Validation of Thermal Cross Sections and Resonance Integrals of SG-23 Evaluated Nuclear Data Library

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1 Introduction

The task of the Working Party on Evaluation Co-operation (WCEC) Subgroup-23 (SG-23) was to assemble, verify and validate an evaluated data library for the minor fission products by reviewing and making use of existing evaluations, running nuclear model calculations and performing selective partial re-evaluation work.

The constants from the k_0 database for neutron activation analysis are routinely used in analytical work. They were generally determined experimentally by direct measurements, and in most cases they were not used in the evaluation process of the cross sections in the evaluated nuclear data files. Therefore, they may be considered as independent integral measurements for the validation of the differential cross section data. The purpose of the exercise presented herein was to compare the thermal capture cross sections and resonance integrals from the SG-23 library to the equivalent values in the k_0 database.

2 Methodology

In the validation exercise only the radiative capture reactions are considered. There are 49 such reaction cross section sets in the SG-23 library, referring either to the total radiative capture cross section, or the excitation cross section of long-lived metastable states.

2.1 Thermal cross sections

Thermal cross sections are related to the k_0 constants for neutron activation analysis (NAA) by the following relation:

$$k_{0,a} = \frac{M_s \Theta_a P_a \sigma_{0,a}}{M_a \Theta_s P_s \sigma_{0,s}} \tag{7}$$

where:

M_x molar mass of the element in sample material,

Θ_x natural atomic abundance of the isotope,

P_x gamma emission probability of the measured gamma ray,

$\sigma_{0,x}$ thermal capture cross section.

Gold is the universal comparator in the k_0-standardisation variant of NAA. Thermal capture cross section of gold of 98.65 barns is assumed. From the published k_0 values [1] and the gamma emission probabilities from Nudat-2.1 the thermal capture cross sections can be calculated. For the present intercomparison the cross sections were taken from [2] and were calculated by the author in the same way. They are compared in Table 1 to the evaluated values by Mughabghab [3], the values in the IRDF-2002 library and the SG-23 library.

There are 49 matching nuclides. Comparison can be made for 30 of them; the remainder refer to the excitation of the long-lived metastable states, for which the corresponding branching ratios are not available in the SG-23 library.

The cross sections (Sig0) and their uncertainties (dSig0) derived from the k_0 database are taken as reference. Differences from this reference (Dif) are given whenever possible. The following conclusions can be drawn:

- 2 nuclides (^{96}Ru and ^{127}I) show severe differences (greater than 20%, marked red in Table 1). It is interesting to note that the value for ^{96}Ru by Mughabghab is in good agreement with the reference.
- 5 nuclides (^{87}Rb, ^{102}Ru, ^{107}Ag, ^{160}Gd and ^{165}Ho) show large differences (greater than 10%, marked magenta in Table 1).
- 5 nuclides (^{75}As, ^{96}Zr, ^{104}Ru, ^{148}Nd and ^{154}Sm) show significant differences (greater than 5%, marked yellow in Table 1).
- 18 nuclides are consistent within the quoted uncertainties.

Table 1: Comparison of thermal capture cross sections from various sources.

Target	Reac	Product	Mughabghab Sig0 [b]	dSig0 [%]	Diff [%]	Kayzero/Nudat Sig0 [b]	dSig0 [%]	SG-23 Sig0 [barns]	Diff [%]	IRDF-2002 Sig0 [barns]	Diff [%]
Ga-71	(n,g)		4.73	3.2	1.7	4.650	0.8	4.735	1.8		
As-75	(n,g)		4.23	1.9	9.9	3.850	4.8	4.092	6.3		
Se-74	(n,g)		51.8	2.3	2.6	50.50	4.8	51.86	2.7		
Se-76	(n,g)	Se-77m	85	8.2		18.90	3.4	85.08			
Br-79	(n,g)	Br-80m	10.32	1.3		8.160	7.5	11.01			
Br-81	(n,g)	Br-82m	2.36	2.1		2.590	1.1	2.367			
Rb-85	(n,g)		0.48	2.1	-4.4	0.502	1.1	0.4939	-1.6		
Rb-87	(n,g)		0.12	25.0	12.1	0.107	6.1	0.1201	12.2		
Sr-86	(n,g)	Sr-87m	1.04	6.7		0.775	0.8	1.006			
Y-89	(n,g)	Y-90m	1.28	1.6		0.0010	1.1	1.278			
Zr-94	(n,g)		0.0499	4.8	-2.2	0.051	2.0	0.04992	-2.1		
Zr-96	(n,g)		0.02	5.0	1.5	0.0197	3.2	0.02118	7.5		
Nb-93	(n,g)	Nb-94m	1.15	4.3		0.863		1.148		1.156	34.0
Mo-98	(n,g)		0.137	3.6	4.6	0.131	2.3	0.1301	-0.7		
Mo-100	(n,g)		0.199	1.5	0.0	0.199	3.1	0.1992	0.1		
Ru-96	(n,g)		0.22	9.1	-4.3	0.230	2.6	0.2902	26.2		
Ru-102	(n,g)		1.21	5.8	5.2	1.150	1.2	1.271	10.5		
Ru-104	(n,g)		0.47	4.3	-5.6	0.498	2.2	0.472	-5.2		
Pd-108	(n,g)	Pd-109m	27.6	1.4		0.170	0.5	8.486			
Pd-110	(n,g)	Pd-111m	0.227	14.1				0.2293			
Ag-107	(n,g)		37.6	3.2	14.3	32.90	4.2	37.63	14.4		
Cd-114	(n,g)		0.34	5.9	5.9	0.321	3.2	0.3363	4.8		
In-113	(n,g)	In-114m	12	9.2				12.14			
In-115	(n,g)	In-116m	202	1.0		160.24	6.2	202.4		166.5	3.9
Sn-112	(n,g)	Sn-113m	0.86	10.5		0.006	1.2	0.8509			
Sn-116	(n,g)	Sn-117m	0.13	23.1		0.146	1.0	0.1278			
Sn-122	(n,g)	Sn-123m	0.139	10.8		0.119	3.0	0.1461			
Sn-124	(n,g)	Sn-125m	0.134	3.7		0.0045		0.1339			
Sb-121	(n,g)	Sb-122m	5.9	3.4		631.00	2.1	5.776			
Sb-123	(n,g)	Sb-124n	4.1	2.4		4.020	0.9	3.877			
Te-130	(n,g)	Te-131m	0.29	20.7		4.060	10.0	0.1954			
I-127	(n,g)		6.2	3.2	52.7	4.060	10.0	6.15	51.5		
Ba-130	(n,g)		8.7	10.3	2.0	8.53	10.0	8.686	1.8		
Ba-132	(n,g)	Ba-133m	6.5	12.3		0.83		6.537			
Ba-138	(n,g)		0.404	9.9	-0.5	0.406	1.0	0.4038	-0.5		
La-139	(n,g)	La-140	9.04	0.4	-4.1	9.423	1.8	9.048	-4.0	9.042	-4.0
Ce-140	(n,g)		0.58	3.4	0.9	0.575	1.0	0.5781	0.5		
Ce-142	(n,g)		0.97	2.1	-0.6	0.98	1.3	0.966	-1.0		
Nd-146	(n,g)		1.41	3.5	-0.7	1.42	4.8	1.49	4.9		
Nd-148	(n,g)		2.58	5.4	8.4	2.38	6.8	2.586	8.7		
Nd-150	(n,g)		1.03	7.8	1.0	1.020	0.0	1.041	2.1		
Sm-154	(n,g)		8.3	6.0	7.8	7.700	2.6	8.401	9.1		
Eu-151	(n,g)	Eu-152m	9200	1.1		3221	11.9	9189			
Gd-152	(n,g)		735	2.7	-2.8	756.00	5.8	735.9	-2.7		
Gd-158	(n,g)		2.2	9.1	-2.7	2.260	24.0	2.204	-2.5		
Gd-160	(n,g)		1.4	21.4	-11.4	1.580	2.0	1.407	-10.9		
Tb-159	(n,g)		23.3	1.7	-2.9	24.00	2.0	23.38	-2.6		
Ho-165	(n,g)		64.7	1.9	10.6	58.50	1.3	64.74	10.7		
Er-170	(n,g)		8.85	3.4	-0.1	8.86	3.9	8.861	0.0		

2.2 Resonance integral to thermal cross section ratio

The Q_0 values in NAA are defined as the ratio of the resonance integral I_0 in a $1/E$ spectrum and the thermal cross section σ_0 corresponding to neutron speed of 2200 m/s. The resonance integrals are less rigorously defined and various definitions can be found in the literature. For our intents and purposes we define the resonance integral by the following:

$$I_0 = \int_{E_{cd}}^{E_3} \sigma(E)\psi(E)\,dE \quad ; \quad \psi(E) = \frac{1}{E},$$

where the lower integration limit E_{cd} is the cadmium cutoff energy of 0.55 eV and the upper integration limit E_3 is chosen at 2 MeV. Therefore

$$Q_0 = \frac{I_0}{\sigma_0}$$

Experimentally, the resonance integral is often measured by the cadmium ratio method, where $t(E)$ is the cadmium transmission function:

$$I_{cd} = \int_0^{\infty} t(E)\sigma(E)\phi^*(E)\,dE\,. \tag{24}$$

The above equation reduces to the previous idealised one if the range of integration is limited from E_{cd} to E_3, the spectrum $\varphi^*(E)$ is pure $1/E$, and $t(E)$ is an idealised Heaviside function:

$$t(E) = \begin{cases} 0 & \text{for } E < E_{cd} \\ 1 & \text{for } E \geq E_{cd} \end{cases} \tag{25}$$

A more realistic form of the cadmium transmission function is:

$$t(E) = e^{N_{cd}\,d\,\sigma_{cd}(E)} \tag{26}$$

where d is the cadmium cover thickness, σ_{cd} is the cadmium cross section and N_{cd} is the number density of cadmium atoms in the cover. It is calculated as:

$$N_{cd} = \frac{\rho_{cd} N_A}{M_{cd}}\,, \tag{27}$$

where ρ_{cd} is the density of cadmium, N_A the Avogadro number and M_{cd} the molar mass of cadmium. Resonance integral defined by equation (23) is a measurable quantity. This is to be compared with the required form evident from equations (4) and (5). The cadmium transmission factor F_{cd} is introduced to compensate for the difference:

$$I = \int_{E_{cd}}^{E_3} \sigma(E)\phi(E)\,dE = \frac{1}{F_{cd}} \int_0^{\infty} t(E)\sigma(E)\phi(E)\,dE\,. \tag{28}$$

From this it follows that:

$$F_{cd} = \frac{\int_0^{\infty} t(E)\sigma(E)\phi(E)\,dE}{\int_{E_{cd}}^{E_3} \sigma(E)\phi(E)\,dE}\,. \tag{29}$$

Deviation of F_{cd} from unity arises from the cadmium transmission function and possibly from the difference in the upper integration limit. The contribution of the later is negligible in the case of $1/E$ spectrum with a small component of the fission neutrons in the spectrum. This is usually the case for irradiation facilities behind a reflector.

The published Q_0 values [1] are compared in Table 2 to the evaluation by Mughabghab [3], the values in the IRDF-2002 library and the SG-23 library.

The Q_0 values and their uncertainties dQ_0 from the k_0 database are taken as reference. Differences from this reference (Dif) are given. Assuming that the branching ratios for the excitation of metastable states are independent of incident particle energies (which is not necessarily valid) the Q_0 values for total capture and for excitation of metastable states are the same. The following conclusions can be drawn:

- 17 nuclides (^{71}Ga, ^{76}Se, ^{89}Y, ^{108}Pd, ^{114}Cd, ^{112}Sn, ^{116}Sn, ^{123}Sb, ^{130}Te, ^{132}Ba, ^{138}Ba, ^{140}Ce, ^{142}Ce, ^{148}Nd, ^{150}Nd, ^{151}Eu and ^{160}Gd) show severe differences (greater than 20%, marked red in Table 2).
- 8 nuclides (^{85}As, ^{86}Sr, ^{94}Zr, ^{102}Ru, ^{110}Pd, ^{113}In, ^{122}Sn and ^{130}Ba) show large differences (greater than 10%, marked magenta in Table 1).
- 8 nuclides (^{77}Br, ^{96}Zr, ^{93}Nb, ^{96}Ru, ^{104}Ru, ^{115}In, ^{121}Sb, and ^{170}Er) show significant differences (greater than 5%, marked yellow in Table 1).
- 6 nuclides (^{85}Rb, ^{87}Rb, ^{127}I, ^{146}Nd, ^{158}Gd and ^{165}Ho) show differences larger than the quoted uncertainties (marked pale yellow in Table 2)
- 10 nuclides are consistent within the quoted uncertainties.

Table 2: Comparison of resonance integral to thermal capture cross section ratios from various sources

Target	Reac	Product	Mughabghab Q0	Mughabghab dQ0 [%]	Mughabghab Diff [%]	Kayzero-96 Q0	Kayzero-96 dQ0 [%]	Fcd	SG-23 Q0	SG-23 Diff [%]	IRDF-2002 Q0	IRDF-2002 Diff [%]
Ga-71	(n,g)		6.596	9.3	-1.4	6.69	1.2		9.340	39.6		
As-75	(n,g)		14.421	8.4	6.0	13.6			15.370	13.0		
Se-74	(n,g)		10.811	11.2	0.1	10.8	6.5		11.160	3.3		
Se-76	(n,g)	Se-77m	0.471	18.2	-38.9	0.77			0.463	-39.8		
Br-79	(n,g)	Br-80m	12.306	12.3	-3.9	12.8			11.690	-8.7		
Br-81	(n,g)	Br-82m	21.186	12.1	9.8	19.3	3		19.570	1.4		
Rb-85	(n,g)		12.292	10.6	-16.9	14.8	2.5		15.380	3.9		
Rb-87	(n,g)		22.500	39.8	-3.4	23.3	3		22.560	-3.2		
Sr-86	(n,g)	Sr-87m	4.615	13.0	12.3	4.11	1.7		4.819	17.3		
Y-89	(n,g)	Y-90m	0.781	11.6	-86.8	5.93	2.3		0.658	-88.9		
Zr-94	(n,g)		5.411	15.9	1.9	5.31	3.3		6.339	19.4		
Zr-96	(n,g)		280.000	8.6	11.3	251.6	1		264.500	5.1		
Nb-93	(n,g)	Nb-94m	7.391	10.2	0.6	**7.35**	**2.7**	**0.985**	8.081	9.9	8.571	16.6
Mo-98	(n,g)		50.365	8.0	-5.2	53.1	6.3		50.320	-5.2		
Mo-100	(n,g)		19.095	4.1	1.6	18.8	4		19.400	3.2		
Ru-96	(n,g)		29.545	15.2	11.5	26.5	3.5		24.960	-5.8		
Ru-102	(n,g)		3.471	8.2	-4.4	3.63			4.264	17.5		
Ru-104	(n,g)		13.617	12.1	6.4	12.8	2.7		13.980	9.2		
Pd-108	(n,g)	Pd-109m	8.841	3.1	-66.8	26.6	1.7		2.868	-89.2		
Pd-110	(n,g)	Pd-111m	13.656	27.0	14.8	11.9	6.7		13.510	13.5		
Ag-107	(n,g)		2.660	51.2	-8.3	2.9			2.925	0.9		
Cd-114	(n,g)		41.471	10.8	28.0	32.4			39.070	20.6		
In-113	(n,g)	In-114m	25.833	18.8	6.7	24.2	1.7		27.360	13.1		
In-115	(n,g)	In-116m	16.337	4.0	-2.8	**16.8**	**1.9**	**0.976**	15.880	-5.5	15.520	-7.6
Sn-112	(n,g)	Sn-113m	33.721	17.4	-30.3	48.4	1.2		35.140	-27.4		
Sn-116	(n,g)	Sn-117m	91.538	31.5	62.6	56.3	1.9		96.320	71.1		
Sn-122	(n,g)	Sn-123m	5.827	15.7	7.9	5.4	2.5		4.446	-17.7		
Sn-124	(n,g)	Sn-125m	59.701	6.2	-0.7	60.1	2.9		60.000	-0.2		
Sb-121	(n,g)	Sb-122m	34.746	13.1	5.3	33	3.5		35.650	8.0		
Sb-123	(n,g)	Sb-124n	30.976	18.2	55.7	19.9			32.960	65.6		
Te-130	(n,g)	Te-131m	1.034	54.0	-42.5	1.8	5.8		1.328	-26.2		
I-127	(n,g)		24.194	9.9	-2.4	24.8	2.7		25.940	4.6		
Ba130	(n,g)		19.540	16.2	-21.2	24.8			20.130	-18.8		
Ba-132	(n,g)	Ba-133m	5.077	21.4	-9.3	5.6			8.258	47.5		
Ba-138	(n,g)		0.792	22.4	-10.0	0.88			0.661	-24.9		
La-139	(n,g)	La-140	1.338	5.4	7.9	1.24	2.4	1.004	1.246	0.5	1.307	5.4
Ce-140	(n,g)		0.931	12.7	12.2	0.83			0.500	-39.8		
Ce-142	(n,g)		1.186	6.4	-1.2	1.2			0.869	-27.6		
Nd-146	(n,g)		16.454	5.7	723	2.0	1.2		1.921	-4.0		
Nd-148	(n,g)		5.426	12.6	6.8	5.08	2.5		6.182	21.7		
Nd-150	(n,g)		13.592	22.1	10.5	12.3	0.8		15.280	24.2		
Sm-154	(n,g)		4.337	17.1	0.9	4.3	7		4.300	0.0		
Eu-151	(n,g)	Eu-152m	0.359	10.2	-47.3	0.68			0.274	-59.8		
Gd-152	(n,g)		2.748	10.6	257	0.77	15		0.743	-3.5		
Gd-158	(n,g)		33.182	18.7	11.0	29.9	3.1		31.220	4.4		
Gd-160	(n,g)		5.286	34.9	38.0	3.83	1.9		5.783	51.0		
Tb-159	(n,g)		17.940	6.5	0.2	17.9	3.8		17.730	-0.9		
Ho-165	(n,g)		10.278	5.2	-5.7	10.9	2.4		10.510	-3.6		
Er-170	(n,g)		4.000	20.1	-9.5	4.42	3.3		4.706	6.5		

3 Conclusions

The identified discrepancies bear no implications as to which dataset is more correct. They simply indicate which nuclides require attention.

There is fairly good consistency between the thermal capture cross sections and the reference. Differences are similar to those observed for the Mughabghab evaluation.

Larger differences are observed for the ratios of the resonance integrals to thermal cross sections. Some of them will require detailed attention. Proper treatment of the energy dependence of the branching ratios may help in some cases, but is not likely to greatly improve the situation.

References

[1] F. De Corte, A. Simonits: Recommended nuclear data for use in the k_0 standardization of neutron activation analysis, Atomic Data and Nuclear Data Tables 85 (2003) 47-67.

[2] F. De Corte: The updated NAA nuclear data library derived from the Y2K k_0-database, Journal of Radioanalytical and Nuclear Chemistry, Vol. 257, No. 3 (2003) 493-499.

[3] S. Mughabghab: Thermal Neutron Cross Sections and Resonance Integrals, International Atomic Energy Agency, INDC(NDS)-440.