red line) of total cross section of natural Ag obtained from non-Bayes' analysis with covariance matrix (Final)

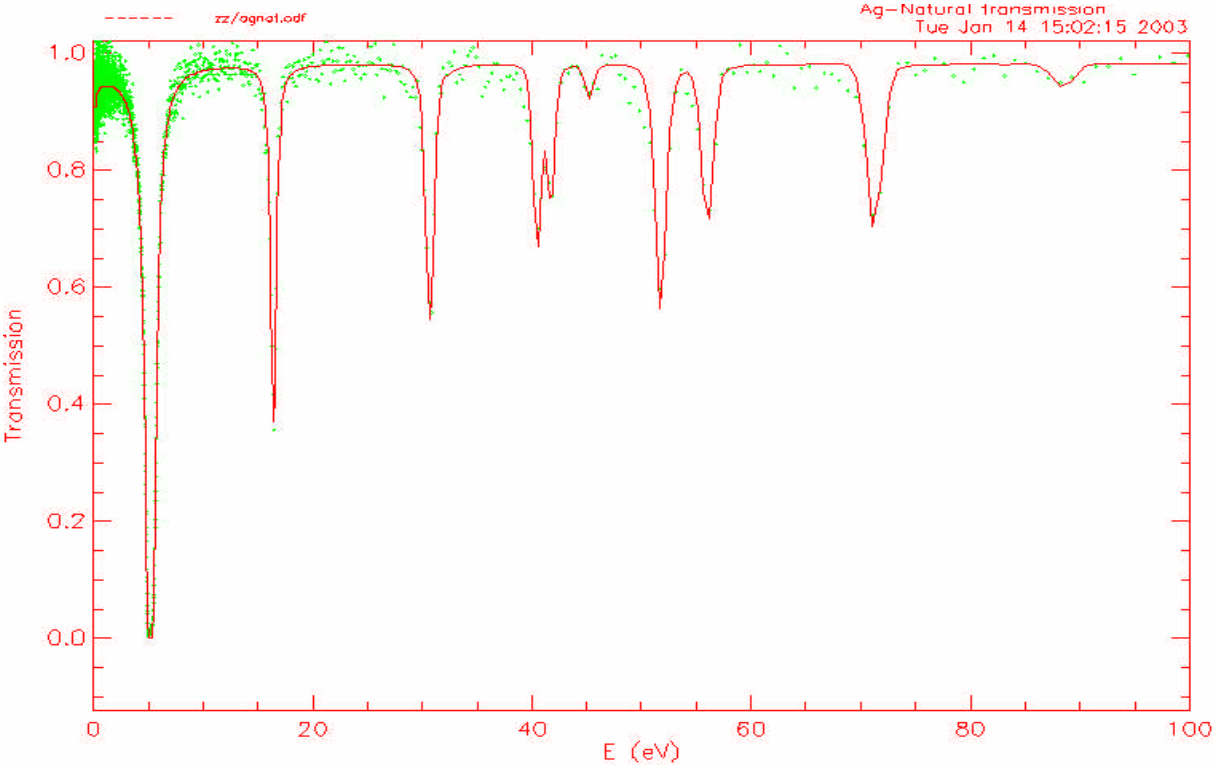

Fig. 3. Measured data (green dot) and SAMMY prediction (red line) of transmission of natural Ag obtained from non-Bayes' analysis with covariance matrix (Final)

Table 1. Covariance Matrix Used in Final SAMMY Non-Bayes' Analysis

E (eV)	$\tilde{A}_{\tilde{a}}$ (meV)	$\tilde{A}_n$ (meV)
4.17255E+01(1)	1.6378E+02(2)	2.5219E+00(3)
5.17560E+01(4)	3.1497E+02(5)	9.7141E+00(6)
8.28273E+01(7)	1.3907E+02(8)	1.8704E-02(9)
1.64233E+01(10)	3.6354E+02(11)	7.5445E+00(12)
4.52644E+01(13)	1.5012E+02(14)	1.8478E+00(15)
1.88985E+01(16)	1.0000E+02(17)	1.4000E-04(18)
2.03227E+01(19)	9.9994E+01(20)	1.6034E-04(21)
3.58258E+01(22)	9.9997E+01(23)	3.8109E-04(24)
4.27514E+01(25)	1.0000E+02(26)	4.6810E-03(27)
6.41974E+01(28)	9.9970E+01(29)	2.6018E-02(30)
7.26666E+01(31)	9.9981E+01(32)	3.6287E-02(33)
6.45649E+01(34)	9.9997E+01(35)	1.0523E-02(36)
5.18570E+00(37)	3.4527E+02(38)	5.9511E+00(39)
3.06739E+01(40)	4.3299E+02(41)	4.4958E+00(42)
4.04917E+01(43)	2.3162E+02(44)	3.7147E+00(45)
7.12595E+01(46)	1.3885E+02(47)	1.2967E+01(48)
8.84744E+01(49)	1.3081E+02(50)	2.2092E+00(51)
9.12748E+01(52)	1.3200E+02(53)	3.3541E-02(54)
5.60480E+01(55)	1.7155E+02(56)	1.9559E+01(57)
8.34020E+01(58)	1.3200E+02(59)	7.4176E-02(60)
3.26940E+01(61)	1.0009E+02(62)	9.1917E-03(63)

(Continued)

Table 1 (Continued) CORRELATION MATRIX FOR OUTPUT PARAMETERS

	STD.DEV. (REL.)		CORRELATION*100													
			1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	2.6383E-02	.001	100														
2	15.68	.096	-1	100													
3	0.1273	.050	-6	13	100												
4	1.8466E-02	.000	0	0	0	100											
5	24.32	.077	0	0	0	1	100										
6	0.2916	.030	0	0	0	2	4	100									
7	0.5979	.007	0	0	0	0	0	0	100								
8	13.91	.100	0	0	0	0	0	0	0	100							
9	1.8703E-03	.100	0	0	0	0	0	0	0	0	100						
10	3.9679E-03	.000	0	0	0	0	0	0	0	0	0	100					
11	10.64	.029	0	0	0	0	0	0	0	0	0	6	100				
12	0.1121	.015	0	0	0	0	0	0	0	0	0	4	57	100			
13	0.1178	.003	0	0	0	0	0	0	0	0	0	0	0	0	100		
14	14.94	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	100	
15	0.1701	.092	0	0	0	0	0	0	0	0	0	0	0	0	2	2	100
16	0.1396	.007	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

(Continued)

Table 1 (Continued) CORRELATION MATRIX FOR OUTPUT PARAMETERS

	STD.DEV.	(REL.)	CORRELATION*100														
			1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
17	10.00	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
18	1.4000E-05	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19	0.1467	.007	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20	10.00	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21	1.6034E-05	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22	0.2330	.007	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23	10.00	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24	3.8105E-05	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25	0.2764	.006	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0
26	10.00	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27	4.6806E-04	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
28	0.4275	.007	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29	9.997	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	2.5996E-03	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
31	0.4941	.007	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
32	9.998	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
33	3.6265E-03	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34	0.4307	.007	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
35	10.00	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36	1.0518E-03	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37	7.6345E-04	.000	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38	3.608	.010	0	0	0	0	-1	0	0	0	0	0	-3	-3	0	0	0
39	4.2924E-02	.007	0	0	0	0	1	0	0	0	0	0	2	1	0	0	0
40	1.0650E-02	.000	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41	24.17	.056	0	0	0	0	0	0	0	0	0	0	-1	-1	0	0	0
42	0.1135	.025	0	0	0	0	0	0	0	0	0	0	-1	-1	0	0	0
43	2.0158E-02	.000	26	-6	-17	0	0	0	0	0	0	0	0	0	0	0	0
44	19.89	.086	10	-2	-12	0	0	0	0	0	0	0	0	0	0	0	0
45	0.1484	.040	18	-8	-15	0	0	0	0	0	0	0	0	0	0	0	0
46	3.8227E-02	.001	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47	13.44	.097	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48	0.6247	.048	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49	0.3361	.004	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50	13.07	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51	0.2119	.096	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

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Table 1 (Continued) CORRELATION MATRIX FOR OUTPUT PARAMETERS

	STD.DEV.	(REL.)	CORRELATION*100														
			1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
52	0.6679	.007	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53	13.20	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54	3.3532E-03	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55	3.1764E-02	.001	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0
56	16.32	.095	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0
57	0.8981	.046	0	0	0	0	-2	-1	0	0	0	0	0	0	0	0	0
58	0.5993	.007	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59	13.20	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	7.4167E-03	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61	0.2138	.007	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62	10.01	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63	9.1999E-04	.100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

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Table 1 (Continued) CORRELATION MATRIX FOR OUTPUT PARAMETERS

	STD.DEV.	(REL.)	CORRELATION*100														
			31	32	33	34	35	36	37	38	39	40	41	42	43	44	45
38	3.608	.010	0	0	0	0	0	0	-7	100							
39	4.2924E-02	.007	0	0	0	0	0	0	14	-91	100						
41	24.17	.056	0	0	0	0	0	0	0	-2	1	5	100				
42	0.1135	.025	0	0	0	0	0	0	0	-2	1	4	49	100			
44	19.89	.086	0	0	0	0	0	0	0	-1	0	0	0	0	5	100	
45	0.1484	.040	0	0	0	0	0	0	0	0	0	0	0	0	6	21	100
46	3.8227E-02	.001	2	0	-1	0	0	0	0	0	0	0	0	0	0	0	0
48	0.6247	.048	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0

(Continued)

Table 1 (Continued) CORRELATION MATRIX FOR OUTPUT PARAMETERS

	STD.DEV.	(REL.)	CORRELATION*100														
			46	47	48	49	50	51	52	53	54	55	56	57	58	59	60
48	0.6247	.048	-2	-9	100												
51	0.2119	.096	0	0	0	1	0	100									
52	0.6679	.007	0	0	0	1	0	0	100								
56	16.32	.095	0	0	0	0	0	0	0	0	0	1	100				
57	0.8981	.046	0	0	0	0	0	0	0	0	0	4	2	100			

Note---Missing lines have zero off-diagonal correlation.

Table 2. Comparison of Resonance Parameters

NuclideJ	g	J	l	E(eV)	Γ_γ (meV)	$g\Gamma_n$ (meV)
Ag-107	0.75	1	0	-11.1 -11.142	141.00[141.50] 108.06	24.585[24.587] 14.613
Ag-107	0.25	0	0	16.30 16.4233±0.0039679	146[134] 363.54±10.64	2.90[2.917] 1.8861±0.028025
Ag-107	0.75	1	1	-[18.9] 18.8985±0.1396	-[100] 100.00±10.00	-[0.000105] 0.000105±0.0000105
Ag-107	0.75	1	1	-[20.3] 20.3227±0.1467	-[100] 99.994±10.00	-[0.00012] 0.00012055±0.000012055
Ag-107	0.75	1	1	-[35.84] 35.8258±0.2330	-[100] 99.997±10.00	-[0.000285] 0.00028582±0.000028579
Ag-107	0.75	1	0	41.5[41.57] 41.7255±0.026383	137 163.78±15.68	4.025[4.5] 1.8914±0.095475
Ag-107	0.75	1	1	-[42.81] 42.7514±0.2764	-[100] 100.00±10.00	-[0.003495] 0.0035108±0.00035105
Ag-107	0.25	1 (0)	0	44.80[44.9] 45.2644±0.1178	147 150.12±14.94	0.87[0.9] 0.46195±0.042525
Ag-107	0.75	1	0	51.40[51.56] 51.7560±0.01846	133 314.97±24.32	17.2[23.4] 7.2856±0.2187
Ag-107	0.75	1	1	-[64.24] 64.1974±0.4275	-[100] 99.970±9.997	-[0.019] 0.019514±0.0019497
Ag-107	0.25	2	1	-[64.74] 64.5649±0.4307	-[100] 99.997±10.00	-[0.0013] 0.026308±0.00026295
Ag-107	0.75	1	1	-[73.21] 72.6666±0.4941	-[100] 99.981±9.998	-[0.027] 0.027215±0.0027199
Ag-107	0.75	1	0	82.600 82.8273±0.5979	139.07 139.07±13.91	0.0014 0.014028±0.0014027
Ag-109	0.75	1	0	5.19[5.145] 5.1857±0.00076345	136.00[143] 345.27±3.608	9.5498[9.65] 4.4633±0.00032193
Ag-109	0.75	1	0	30.4[30.6] 30.6739±0.010650	130 432.99±24.17	5.50[6.33] 3.3719 ±0.085125
Ag-109	0.75	1	1	-[32.7] 32.6940±0.2138	-[100] 100.09±10.01	-[0.007] 0.0068938±0.00068999
Ag-109	0.75	1	0	40.1[40.3] 40.4917±0.020158	131 231.62±19.89	3.75[3.24] 2.7860±0.1113
Ag-109	0.25	0	0	55.7[55.8] 56.0480±0.031764	139 171.55±16.32	9.3[11.62] 4.8898±0.22453
Ag-109	0.75	1	0	70.8[71.0] 71.2595±0.038227	120 138.85±13.44	20.0[22.55] 9.7253±0.46853
Ag-109	0.25	0	0	83.50 83.402±0.5993	132 132±13.20	0.00185 0.018544±0.0018542
Ag-109	0.75	1	0	87.7 88.4744±0.3361	130 130.81±13.07	4.70[4.87] 1.6569±0.15893
Ag-109	0.75	1	0	91.50 91.2748±0.6679	132 132±13.20	0.0250 0.025156±0.0025149

Note: Reference 6 data is given only when it is different from ENDF/B-VI release 8 data.

Legend:

ENDF/B-VI release 8 Data [LANDOLT-BOERNSTEIN Data[6]]

KAERI's result