EVALUATION OF THE ^{233}U NEUTRON CROSS SECTIONS IN THE RESOLVED RESONANCE ENERGY RANGE

L. C. Leal,* H. Derrien, K. H. Guber,** J. A. Harvey, and N. M. Larson

Oak Ridge National Laboratory, P. O. Box 2008, Oak Ridge, TN 37831 USA

A resonance analysis of the ^{233}U data in the neutron energy range from thermal to 600 eV were done with the SAMMY computer code. The analysis included the most recent high-resolution neutron transmission and fission data in particular those data measurements performed at ORELA. The Reich-Moore resonance formalism and the Bayes' approach of the SAMMY code were used to analyze the experimental data leading to a set of 769 s-wave resonances for which 738 resonances are in the energy range from thermal to 600 eV and 31 resonances placed as negative energies and above 600 eV. Benchmark calculations were done to test the performance of the ORNL ^{233}U evaluation and comparisons were done with results of calculations obtained with current ^{233}U evaluation on the ENDF/B-VI library.

I. INTRODUCTION

The first multilevel-multichannel resonance analyses of the ^{233}U neutron cross sections were performed by Moore and Reich[1] and by Vogt[2] in the energy region below 12 eV. Bergen and Silbert[3] extended the analysis to the energy range of 20 eV to 60 eV. These analyses used both the single level and multilevel-multichannel formalism; It was shown that the variation of the ratio of the capture cross section to the fission cross section, the α value, could not be reproduced by the single level parameters. A more extensive work was performed by Reynolds and Steiglitz[4] who used the least-squares fitting code MULTI[5] for the analysis of the fission and capture cross sections of Weston *et al.*[6] in the energy region from thermal to 60 eV. The resonance parameters of Reynolds and Steiglitz evaluation were converted to Adler-Adler parameters by deSaussure with the code POLLA for the ENDF/B-V library and are still used in the current version of the ENDF/B-VI. A single level Breit-Wigner and Adler-Adler analyses of the ^{233}U neutron cross sections were also performed by Kolar *et al.*,[7] Cao *et al.*,[8] and Nizamuddin.[9] The results of the single level analysis of Nizamuddin *et al*. in the energy range from thermal to 100 eV were used with a large background contribution in the first version of ENDF/B-V and JENDL-3. None of these evaluations proved to be satisfactory. In the early 90s an R-matrix evaluation of the ^{233}U cross section was done by Derrien[10] at the Japan Atomic Energy Commission (JAERI, Tokai-Mura, Japan) using the SAMMY computer code. Due to poor experimental resolution of the available data in the high energy range, the analysis was performed only up to 150 eV. The JAERI evaluation, which is used in the current version of the Japanese Evaluated Nuclear Data Library (JENDL) and of the European file JEF, brought a large improvement compared to the previous evaluations by allowing accurate calculations of the cross sections over the energy range up to 150 eV. The present evaluation extends the energy range up to 600

* Phone 865-574-5281, fax 865-574-3527, email leallc@ornl.gov

**TUV Energie- und Systemtechnik GmbH Baden Wurtemberg, Postfach 10 32 62 , D-68032 Mannheim, Germany

eV and improves the accuracy of the resonance parameters, taking advantage of the excellent experimental conditions of new ORNL neutron transmission and fission cross data.

II. EXPERIMENTAL DATA DESCRIPTION

Several experimental data were used in the ^{233}U evaluation. To enable a SAMMY analysis of the ^{233}U cross sections at energies above 150 eV two high resolution measurements were performed at the Oak Ridge Electron Linear Accelerator (ORELA). Neutron transmission measurements with samples cooled to 11 K to reduce the Doppler effect, at a flight path of 79.8 m, were done by Guber *et al.*[11] The transmission measurements done with the sample cooled to 11 K has led to a reduction of the width of the resonances by a factor of two compared with the experiments at room temperature. Two sets of measurements were done with different sample thicknesses: (1) a set of measurements with a sample of 0.00298 at/b in the energy region 0.5 eV to 80 eV; (2) a set of measurements of 0.0119 at/b in the energy range 6 eV to 300 keV. In addition to the transmission measurements, two sets of fission cross section measurements at a flight path of 80 m were also carried out by Guber *et al.*[12] in the energy ranges of 0.5 to 80 eV with a Cd filter and another in the energy range from 10 eV to 700 keV with a ^{10}B filter, respectively. The fission cross section measurements at the 80 m flight-path have much better resolution than of any previous fission measurements. These ORELA transmission and fission measurements were the primary data used in the ^{233}U evaluation in the energy range from 0.5 to 600 eV. Twelve measurements were included in the evaluation as shown in **Table 1**. Four of these measurements are the ORNL transmission and fission cross section done by Guber *et al.* as explained above, transmission measurements done by Harvey *et al.*[13] in 1979, transmission measurements done by Moore *et al.*[14] in 1960, and transmission measurements done by Pattenden and Harvey[15] in 1963. There are two sets of simultaneous measurements of capture and fission data performed by Weston *et al.*[16] in 1970. There are fission cross-section measurements done by Blons[17] in 1973, fission measurements done by Deruyter and Wagemans[18] done in 1974, and Wagemans *et al.*[19] in 1998.

In addition to the microscopic data (from TOF measurements) a variety of integral quantities are available within SAMMY.[20] These integral quantities are calculated by integrating over the microscopic absorption, fission and capture cross sections. The integral quantities used in the ^{233}U evaluation were the Westcott factor, the K_1 value, the resonance integral I_x, and the capture to fission ratio, the α ratio. These quantities are defined as follows:

1. Westcott factor:
$$g_w = \frac{2}{\sqrt{x}} \frac{\sigma_x}{\sigma_{0x}}$$

where $_{0x}$ and σ_{0x} are the Maxwellian-averaged cross sections and the cross sections at 0.0253 eV.

2. K_1 factor
$$K_1 = \nu\sigma_{0f} g_f - \sigma_{0\alpha} g_a$$

3. Resonance Integral
$$I_x = \int_{0.5eV}^{20MeV} \frac{\sigma_x}{E} dx$$

4. α Ratio $$\alpha = \frac{I_c}{I_f}$$

Some of the evaluated integral values for ^{233}U are given in **Table 2**.

III. RESULTS OF THE ANALYSIS

The analysis of the ^{233}U transmission and cross sections provided a set of resonance parameters that describe the experimental cross sections very well up to 600 eV. Comparison of the experimental data with calculations performed using the resonance parameters are shown in **Figures 1, 2, and 3**. Figure 1 shows a comparison of the total cross sections in the neutron energy region from 0.01 eV to 1 eV. The data are from Harvey *et al*. (bottom curve), Moore *et al*. (middle curve), and Pattenden *et al*. (top curve). For clarity of the display the data of Moore *et al*. was multiplied by 10 and the Pattenden *et al*. data was multiplied by 100. Figure 2 shows a comparison of the fission and the capture cross sections in the energy range from 0.01 eV to 1 eV. The data are, from bottom to top, Weston *et al*. capture, Weston *et al*. fission, Wagemans *et al*. fission (multiplied by 10), and Deruyter *et al*. fission (multiplied by 100). The total, fission, and capture thermal values are shown in **Table 3**. The Axton standard values and the ENDF/B-VI standard values are also shown in Table 3.

Figure 3 shows a comparison for the total and fission cross sections in the energy range from 50 eV to 75 eV. The experimental data are, from the bottom of the figure, the fission data of Weston *et al*. multiplied by 0.09, the fission data of Blons *et al*. multiplied by 0.3, the ORELA fission of Guber *et al*. and the ORELA total cross section of Guber *et al*. multiplied by a factor of 3. Figure 4 shows a comparison of the total and fission cross sections in the energy range 550 eV and 600 eV. The experimental data are, from the bottom of the figure, the fission cross section of Weston *et al*. multiplied by 0.09, the fission cross section of Blons *et al*. multiplied by 0.3 and the ORELA fission of Guber *et al*., and the ORELA total cross section of Guber *et al*. multiplied by 3. As can be seen the theoretical calculation provides an excellent representation of the experimental data.

IV. BENCHMARK CALCULATIONS

Benchmark calculations were done to test the performance of the ORNL ^{233}U evaluation and comparisons were made with calculations obtained with the current ENDF/B-VI library ^{233}U evaluation. The evaluations were used to calculate various benchmark systems in the thermal energy region, intermediate energy region, and high energy region. The ^{233}U library was obtained by replacing the resonance region evaluation with the present ORNL ^{233}U resonance evaluation. The library obtained will be referred to as the ORNL library. Benchmark calculations were performed using the ORNL and ENDF data library and the multiplication factors (k_{eff}) were obtained. The selected energy group structure used in the calculations is the 199-group VITAMIN-B6 cross-section library.[21] The data libraries were processed using the NJOY code system, whereas the benchmark calculations were performed with the Monte Carlo code KENO.Va. A total of 27 benchmark calculations were performed, namely, 6 benchmarks in the thermal region, 11 benchmarks in the intermediate energy region and 10 benchmarks in the fast energy region. The six thermal benchmarks are available from the Cross Section Evaluation Working Group (CSEWG). The CSEWG thermal benchmarks, the ORNL series, are unreflected spheres of ^{233}U with H/U ratio in the range of 1533 to 1986. The 11 benchmarks in the intermediate energy region, the ^{233}U-SOL-INTER-001 series also known as *Falstaff*, are from the ICSBEP.[22] They are aqueous solutions of ^{233}U in the form of uranyl-fluoride in spheres with reflectors of Be, CH_2 and $BeCH_2$ composites. The *Falstaff* benchmarks were done in the late 1950's using 8 types of stainless steel spheres with an inner radius varying from 7.87 cm to 12.45 cm. The 10 fast critical benchmark experiments are the 9 CSEWG ^{233}U-MET-FAST in which the ^{233}U-MET-FAST-001 is known as JEZEBEL-23 and the FLATTOP-23 benchmark. They are spheres of highly enriched ^{233}U (98.2 wt %) either unreflected, as for instance ^{233}U-MET-FAST-001 also known as JEZEBEL-2, or spheres with reflectors such as highly enriched uranium, nickel, tungsten, or beryllium.

The calculated k_{eff} obtained with the KENO.Va code are shown in **Tables 4–6** for the ORNL and ENDF libraries. The results of the k_{eff} for the thermal critical benchmark experiments are displayed in Table 4. The results shown in this table indicate that the calculations using the two libraries are compatible, with the ENDF results being lower than the ORNL thermal benchmarks results. The resulting k_{eff} shown in Table 5 are very close for the two cross section libraries used, namely, ENDF and ORNL data libraries. The results of the k_{eff} for the fast critical benchmark experiments are displayed in Table 6, which indicates that the k_{eff} calculated using the ORNL evaluations are greatly improved relative to the ENDF results.

V. Conclusions

An R-matrix evaluation of the ^{233}U transmission and neutron cross sections up to 600 eV has been completed using the SAMMY computer code. High resolution data measurements at ORELA, in particular transmission measurements performed with a target sample cooled to 11 K and fission cross section measurements, were used in the evaluation for the determination of resonance energies above 150 eV up to 600 eV. The evaluation has been tested by performing calculations of critical benchmark experiments and good results were obtained.

Acknowledgment

This work was sponsored by the Office of Environmental Management, U.S. Department of Energy, under contract DE-AC05-00OR22725 with UT-Battelle, LLC. The authors are particularly indebted to Hoyt Johnson, DOE, Washington, DC, for his support.

References

1. M. S. Moore and C. W. Reich, *Phys. Rev.* **118,** 718(1960).
2. E. Vogt, *Phys. Rev*. **118**, 524(1960).
3. D. W. Bergen and M. G. Silbert, *Phys. Rev.*, **166**, 1178(1960).
4. J.T. Reynolds and M.G. Steiglitz, Knolls Atomic Power Laboratory Report KAPL-M-7323 (1973).
5. G. F. Auchampaugh, *MULTI, A FORTRAN Code for Least-Squares Shape Fitting of Neutron Cross Section Data Using the Reich-Moore Multilevel Formalism,* LA-5473-MS, Los Alamos Scientific Laboratory, 1974.

6. L. W. Weston, R. Gwin, G. De Saussure, R. R. Fullwood, R. W. Hockenbury, *Nucl. Sci. Eng.,* 34, 1 (1968).

7. W. Kolar, G. Carraro and G. Nastri, *Proc. 2nd Int. Conf. On Nuclear Data for Reactors, Helsinki, June 15-19, 1970,* Vol.1, p.387 (1970).

8. M. G. Cao, E. C. Migneco, J. P. Theobald and M. Merla, *Proc. 2nd Int. Conf. On Nuclear Data for Reactors, Helsinki, June 15-19, 1970,*Vol.1, p.419 (1970).

9. S. Nizamuddin, J. Blons, *Nucl. Sci. Eng.,* **54**, 116 (1974).

10. H. Derrien, *J. of Nuc. Sci. and Tech*., **31**, 5, 379, May 1994.

11. K. H. Guber, R. R. Spencer, L. C. Leal, P. E. Koehler, J. A. Harvey, R. O. Sayer, H. Derrien, T. E. Valentine, D. E. Pierce, V. M. Cauley, and T. A. Lewis, submitted to *Nucl. Sci. Eng.* ***139***, (2001).

12. K. H. Guber, R. R. Spencer, L. C. Leal, J. A. Harvey, N. W. Hill, G. Dos Santos, R. O. Sayer, and D. C. Larson, *Nuc. Sci. Eng*. **135**, 1(2000).

13. J. A. Harvey, C. L. Moore, N. W. Hill, *Proc. Int. Conf. on Neutron Cross Section for Technology, Knoxville, Oct. 22-26, 1979,* NBS Special Publication 594, p. 690 (1980).

14. M. S. Moore, M. G. Miller and O. D. Simpson, *Phys. Rev*., **118**, 714 (1960).

15. N. J. Pattenden and J. A. Harvey, *Nuc. Sci. Eng.,* **17**, 404 (1963).

16. L. W. Weston, R. Gwin, G. De Saussure, R. W. Ingle, J. H. Todd, C. W. Craven, R. W. Hockenbury, R. C. Block, *Nuc. Sci. Eng.* 42, 143 (1970).

17. J. Blons, *Nucl. Sci. Eng.,* 51, 130 (1973).

18. A. J. Deruyter and C. Wagemans, *Nucl. Sci. Eng.* 54, 423 (1974)

19. C. Wagemans, P. Shillebeeckx, A. J. Deruyter and R. Barthelemy, *Proc. Int. Conf. on Nuclear Data for Science and Technology, Mito, May 30-June 3, 1988*, P. 91 (1988).

20. N. M. Larson, *Updated User' Guide for SAMMY: Multilevel R-Matrix Fits to Neutron Data Using Bayes' Equations*, ORNL/TM-9179/R4 (December 1998). See also ORNL/TM-9170/R5.

21. J. E. White, R. Q. Wright, D. T. Ingersoll, R. W. Roussin, N. M. Greene, and R. E. MacFarlane, "VITAMIN-B6: A Fine-Group Cross Section Library Based on ENDF/B-VI for Radiation Transport Applications," pp. 733-36 in *Nuclear Data for Science and Technology: Proceedings of the International Conference, Gatlinburg, Tennessee, May 9-13, 1994*, ed., J. K. Dickens, Oak Ridge National Laboratory, 1995.

22. *International Handbook of Evaluated Criticality Safety Benchmark Experiments*, NEA/NSC/DOC (95) 03, Nuclear Energy Agency, Organization for Economic Cooperation and Development (Sep. 1999).

Table 1. Selected Measurements for ^{233}U evaluation

Author	Energy Region Analyzed (eV)	Main Features
Moore *et al*., 1960	0.020 - 15.0	Transmission; chopper, TOF 15.7 m Sample 0.0037 and 0.0213 at/b
Pattenden and Harvey, 1963	0.080 - 15.0	Transmission; chopper, TOF 45 m Sample 0.00057, 0.00308, 0.01219 at/b
Weston *et al*., 1968	1.0 - 600.0	Simultaneous measurements of capture and fission, Linac TOF 25.2 m
Weston *et al*., 1968	0.020 - 1.0	Simultaneous measurements of capture and fission, Linac TOF 25.6 m
Blons, 1973	4.0 - 600.0	Fission, Linac, TOF 50.1 m, Sample at Liquid Nitrogen Temperature
Deruyter and Wagemans, 1974	0.020 - 15.0	Fission, Linac, TOF 8.1 m
Harvey *et al*., 1979	0.020 - 1.2	Transmission, Linac, TOF 17.9 m Sample 0.00605 and 0.0031 at/b
Wagemans *et al*., 1988	0.002 - 1.0	Fission, Linac, TOF 8.1 m
Guber *et al*., 1998	1.0 - 80.0	Transmission, Linac, TOF 80 m Cd filter, Sample Temperature 11 K Sample thickness 0.00298 at/b
Guber *et al*., 1998	7.0 - 600.0	Transmission, Linac, TOF 80 m ^{10}B filter, Sample Temperature 11 K Sample thickness 0.0119 at/b
Guber *et al*., 1998	1.0 - 80.0	Fission, Linac, TOF 80 m Cd filter
Guber *et al*., 1998	7.0 - 600.0	Fission, Linac, TOF 80 m ^{10}B filter

Table 2. Evaluated Integral Quantities

Quantity	ENDF/B-VI Standard	Axton Standard	BNL	Present Work
g_a	0.9996 ± 0.0011	0.9995 ± 0.0011	0.9996 ± 0.0015	1.00325
g_f	0.9955 ± 0.0014	0.9955 ± 0.0014	0.9955 ± 0.0011	1.00045
I_a			897 ± 20	917.45
I_f			760 ± 17	777.82
K_1	742.60 ± 2.40	742.25 ± 2.37	738	746.77

Table 3. Thermal Values of the Cross Section (0.0253 eV)

Data	ORNL Evaluation	Axton Standard	ENDF/B-VI Standard
Fission	530.70	530.70 ± 1.34	531.14 ± 1.33
Capture	45.22	45.52 ± 0.70	45.51 ± 0.68
Elastic	12.18	12.19 ± 0.67	12.13 ± 0.66

Table 4. Test of the ^{233}U evaluation with thermal energy benchmarks using KENO.Va code

199-group (VITAMIN/B-6)		
Benchmark	ENDF/B-6	ORNL
ORNL-5	0.9964 ± 0.0008	1.0006 ± 0.0009
ORNL-6	0.9962 ± 0.0009	0.9997 ± 0.0008
ORNL-7	0.9948 ± 0.0008	0.9996 ± 0.0008
ORNL-8	0.9963 ± 0.0008	1.0000 ± 0.0009
ORNL-9	0.9950 ± 0.0008	0.9998 ± 0.0007
ORNL-11	0.9951 ± 0.0005	0.9987 ± 0.0006

Table 5. Test of the ^{233}U evaluation with intermediate energy benchmarks using KENOV.a code

199-group (VITAMIN/B-6)		
Sphere No.	ENDF/B-6	ORNL
1	0.9899 ± 0.0003	0.9908 ± 0.0003
2	0.9855 ± 0.0003	0.9858 ± 0.0003
3	0.9859 ± 0.0003	0.9866 ± 0.0003
3	0.9946 ± 0.0003	0.9963 ± 0.0003
4	0.9892 ± 0.0003	0.9898 ± 0.0003
4	0.9884 ± 0.0003	0.9894 ± 0.0003
5	0.9858 ± 0.0003	0.9874 ± 0.0003
5	1.0019 ± 0.0003	1.0032 ± 0.0003
5	0.9831 ± 0.0003	0.9834 ± 0.0003
6	0.9823 ± 0.0003	0.9842 ± 0.0003
6	0.9833 ± 0.0003	0.9842 ± 0.0003

Table 6. Test of the ^{233}U evaluation with fast energy benchmarks using KENO.Va code

199-group (VITAMIN/B-6)		
Benchmark	ENDF/B-6	ORNL
^{233}U-MET-FAST-001 (JEZEBEL-23)	0.9983 ± 0.0010	0.9974 ± 0.0010
^{233}U-MET-FAST-002-a	0.9931 ± 0.0008	0.9997 ± 0.0010
^{233}U-MET-FAST-002-b	0.9939 ± 0.0010	0.9979 ± 0.0009
^{233}U-MET-FAST-003-a	0.9956 ± 0.0010	0.9979 ± 0.0011
^{233}U-MET-FAST-003-b	0.9946 ± 0.0010	0.9977 ± 0.0010
^{233}U-MET-FAST-004-a	0.9961 ± 0.0010	0.9999 ± 0.0011
^{233}U-MET-FAST-004-b	0.9952 ± 0.0009	0.9985 ± 0.0009
^{233}U-MET-FAST-005-a	1.0022 ± 0.0010	0.9969 ± 0.0009
^{233}U-MET-FAST-005-b	1.0024 ± 0.0010	1.0037 ± 0.0010
FLATTOP-23	1.0024 ± 0.0010	1.0048 ± 0.0010

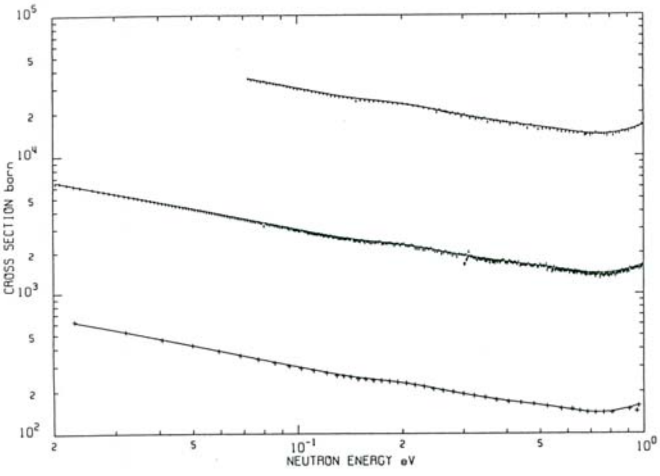

Figure 1. The total cross section in the neutron energy range 0.01 to 1 eV. The experimental data are represented by the error bars. The solid lines are the data calculated by the resonance parameters. The experimental cross sections are, from the bottom of the figure, Harvey *et al*. data, Moore *et al*. data (multiplied by 10) and Pattenden *et al*. data (multiplied by 100).

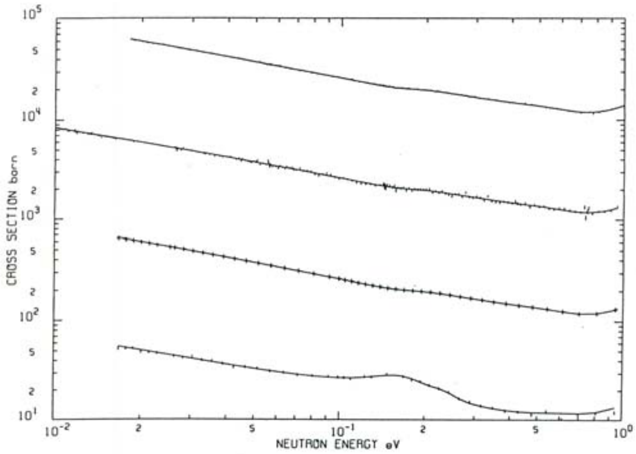

Figure 2. The fusion and capture cross sections in the energy range 0.01 to 1 eV. The experimental data points are represented by the error bars. The solid lines are the data calculated from the resonance parameters. The experimental cross sections are, from the bottom of the figure, Weston *et al*. capture, Weston *et al*. fission, Wagemans *et al*. fission (multiplied by 10), and Deruyter *et al*. fission (multiplied by 100).

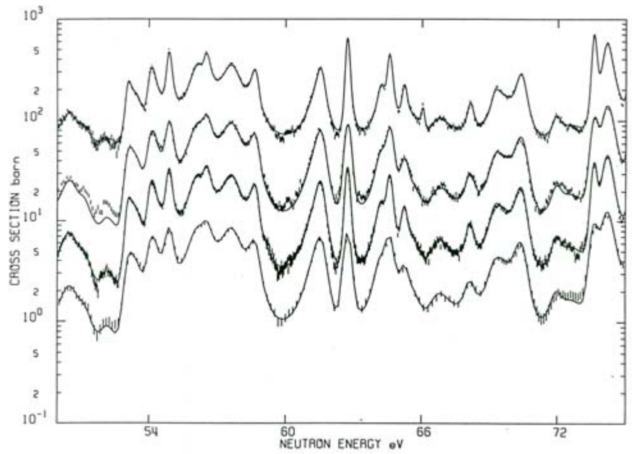

Figure 3. Total and fission cross section in the energy range 50 eV to 75 eV. The solid lines represent the cross sections calculated from the resonance parameters. The experimental data are, from the bottom of the figure: Weston *et al*. fission (multiplied by 0.09), Blons *et al*. fission (multiplied by 0.30), ORELA fission and ORELA total cross sections (multiplied by 3.0).

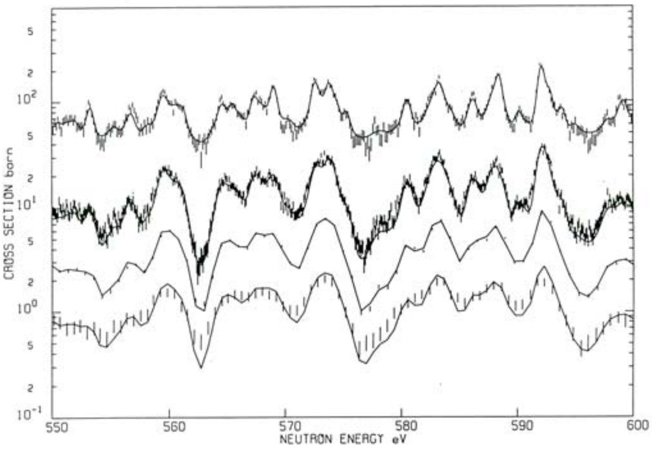

Figure 4. Total and fission cross sections in the energy range 550 eV to 600 eV. The solid lines represent the cross sections calculated from the resonance parameters. The experimental data are, from the bottom of the figure: Weston *et al.* (multiplied by 0.09), Blons *et al.* (multiplied by 0.30), ORELA fission cross sections and ORELA4 total cross section (multiplied by 3.0).