CONF-841118--5

BNL-NCS-35522

A LEAST SQUARES FIT OF THERMAL DATA FOR FISSILE NUCLEI

BNL-NCS--35522

DE85 004712

M. Divadeenam and J. R. Stehn
National Nuclear Data Center
Brookhaven National Laboratory

Since the paper of the above title was written[1], we have learned of one new set of measurements that would have been included had we known of it: Gwin, Spencer and Ingle's measurement of the nu-prompt ratios of the four fissile materials with respect to ^{252}Cf. Their recently published paper[2] reports revised final results for ^{233}U, ^{235}U and ^{239}Pu and includes a measurement on $\bar{\nu}_p(241)/\bar{\nu}_p(252)$ that was not attempted previously. In some of the fitted results reported here, we have replaced their earlier 1978/1981 values by the final 1984 set[2]. The replacement has appreciable effect on some of the parameters.

	$\bar{\nu}_p(233)/\bar{\nu}_p(252)$	$\bar{\nu}_p(235)/\bar{\nu}_p(252)$	$\bar{\nu}_p(239)/\bar{\nu}_p(252)$	$\bar{\nu}_p(241)/\bar{\nu}_p(252)$
83 Fit	0.6615±0.0010	0.6407±0.0008	0.7636±0.0016	0.7771+0.0018
78/81	0.6630±0.0020	0.6441±0.0019	0.7650±0.0030	----
1984	0.6597±0.0018	0.6443±0.0014	0.7655±0.0014	0.7820±0.0018

Another revised value that we have used here is Axton's 1984 revision[4] (3.7509±0.0107) of his 1982 ^{252}Cf $\bar{\nu}_p$ value (3.744±0.021). The effect of including the revised result is not appreciable.

Ever since the 1962 critical experiments of Gwin and Magnuson[5] on spherical and cylindrical volumes of uranyl nitrate (both ^{233}U and ^{235}U), their interpretation has been a quandary. The approximations used by the authors have changed with time; each has separately proposed different approaches[6,7,8]. Reactor theorists Ullo and Hardy[9] have made a thorough study with a multigroup code and using the best set of cross-sections available at the time (ENDF/B-IV). Hardy[10] recently has further analyzed their calculation to bring out the best approximation to 2200 m/sec cross sections and he has used a more recently evaluated[11] hydrogen cross section value. We have made separate fits both with Gwin's and with Hardy's latest suggested parameters. Gwin's 1984 interpretation gives results slightly different from our previous paper, but Hardy's results cause appreciable changes (see below) in some of the parameters.

Parameter	Input: 1983 Fit[1]	Input: Gwin[8]	Input: Hardy[10]	Output: 1983 Fit	Output: Gwin	Output: Hardy
$(\hat{n}_3-1)\hat{\sigma}_a(3)$	740.4±8.6	741.4±5.0	744.7±4.0	738.4±2.4	739.1±2.3	741.0±2.1
$(\hat{n}_5-1)\hat{\sigma}_a(5)$	724.1±10.0	712.0±4.0	722.7±3.9	712.7±2.1	712.2±2.0	715.3±2.0

To show the greatest possible effect of the new data and the new interpretations, we used only Hardy's interpretation of the critical assembly results. The net result of using the three new inputs[2,4,10] is seen in Table 1, which is Table 36 of our Annals of Nuclear Energy paper with the changes Δ indicated for each quantity in an additional column for each nucleus.

Of all the changes from the 1983 fit two of the changes Δ are greater than the corresponding uncertainty in the 1983 fit: $\bar{\nu}_t(235)$ and $\bar{\nu}_t(241)$. Gwin's higher value for $\bar{\nu}_p(241)/\bar{\nu}_p(252)$ when combined with the single other measured value resulted in a clear increase in $\bar{\nu}_t(241)$ to 2.9461±0.0056.

It is of interest that the statistical self-consistency of the fitting process was improved when the three new sets of values were included in the fit. As was stated on p. 395 of our paper, we had found the goodness-of-fit parameter, χ^2, to be only 85.8 for the 97 degrees of freedom available. We had observed that such a result might be taken to mean that the input errors had a tendency to be unduly large. With the present fit, however, χ^2=99.3 for the 98 degrees of freedom; and thus the input errors are just the right size. We had not sufficiently allowed for the breadth of the χ^2 distribution!

We are grateful to Dr. E. J. Axton for a table of his fitted values[12] that take into account both 2200 m/s and Maxwellian input data. His values are thus directly comparable with those of other evaluators, and we use them here in a repeat of the history of thermal constant evaluations. Tables 2-5 below are the same as Tables 30-34 of our paper except that Axton's newer values replace his 2200 m/s values.

The most striking aspect of the last columns of these tables, which show the range of variation among the various evaluations, is the 26%-34% range of scattering cross sections. This is in large part an artifact, despite considerable differences among the different evaluators. (We ourselves have produced the extrema in three of the four tables because we have chosen not to include data on the scattering of neutrons by atoms bound in crystalline structures). Nevertheless, σ_s appears in the fitting process only as a small subtractive quantity in the relation $\sigma_a=\sigma_t-\sigma_s$, which is the most direct way to calculate σ_a. Here it is the difference in barns, not in percent, that counts. These differences, not exceeding 4 barns, are less than 1% of σ_a. Ranges of up to 7% occur with σ_γ and with α, and those truly reflect the historic difficulties in measuring these two quantities. Other quantities appear to be agreed upon within about 1% by all evaluators. It is pleasing to see that the two most recent evaluations, Axton's and ours, agree very well.

The present work was supported by the U.S. Department of Energy.

Table 1

Least-Squares fit of 2200 m/sec Constants
A comparison of the 1983 Fit and the present Fit

Quantity	^{233}U	Δ	^{235}U	Δ	^{239}Pu	Δ	^{241}Pu	Δ
σ_s(b)	12.6±0.3	-0.0	14.0±0.5	-0.1	7.3±0.4	-0.0	9.1±1.0	-0.0
σ_a(b)	574.7±1.0	+0.4	680.9±1.1	+0.5	1017.3±2.9	+0.7	1369.4±7.7	+1.6
σ_f(b)	529.1±1.2	+0.5	582.6±1.1	+0.3	748.1±2.0	+0.1	1011.1±6.2	-1.4
σ_γ(b)	45.5±0.7	-0.1	98.3±0.8	+0.3	269.3±2.2	+0.6	358.2±5.1	+2.9
g_a	0.9996±0.0011	+0.0002	0.9788±0.0008	+0.0000	1.0784±0.0024	-0.0001	1.0442±0.0020	-0.0001
g_f	0.9955±0.0015	+0.0002	0.9761±0.0012	+0.0005	1.0558±0.0023	+0.0003	1.0440±0.0049	+0.0015
η	2.2957±0.0040	+0.0002	2.0751±0.0033	+0.0024	2.1153±0.0052	+0.0017	2.1686±0.0080	+0.0014
α	0.0861±0.0015	-0.0002	0.1687±0.0015	+0.0004	0.3600±0.0032	+0.0007	0.3543±0.0057	+0.0034
$\bar{\nu}_t$	2.4933±0.0039	-0.0002	2.4251±0.0034	+0.0036	2.8768±0.0057	+0.0039	2.9369±0.0073	+0.0092

$^{252}Cf\ \bar{\nu}_t = 3.7675\pm0.0040$ Δ=±0.0007

Table 2

2200 m/s Thermal Constants for ^{233}U

Quantity	Westcott (1965)	Hanna (1965)	Steen (1972)	Lemmel (1975/82)	Axton (1984)	ENDF-V	Present (1983)	% Range $\frac{\text{(Max-Min)}^{+}}{\text{Present}}$
g_a	---	0.9965 ±0.0013	0.9990	1.0008 ±0.0018	0.9996 ±0.0011	0.9990	0.9996 ± 0.0011	0.4
g_f	---	0.9950 ±0.0021	0.9966	0.9967 ±0.0017	0.9952 ±0.0015	0.9966	0.9955 ± 0.0015	0.2
σ_s	---	10.7 ± 1.8	14.4 ± 4.3	13.3* ± 0.7	13.3* ± 0.9	12.6	12.6 ± 0.3	29.4
σ_a	576.3 ± 2.3	577.6 ± 1.8	571.0 ± 2.5	575.2 ± 1.3	575.1 ± 1.3	574.5	574.7 ± 1.0	1.1
σ_f	527.7 ± 2.1	530.6 ± 1.9	525.1 ± 2.4	529.9 ± 1.4	529.6 ± 1.4	528.7	529.1 ± 1.2	1.3
σ_γ	48.6 ± 1.5	47.0 ± 0.9	45.9 ± 0.2	45.3 ± 0.9	45.5 ± 0.7	45.8	45.5 ± 0.7	6.8
η	2.284 ±0.008	2.2844 ±0.0063	2.297 ±0.007	2.283 ±0.006	2.2979 ±0.0111	2.296	2.2957 ± 0.0040	0.6
α	0.0921 ±0.0029	0.0885 ±0.0018	0.0874 ±0.0005	0.086 ±0.002	0.0859 ±0.0015	0.0866	0.0866 ± 0.0015	7.1
$\bar{\nu}_t$	2.494 ±0.069	2.474 ±0.060	2.498 ±0.008	2.479 ±0.006	2.4952 ±0.0046	2.495	2.4933 ± 0.0039	0.8
$\bar{\nu}_t$ (252)	3.772 ±0.015	3.765 ±0.012	3.783 ±0.014	3.746 ±0.009	3.7656 ±0.0049	3.766	3.7675 ± 0.0040	1.0

+ – ENDF/B-V values were not considered in estimating the % range.

* – The σ_s corresponds to liquid sample values

Table 3

2200 m/s Thermal Constants for ^{235}U

Quantity	Westcott (1965)	Hanna (1969)	Leonard (1976)	Lemmel (1975/82)	Axton (1984)	ENDF-V	Present (1983)	% Range (Max-Min)+ / Present
g_a	---	0.9787 ±0.0010	0.9782	0.9797 ±0.0025	0.9787 ±0.0008	0.9781	0.9788 ±0.0008	0.2
g_f	---	0.9766 ±0.0016	0.9775 ±0.0011	0.9758 ±0.0014	0.9762 ±0.0012	0.9775	0.9761 ±0.0012	0.2
σ_s	---	17.6 ± 1.5	14.7	16.1* ± 1.1	16.4* ± 1.1	14.7	14.0 ± 0.5	25.7
σ_a	679.9 ± 2.3	678.5 ± 1.9	681.9	680.9 ± 1.7	681.2 ± 1.4	681.9	680.9 ± 1.1	0.5
σ_f	579.5 ± 2.0	580.2 ± 1.8	583.5 ± 1.7	583.5 ± 1.3	582.7 ± 1.2	583.5	582.6 ± 1.1	0.5
σ_γ	100.5 ± 1.4	98.3 ± 1.1	98.4 ± 0.8	97.4 ± 1.6	98.4 ± 0.8	98.4	98.3 ± 0.8	2.2
η	2.071 ±0.007	2.0719 ±0.0060	2.0713 ±0.0025	2.071 ±0.006	2.0794 ±0.0086	2.085	2.0751 ±0.0033	0.4
α	0.1734 ±0.0025	0.1694 ±0.0021	0.1686 ±0.0014	0.167 ±0.003	0.1689 ±0.0015	0.1686	0.1687 ±0.0015	2.8
$\bar{\nu}_t$	2.430 ±0.008	2.4229 ±0.0066	2.4205	2.416 ±0.005	2.4308 ±0.0040	2.437	2.4251 ±0.0034	0.6
$\bar{\nu}_t$ (252)	3.772 ±0.015	3.7653 ±0.0012	---	3.746 ±0.009	3.7656 ±0.0049	3.766	3.7675 ±0.0040	1.0

+ ENDF/B-V values were not considered in estimating the % range.
* The σ_s corresponds to liquid sample values

Table 4

2200 m/s Thermal Constants for ^{239}Pu

Quantity	Westcott (1965)	Hanna (1969)	Leonard (1981)	Lemmel (1975/82)	Axton (1984)	ENDF-V	Present (1983)	% Range $\frac{(Max-Min)^{+}}{Present}$
g_a	---	1.0752 ±0.0030	1.0762	1.0808 ±0.0039	1.0782 ±0.0024	1.0764	1.0784 ±0.0024	0.5
g_f	---	1.0548 ±0.0030	1.0535 ±0.0015	1.0555 ±0.0024	1.0562 ±0.0023	1.0582	1.0558 ±0.0023	0.3
σ_s	---	8.5 ±2.0	6.6 ±0.7	8.0* ±1.0	7.9* ±1.0	8.0	7.3 ±0.4	26.0
σ_a	1008.1 ± 4.9	1012.9 ± 4.1	1028.6 ± 5.1	1011.2 ± 4.1	1018.0 ± 3.0	1011.9	1017.3 ± 2.9	2.0
σ_f	742.4 ± 3.5	741.6 ± 3.1	754.8 ± 4.5	744.0 ± 2.5	747.8 ± 2.0	741.7	748.1 ± 2.0	1.8
σ_γ	265.7 ± 3.7	271.3 ± 2.6	273.8 ± 2.7	267.2 ± 3.3	270.2 ± 2.2	270.2	269.3 ± 2.2	3.0
η	2.114 ±0.010	2.1085 ±0.0066	2.1110 ±0.0081	2.106 ±0.007	2.1142 ±0.0118	2.119	2.1153 ±0.0052	0.4
α	0.3580 ±0.0054	0.3659 ±0.0039	0.3627 ±0.0043	0.359 ±0.005	0.3614 ±0.0031	0.3643	0.3600 ±0.0032	2.2
$\bar{\nu}_t$	2.871 ±0.0014	2.8799 ±0.0090	2.8766 ±0.0125	2.862 ±0.008	2.8781 ±0.0058	2.891	2.8768 ±0.0057	0.6
$\bar{\nu}_t$ (252)	3.772 ±0.015	3.765 ±0.012	---	3.746 ±0.009	3.7656 ±0.0049	3.766	3.7675 ±0.0040	0.7

+ ENDF/B-V values were not considered in estimating the % range.
* The σ_s corresponds to liquid sample values

Table 5

2200 m/s Thermal Constants for ^{241}Pu

Quantity	Westcott (1965)	Hanna (1969)	Leonard (1981)	Lemmel (1975/82)	Axton (1984)	ENDF-V	Present (1983)	% Range (Max-Min)+ / Present
g_a	---	1.0376 ±0.0 [illegible]	---	1.0392 ±0.0028	1.0441 ±0.0019	1.043	1.0442 ±0.0020	0.6
g_f	---	1.0486 ±0.0053	---	1.0442 ±0.0048	1.0452 ±0.0049	1.0452	1.0440 ±0.0049	0.4
σ_s	---	12.0 ± 2.6	11.6	12.0* ± 2.6	12.2* ± 2.6	11.0	9.1 ±1.0	34.1
σ_a	1391 22	1375.4 ± 8.6	1368.5	1378 ±0.09	1371.8 ± 7.8	1376.4	1369.4 ± 7.7	1.6
σ_f	1009 9	1007.3 ± 7.2	1003.8	1015 ±0.07	1011.7 ± 6.2	1015.0	1011.1 ± 6.2	1.1
σ_γ	382 21	368.1 ± 7.8	364.7	267.2 ± 3.3	360.1 ± 4.6	361.4	358.2 ± 5.1	6.6
η	2.154 ±0.036	2.149 ±0.014	2.166	2.155 ±0.010	2.1684 ±0.0245	2.178	2.1686 ±0.0080	0.9
α	0.379 ±0.021	0.3654 ±0.0090	0.3633	0.357 ±0.007	0.3559 ±0.0051	0.3560	0.3543 ±0.0057	7.0
$\bar{\nu}_t$	2.969 ±0.023	2.934 ±0.012	2.9528	2.924 ±0.010	2.9402 ±0.0063	2.953	2.9369 ±0.0073	1.5
$\bar{\nu}_t$ (252)	3.772 ±0.015	3.765 ±0.012	---	3.746 ±0.009	3.7656 ±0.0049	3.766	3.7675 ±0.0040	1.0

+ ENDF/B-V values were not considered in estimating the % range.
* The σ_s corresponds to liquid sample values

References

1. Divadeenam, M., and Stehn, J. R. (1984), Ann. of Nucl. Energy, 11, 375.

2. Gwin, R., Spencer, R. R., and Ingle, R. W. (1984), Nucl. Sci. Engng. 87, 381.

3. Gwin, R. et al, (1978), ORNL/TM-6246; (1981), ORNL/TM-7988.

4. Axton, E. J. (1984), private communication, preprint submitted to Metrolegia.

5. Gwin, R. and Magnuson, D. W. (1962), Nucl. Sci. Engng. 12, 364.

6. Magnuson, D.W. (1971), Nucl. Sci. and Engng. 44, 266.

7. Gwin, R., (1976), Nucl. Sci. and Engng. 61, 428.

8. Gwin, R., (1984), private communication.

9. Ullo, J.J. and Hardy, Jr., J. (1977), WAPD-TM-1299.

10. Hardy, Jr., J., (1984), private communication.

11. Mughabghab, S. F., Divadeenam, M. and Holden, N. E., (1981), Neutron Cross Sections: Vol. 1, Neutron Resonance Parameters and Thermal Cross Sections, Part A, Academic Press, N.Y.