Evaluation of ^{231}Pa and ^{233}Pa Resonance Parameters and Covariance in the Resolved Resonance Region

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As part of the International Atomic Energy Agency (IAEA) coordinated research program (CRP) on the thorium-uranium fuel cycle, an evaluation of the resonance parameters and covariance data for ^{231}Pa and ^{233}Pa in the resolved resonance region was performed.

EVALUTION OF ^{231}Pa

The ^{231}Pa Multilevel Breit-Wigner (MLBW) resonance parameters, listed in the Mughabghab compilation,[1] are given in the energy range 0 to 104 eV. Above 60 eV no fission widths are given. The MLBW parameters were converted into the Reich-Moore (RM) formalism, and the fission widths above 60 eV were set equal to the average value obtained below 60 eV. The SAMMY computer code[2] was then used to adjust the neutron, gamma, and fission widths by fitting the experimental total cross section of Simpson[3] while maintaining the capture and fission cross section obtained with the Mughabghab MLBW parameters. Figure 1 shows the fitting of the total cross section of Simpson in the energy range from 5 to 15 eV and also a comparison of the fission cross section calculated with the RM and MLBW formalisms. The square symbol in the upper curve is the experimental total cross section of Simpson, and the solid line is the RM calculation with the resonance parameters. In the lower curve the star symbol is the calculated fission cross section with MLBW formalism whereas the solid line represents the RM calculations. The total cross section at thermal (0.0253 eV) calculated with the RM resonance parameters is 211.87 b, compared with 211.0 ± 2.2 b quoted by Mughabghab. The calculated capture and fission cross sections at thermal are, respectively, 200.63 and 0.021 b, compared with 200.62 ± 2.3 b and 0.020 ± 0.001 b as quoted by Mughabghab.

In addition to the RM resonance evaluation of ^{231}Pa, resonance covariance data were also obtained. The covariance data were converted into the ENDF format using the LCOMP=1 option and processed with the PUFF-IV[5] and ERRORJ[4] codes for use in uncertainty analysis calculations.

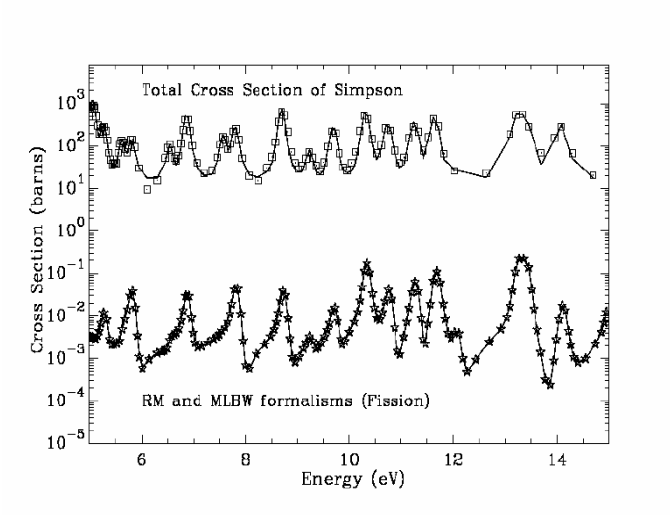

Fig 1. Comparison of the experimental total cross section of Simpson with calculations done with the RM resonance parameters (upper curve). The bottom curve represents the comparison of the RM and MLBW fission cross section.

EVALUATION OF ^{233}Pa

An MLBW resonance evaluation was performed by Morogovskij[6] in the energy range 0 to 106.6 eV. There are two s-wave resonance spin states for ^{233}P, namely, J=1 and J=2. In the Morogovskij evaluation the two spin states were mixed and represented by the single spin state of J=1.5. In the evaluation done in this work, the MLBW resonance parameters were converted into the RM representation. The spin assignment was performed from statistical analysis of the parameters and from a literature search. The RM resonance parameters were used in a SAMMY analysis to fit the experimental total cross section of Simpson. The total and capture cross sections calculated at thermal with the RM resonance parameters are 54.9 and 42.5 b, respectively. The thermal total cross section agrees well with the experimental value 55.0 ± 3.0 b given by Simpson.[7] The thermal capture cross section does not agree with the Simpson value of 39.5 ± 1.2. However, it does agree with the value given by Belanova[8]: 43 ± 11. In addition to the resonance parameter evaluation, resonance covariance data were also generated. Table I shows the total and capture cross section calculated with the computer code SAMMY in the 44-group structure of the SCALE system with a constant flux spectrum. Also shown are the group cross-section

uncertainties calculated using the resonance covariance data. Only 29 of the 44 groups are show in Table I. It can be seen that the cross-section uncertainties for groups 4 and 5 (thermal groups) are consistent with experimental values. The large uncertainties at low-energy groups can be attributed to uncertainties in the negative-energy bound level at energy −0.108 eV.

Table I. Total and Capture Group Cross Sections and Uncertainties

Emin (eV)	Emax (eV)	σ_γ (b)	$\delta\sigma_\gamma$ (b)	σ_t (b)	$\delta\sigma_t$ (b)
106.6	100.0	34.75	0.19	54.83	0.39
100.0	30.0	36.46	0.19	53.59	0.24
30.0	10.0	53.12	0.32	68.29	0.35
10.0	8.1	176.08	2.45	191.14	2.55
8.1	6.0	25.96	0.27	39.57	0.29
6.0	4.75	155.84	2.06	171.46	2.11
4.75	3.0	168.71	2.39	183.87	2.45
3.0	1.77	138.11	2.14	152.77	2.16
1.77	1.0	848.10	12.56	867.09	12.94
1.0	0.625	23.17	0.31	34.39	0.35
0.625	0.4	10.40	0.15	22.21	0.33
0.4	0.375	9.83	0.21	21.21	0.44
0.375	0.35	9.87	0.22	21.87	0.47
0.35	0.325	9.96	0.25	21.99	0.52
0.325	0.275	10.21	0.31	22.29	0.59
0.275	0.25	10.62	0.38	22.74	0.69
0.25	0.225	11.02	0.45	23.17	0.78
0.225	0.2	11.55	0.53	23.74	0.90
0.2	0.15	12.75	0.73	24.97	1.12
0.15	0.1	15.52	1.18	27.79	1.64
0.1	0.07	19.78	1.91	32.10	2.45
0.07	0.05	24.81	2.81	37.16	3.42
0.05	0.04	29.79	3.74	42.17	4.39
0.04	0.03	34.94	4.71	47.35	5.39
0.03	0.0253	40.32	5.73	52.73	6.43
0.0253	0.01	54.06	8.32	66.50	9.06
0.01	0.0075	77.97	12.79	90.47	13.57
0.0075	0.003	104.83	17.69	117.38	18.49
0.003	0.00001	261.05	45.52	274.63	46.41

In conclusion, as part of the IAEA/CRP, evaluations of the resonance parameters and covariance data for ^{231}Pa and ^{233}Pa were performed in the resolved resonance region. Evaluations of the resonance parameters were performed based on the RM formalism. The evaluations fit well the experimental data. In addition, the thermal values and their uncertainties are reproduced. The evaluations can be retrieved from the IAEA nuclear data section. The addition of uncertainty information will permit the users to perform sensitivity calculation and to propagate error uncertainties in k_{eff} calculations.

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