IEC - 142

Final Report on Evaluation of the ^{235}U Cross Sections

L. C. Leal, H. Derrien, R. Q. Wright, and N. M. Larson
January 10, 1996

INTRODUCTION

The intent of this report is to provide a description of the effort undertaken in the period from August to December 1995 in continuation of the reevaluation of the ^{235}U cross sections in the resolved energy range to address criticality safety problems. The various tasks accomplished are described; included are the following: An excellent representation has been obtained for the high resolution transmission (or total cross section), fission cross section, and capture cross section data, with a single set of resonance parameters covering the energy range from 0 to 2250 eV. In addition to the analysis of the differential data, extensive integral data tests have been performed to insure that the resonance parameters properly reproduce integral quantities, especially in the intermediate energy range which is of concern to criticality safety applications. Calculated and measured quantities show excellent agreement.

As part of the evaluation procedure, a preliminary version of the ^{235}U resonance parameter set was distributed to members of the Data Testing Committee of the Cross Section Evaluation Working Group (CSEWG). Several of those members processed the data and provided input and suggestions which were examined for inclusion in the final adjustment. After several iterations the ^{235}U evaluation was completed.

GENERAL DESCRIPTIONS

Parametric representation of neutron cross sections in the resonance range is the approach that best provides a way to characterize the resonance effects and the detailed structure of the cross sections in the resolved energy region. To obtain a single set of resonance parameters which represents all the cross section components of a given isotope in a given energy range, the evaluator must analyze different types of experimental data. The resonance parameters obtained in the differential analyses are used to provide cross section "data" for various neutronic applications (which include reactor analysis and design as well as criticality safety calculations). Results of calculations performed in the study of these nuclear systems are in general based on averaging the cross section data over the energy spectrum characteristic of the system under consideration. In addition to the differential data analysis, integral tests must be performed to assess whether the differential data are adequate for integral calculations. This report describes the differential and integral evaluation of the ^{235}U cross sections in the resolved energy range from 0 to 2250 eV, with a goal of resolving the capture-to-fission ratio which is of importance to the criticality safety problem. Results of this evaluation are expected to greatly improve predictability of the criticality safety margin for nuclear systems in which ^{235}U is present.

DIFFERENTIAL DATA EVALUATION

DATA SELECTION

To evaluate the ^{235}U cross sections in the energy range from 0 to 2250 eV, several high-resolution data sets were analyzed with the computer code SAMMY.[1] SAMMY is a multilevel multichannel R-matrix resonance analysis program based on the Bayes approach; the Reich-Moore formalism[2] was used for cross section generation. New features in SAMMY, such as its availability on an IBM/RISC6000 workstation, have proven invaluable in permitting use of a large number of resonance levels; thus the eleven disjoint resonance parameter sets in the current ENDF evaluation have now been replaced by one single set of parameters.

Various measurements were examined for inclusion in the evaluation of the ^{235}U cross sections; the selected measurements are shown in Table 1. The low energy data of Wagemans[3] were used to determine the cross section at thermal (0.0253 eV); these data sets include capture and fission cross sections as well as eta data (defined as $\eta = \nu\,\sigma_f/\sigma_a$). Below 1 eV the transmission data of Spencer[4] were used to determine both the shape of the total cross section and the value of the total cross section at thermal energy. Because of poor resolution at high energies the fission cross section data of Gwin[5] and Schrack[6] were used only below 20 eV. Three transmission data sets of Harvey[7] were used from 0.4 eV to 2250 eV to determine the shape of the total cross section; because they were high resolution, these transmission data were carefully analyzed with SAMMY to obtain the best fit to the total cross section. Two fission cross section data sets of Weston,[8] taken at two different flight paths, were utilized to determine the shape of the fission cross section from 14 eV to 2250 eV. To determine the shape of the capture cross section two sets of experimental data were used, data of de Saussure[9] and data of Perez.[10] The de Saussure data were used in the entire energy range (to 2250 eV) whereas the Perez data were used only below 200 eV (above this energy the data are given as averaged cross sections). Previous ^{235}U evaluations used the capture cross section data of de Saussure in the analyses only below 50 eV; in the present evaluation the higher-energy data have been found to be important in addressing the capture-to-fission ratio problem.

To obtain a set of resonance parameters that simultaneously fits several experimental data sets, in a typical SAMMY run the data are entered sequentially in arbitrary order. The resonance parameters obtained from the final run in the sequence give a reasonable fit for all data entered into the run. Convergence is achieved when the χ^2 of each run is decreased. In general the high-resolution data analyzed in the sequence (e.g., the transmission data of Harvey) serve as a reference with which the remaining data should be consistent. The capture cross section data of Perez was found to be consistent with the other data. However, the capture cross section data of de Saussure needed to be renormalized in order to be consistent with the others.

RESULTS OF THE DIFFERENTIAL ANALYSIS

General Comments

Neutron cross sections in the energy range from 0 to 2250 eV are represented by a single set of resonance parameters containing 3167 energy levels. There are fourteen bound levels which simulate the negative energy levels; these levels determine the shape of the cross section at low energy and describe also the effect of the potential cross section. Above 2250 eV fourteen energy levels were added to simulate the contribution from all higher-energy resonances. Together these twenty-eight levels give a good representation of the potential cross section in the energy range 0 to 2250 eV.

In the current ^{235}U evaluation in ENDF/B-VI[11] a different scattering radius is given for each of eleven disjoint sets of resonance parameters; however, in the present evaluation one single radius is used for the entire energy range. (This is more physically sound since R-matrix theory permits the scattering radius to vary with spin and parity but not with energy.) The scattering radii were determined by having SAMMY fit the Harvey transmission data, varying the radii, in twelve energy ranges from 22 eV to 1700 eV; the average radius obtained (9.602±0.050 F) was then used throughout the rest of the analysis.

Data Fitting for Energy E < 100 eV

The first several figures illustrate the excellent agreement between the cross section calculated with the evaluated ^{235}U resonance parameters and the experimental data. Solid lines represent the calculated results whereas either vertical lines or symbols represent the experimental data. Figure 1 shows the calculated η compared with measurements performed in the Central Bureau for Nuclear Measurements Electron Accelerator of Geel (Belgium)[12] and at the Institut Laue-Langevin reactor (ILL) at Grenoble.[13] Note that the shape of η agrees well with experiment; this agreement is important since it impacts calculation of the Doppler coefficient of reactivity in thermal reactors.[14] Figure 2 shows comparisons of theoretical and experimental fission and total cross sections in the energy range from 0.001 eV to 1.0 eV; for clarity some of the data were shifted upward as indicated in the figure. The data shown in Fig. 2 are fission cross section data of Wagemans, Gwin, Schrack, and the total cross section data of Spencer. As can be seen, the theoretical calculations reproduce the data very well at these low energies. In Figures 3, 4, and 5, the high-resolution transmission data of Harvey are shown up to 100 eV; the two transmission data sets (thicknesses 0.03269 atom/barn and 0.002335 atom/barn) taken at the 80-m flight path station were displaced by 0.5 and 0.75 respectively. Figures 6, 7, and 8 show the comparison of the calculated fission cross section with data of Perez, de Saussure, Gwin, Schrack, and Weston (18 m flight path) up to 100.0 eV. The Weston data are those taken at the 18-m flight path station. Figures 9, 10, and 11 show the theoretical capture cross section compared with the experimental data of Perez and de Saussure below 100.0 eV.

Data Fitting for Energies between 100 eV and 2250 eV

From 100 eV to 2250 eV the transmission data of Harvey taken at the 80-m flight path station were used to determine the total cross section. The fission data of Weston at the 18-m flight path were used up to 2250 eV; unfortunately the high resolution fission data of Weston at the 80-m flight path were not available above2000 eV. The capture data of Perez were used up to 200 eV; the capture data of de Saussure were utilized up to 2250 eV. Figure 12 shows comparisons of calculation and measurement of the total cross section, in the energy range from 100 eV to 200 eV. (Experimental total cross sections were derived from the transmission data assuming the sample thickness 0.03269 atoms/barn.) Also shown in Fig. 12 are the fission cross section of Weston for two flight paths (18 m and 86 m), the fission data of Perez, and the fission data of de Saussure. Comparisons of theoretical vs. experimental capture cross section data of Perez and de Saussure in the energy range 100 eV and 200 eV are shown in Fig. 13.

Figures 14 to 21 show comparisons of calculated vs. measured total cross sections of Harvey, two fission data sets of Weston, and capture data of de Saussure, in the energy range from 200 eV to 2000 eV. Figure 22 shows comparisons of the total cross section data of Harvey and the fission data of Weston for measurements on the 18-m flight path. As indicated in the plot, the data were displaced for clarity.

INTEGRAL TESTS

To evaluate the ability of the resonance parameters to generate pointwise and groupwise data for applications in integral calculations, several calculations were performed for a variety of benchmark systems with distinct characteristic energy-dependent neutron spectra. The set of resonance parameters in this evaluation impacts primarily systems with neutron spectra in the intermediate energy range which are important for criticality safety applications. The new evaluation addresses the capture-to-fission ratio in regard to the predictability of criticality safety margins for systems with intermediate energy spectra. The calculations of the effective multiplication factors, k_{eff}, for various benchmark systems are presented in Table 2. Two other results are also included in Table 2, those being the calculations corresponding to the ^{235}U evaluation in the ENDF/B-V library and the present ENDF/B-VI release 3 ^{235}U evaluation. The first five benchmarks are the ORNL thermal critical solution spheres, namely ORNL-1, -2, -3, -4, and -10. These are unreflected spheres of ^{235}U as uranyl nitrate and H_2O solutions. The L-series are benchmarks similar to the ORNL series except that they include both reflected and unreflected spheres of ^{235}U as uranyl fluoride and H_2O solutions. The BAPL-1, -2, and -3 benchmarks are 1.3 wt% enriched uranium-oxide rods in a triangular-pitch lattice. The HISS(HUG), UH3-UR, and UH3-NI assemblies are intermediate spectrum benchmarks. These benchmarks are very important for criticality safety applications.

Comparisons of calculations for the thermal ORNL spheres, L-series, and BAPL benchmarks, for the present ^{235}U evaluation and the evaluation in the ENDF/B-VI release 3, show practically no change in the calculated k_{eff} when compared with the release 3 evaluation. However, results for the three intermediate spectrum benchmarks, HISS(HUG), UH3-UR, and UH3-NI, are greatly improved relative to the earlier versions of ENDF/B. This change is significant with regard to fissile material storage and transportation applications.

The capture-to-fission ratio has also been addressed in the present ^{235}U evaluation. The fission resonance integral and the capture resonance integral calculated with the present evaluation are 275.65 barns and 140.35 barns, respectively, which lead to resonance α (capture-to-fission ratio) of 0.5092 compared to 0.513±0.015 obtained from integral measurements.[15]

SUMMARY

All available ^{235}U differential data below 2250 eV have been incorporated into a complete resonance parameter analysis, yielding a single set of resonance parameters; this one set provides reasonable agreement with experiment in all cases. These resonance parameters were then used for calculations of integral quantities, and comparisons made with integral measurements. A few minor adjustments were then made to the resonance parameters to improve the fit to integral data without degrading the fit to the differential data. The resulting resonance parameter set gives consistently good agreement with both the differential and the integral measurements.

Reference	Energy Range (eV)	Data
Wagemans (Geel/1988)	0.001 to 0.4	Fission at 8 m
Spencer (ORNL/1984)	0.01 to 1.0	Transmission at 18 m. Sample of 0.001468 atom/barn.
Gwin (ORNL/1984)	0.01 to 20.0	Fission at 25.6 m
Schrack (RPI/1988)	0.02 to 20.0	Fission 8.4 m
Harvey (ORNL/1986)	0.4 to 68.0	Transmission at 18 m. Sample cooled to 97 K. Sample of 0.03269 atom/barn.
Harvey (ORNL/1986)	4.0 to 2250.0	Transmission at 80 m. Sample cooled to 97 K. Samples of 0.002335 atom/barn and 0.03269 atom/barn.
Weston (ORNL/1984)	14.0 to 2250.0	Fission at 18.9 m
Weston (ORNL/1992)	100.0 to 2000.0	Fission at 86.5 m
de Saussure (RPI/1967)	0.01 to 2250.0	Capture at 25.45 m
Perez (ORNL/1972)	0.01 to 200.0	Capture at 39.7
Wartena (Geel/1987)	0.0018 to 1.0	η, Eta
Weigmann (ILL/1990)	0.0015 to 0.15	η, Eta

Table 1. Data used in the ^{235}U cross section evaluation

BENCHMARK	ENDF/B-V	ENDF/B-VI.3	NEW EVALUATION
ORNL-1	1.0007	0.9974	0.9972
ORNL-2	1.0005	0.9972	0.9970
ORNL-3	0.9975	0.9943	0.9940
ORNL-4	0.9989	0.9958	0.9955
ORNL-10	0.9993	0.9971	0.9970
L-7	1.0082	1.0006	1.0003
L-8	1.0088	1.0050	1.0046
L-9	1.0052	1.0020	1.0017
L-10	1.0062	0.9986	0.9981
L-11	1.0035	0.9997	0.9995
BAPL-1	0.9947	0.9975	0.9970
BAPL-2	0.9965	0.9976	0.9971
BAPL-3	0.9987	0.9983	0.9979
HISS(HUG)	1.0254	1.0133	1.0085
UH3-UR	1.0121	1.0102	1.0057
UH3-NI	1.0228	1.0176	1.0130

Table 2. ORNL k_{eff} Calculations

REFERENCES

1. N. M. Larson, "Updated Users' Guide for SAMMY: Multilevel R-matrix Fits to Neutron Data Using Bayes' Equation," ORNL/TM-9179, Martin Marietta Energy System, Inc., Oak Ridge Natl. Lab., (August 1984); see also ORNL/TM-9179/R1 (July 1985) and ORNL/TM-9179/R2 (June 1989).

2. C. W. Reich and M. S. Moore, Phys. Rev. 111, 929 (1958).

3. C. Wagemans at al., "Subthermal Fission Cross-Section Measurements for ^{233}U, ^{235}U, and ^{23}Pu," Int. Conf. Nuclear Data for Science and Technology, Mito, 1988;

4. R. R. Spencer, J. A. Harvey, N. W. Hill, and L. W. Weston, Nucl. Sci. Eng. **96**, 318 (1987).

5. R. Gwin, R. Spencer, R. W. Ingle, J. H. Todd, S. W. Scoles, Nucl. Sci. Eng. **88**, 37 (1984).

6. R. C. Schrack, "Measurement of the ^{235}U(n,f) Reaction from Thermal to 1 KeV," Int. Conf. Nuclear Data for Science and Technology, Mito, 1988.

7. Harvey, J. A., Hill, N. W., Perey, F. G., Tweed, G. L., and Leal, L., Proc,. Int. Conf. On Nuclear Data for Science and Technology, May 30-June 3, 1988, Mito, p. 115 (1988).

8. Weston, L. and Todd, J. H., Nucl. Sci. Eng., **88** 567 (1984).

9. G. de Saussure, R. Gwin, L. W. Weston, and R. W. Ingle, "Simultaneous Measurements of the Neutron Fission and Capture Cross Section for ^{235}U for Incident Neutron Energies from 0.4 eV to 3 keV," ORNL-TM-1804, Oak Ridge National Laboratory (1967).

10. Perez, R. B., de Saussure, G., Silver, E. G., "Simultaneous Measurements of the Neutron Fission and Capture Cross Section for ^{235}U for Neutron Energies from 8 eV to 10 keV," Nucl.Sci. Eng., **52**, 46 (1973).

11. De Saussure, G., Leal, L. C., Perez, R. B., Larson, N. M., and Moore, M. S., Nucl. Sci. Eng., **103**, 109 (1989).

12. J. A. Wartena, H. Weigmann, and C. Burkholz, report IAEA Tecdoc 491 (1987) p. 123.

13. H. Weigmann, P. Geltenbort, B. Keck, K. Schreckenbach, and J. A. Wartena, Proc. Intern. Conf. On the Physics of Reactors, Marseille 1990, Vol., PI, p. 33.

14 J. Bouchard, C. Golinelli, and H. Tellier, Proc. Intern. Conf. Nuclear Data for Science and

Technology," Antwerp, Belgium Sept. 6-10, 1982.

15. J. Hardy, "^{235}U Resonance Fission Integral and Alpha based on Integral Measurements, ENDF-300, Sec. B.1, Brookhaven National Laboratory (1979).

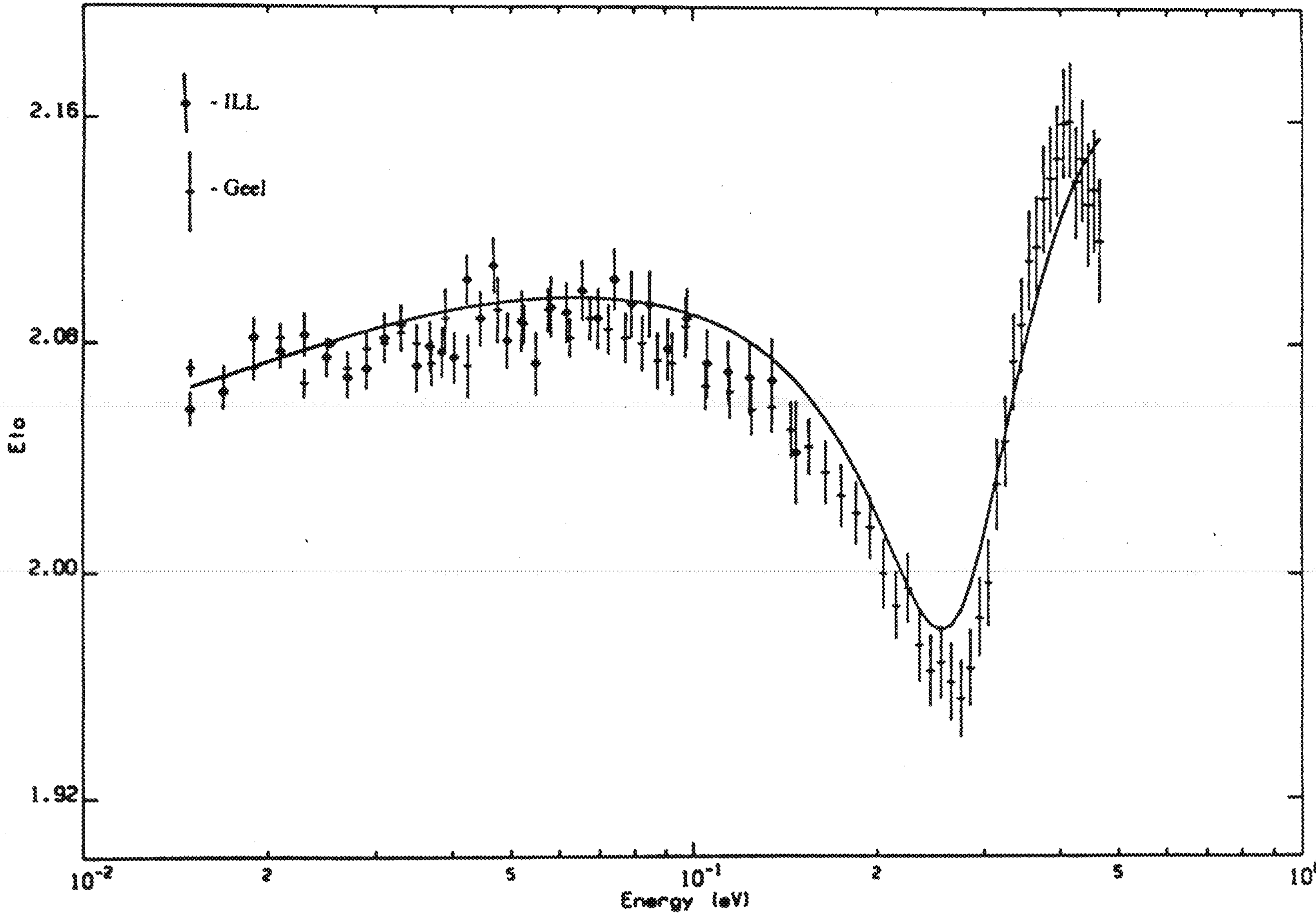

Figure 1.Experimental (symbols) and theoretical (solid curve) values of η for ^{235}U. Theoretical values were calculated from the final set of resonance parameters as described in this report.

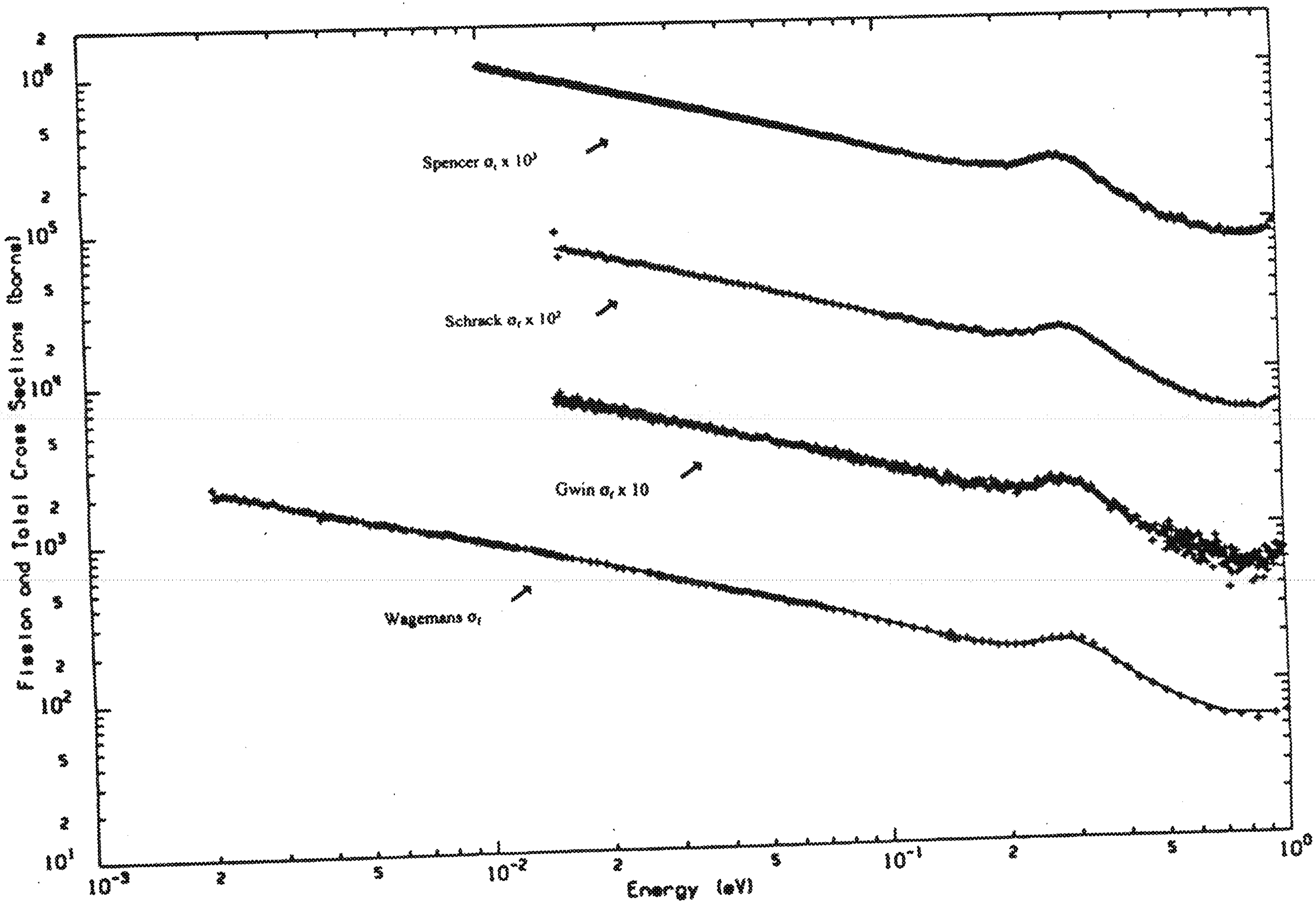

Figure 2. Total (top curve) and fission (lower three curves) cross sections below 1 eV. Measured values are represented by symbols, theoretical values by the solid curve.

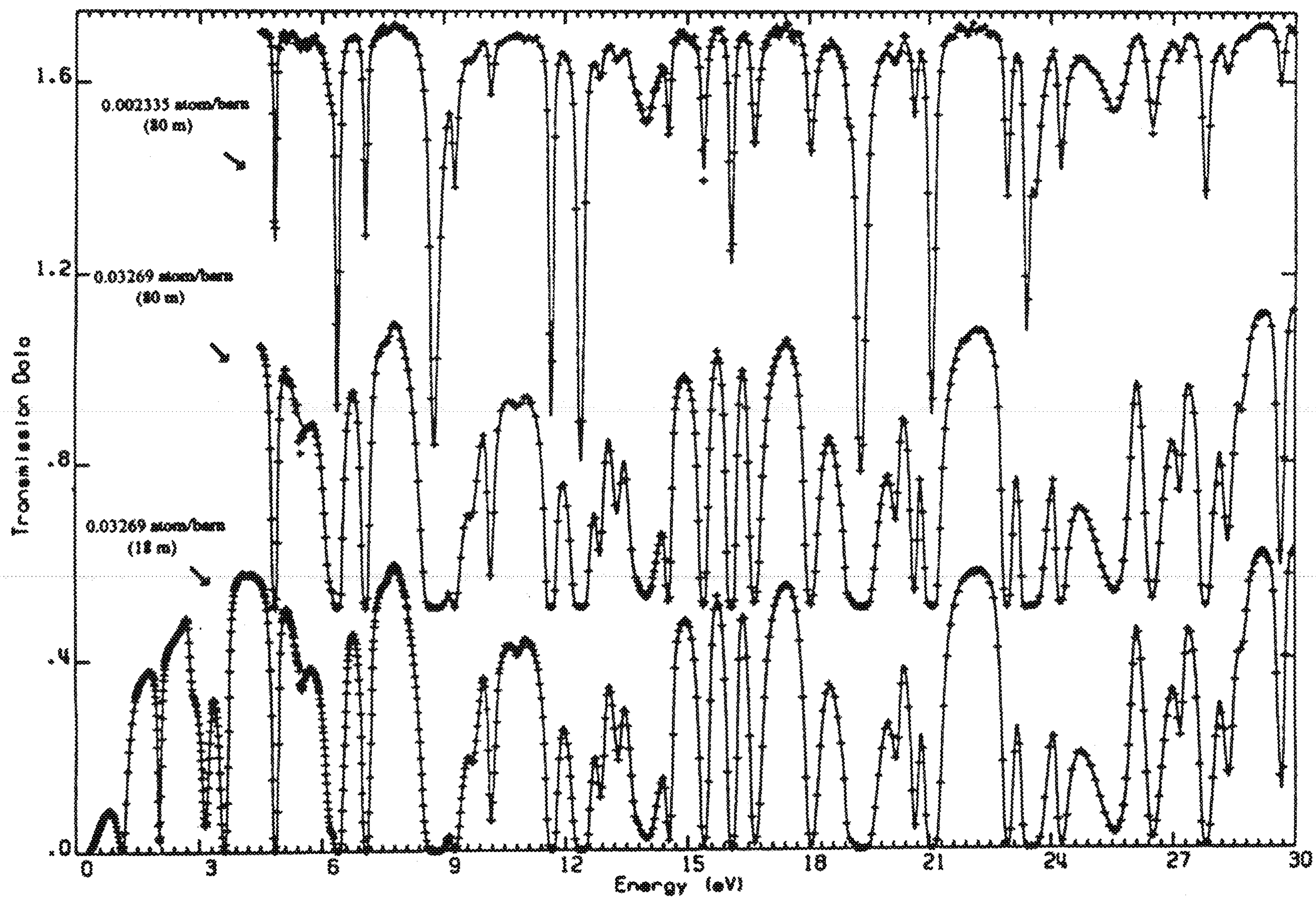

Figure 3. Transmission data (symbols) and calculated values (solid curve) from 0 to 30 eV.

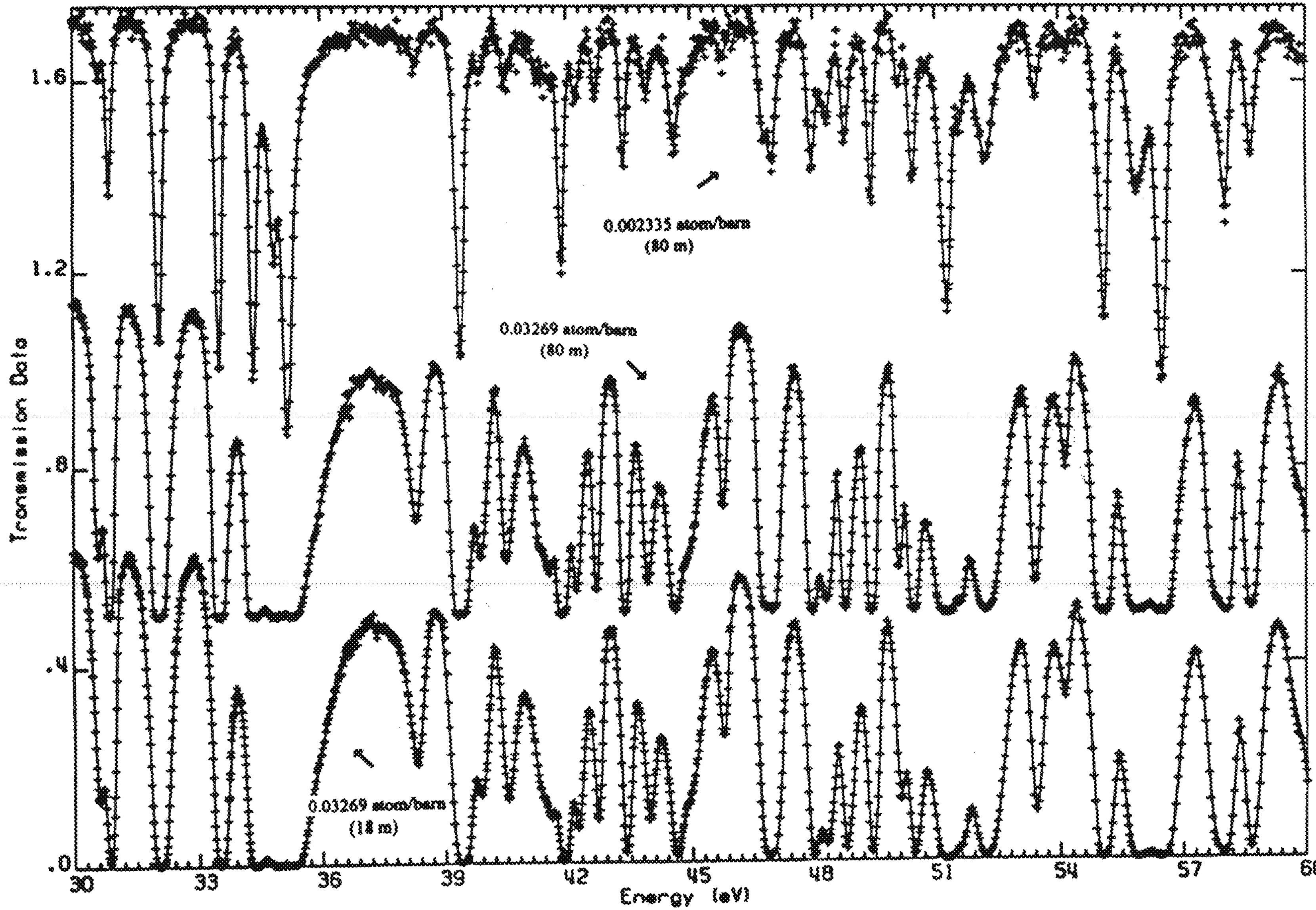

Figure 4. Transmission data (symbols) and calculated values (solid curve) from 30 to 60 eV.

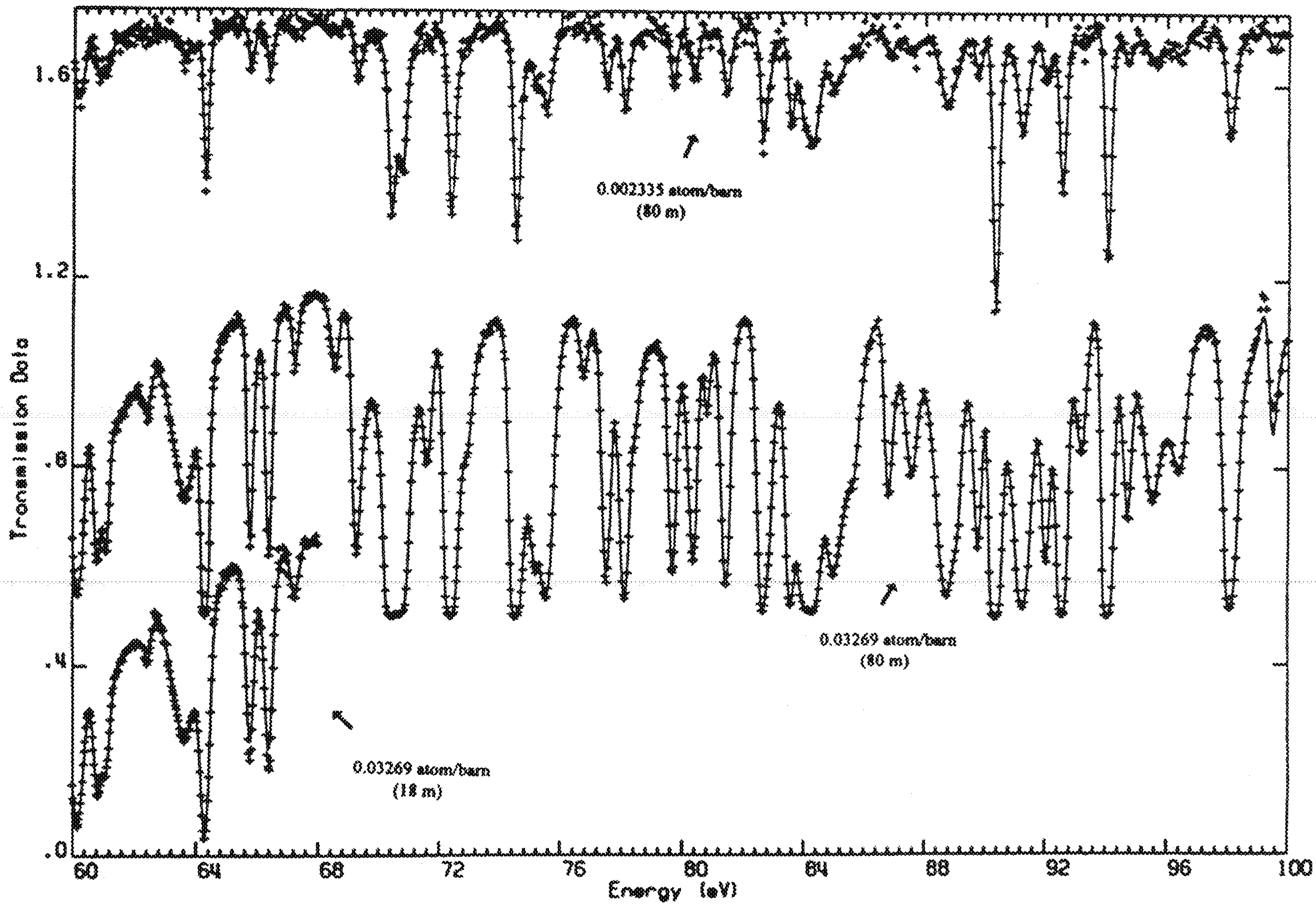

Figure 5. Transmission data (symbols) and calculated values (solid curve) from 60 to 100 eV.

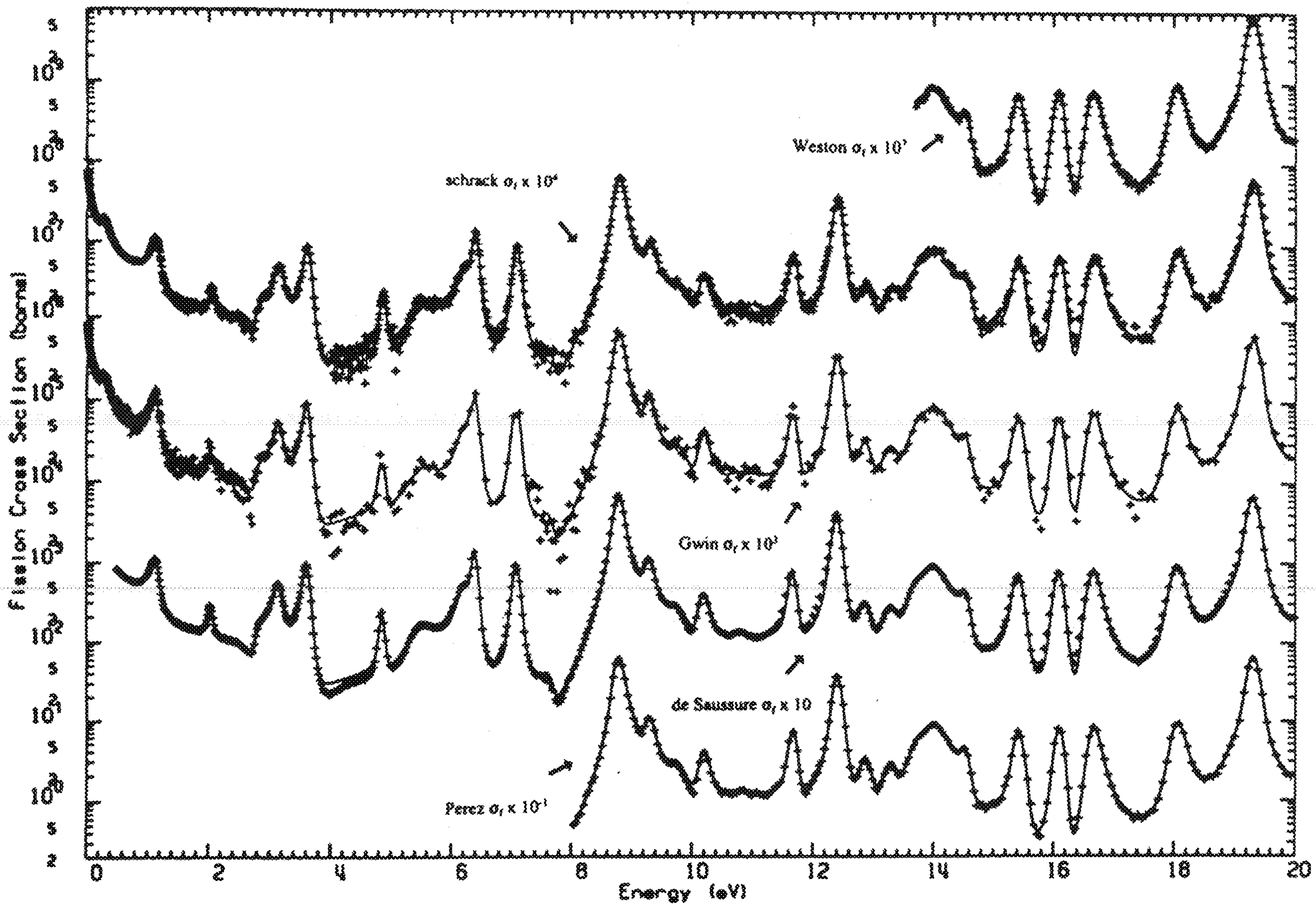

Figure 6. Fission cross section data (symbols) vs calculated values (solid curve) from 0 to 20 eV.

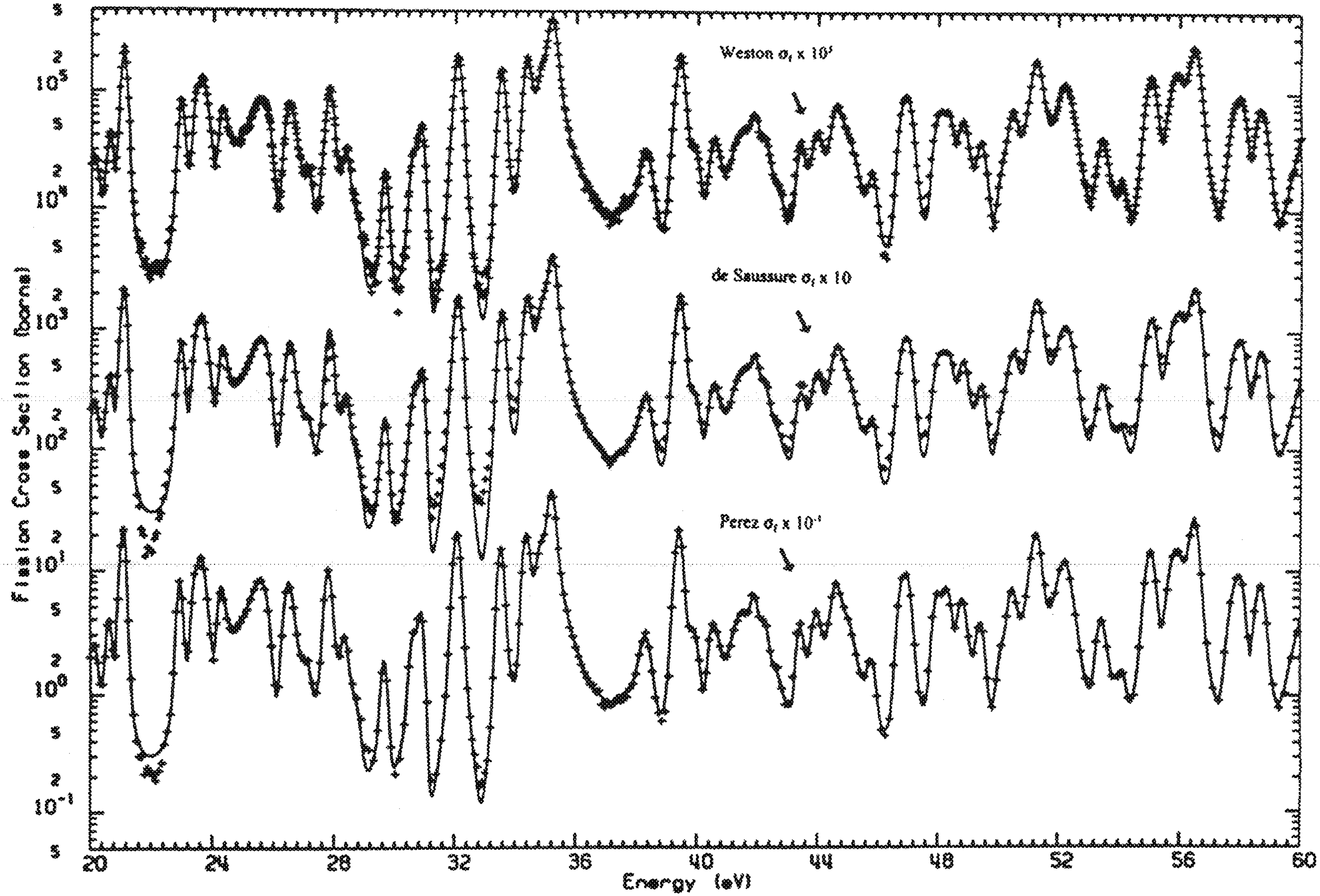

Figure 7. Fission cross section data (symbols) and calculated values (solid curves) from 20 to 60 eV.

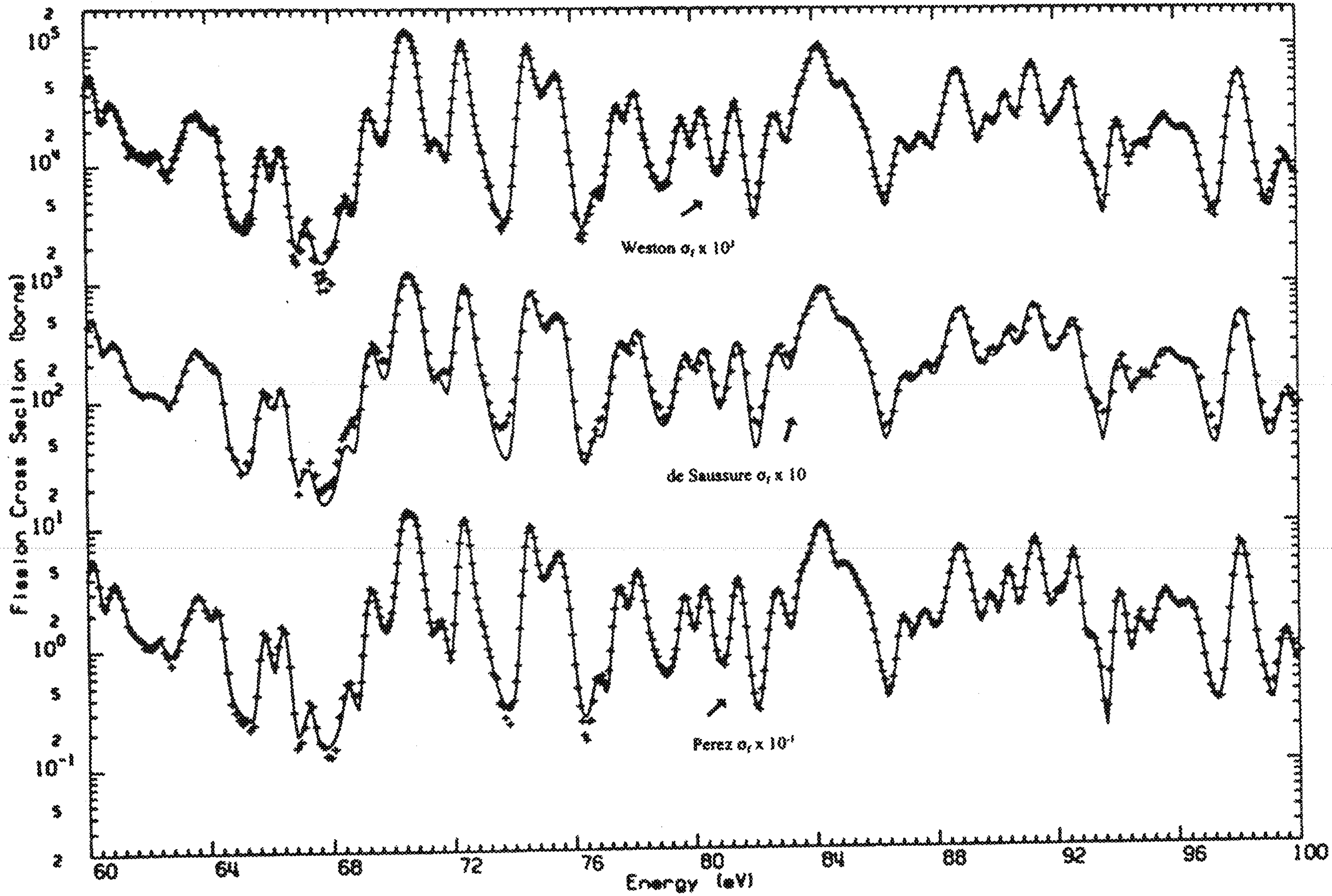

Figure 8. Fission cross section data (symbols) and calculated values (solid curves) from 60 to 100 eV.

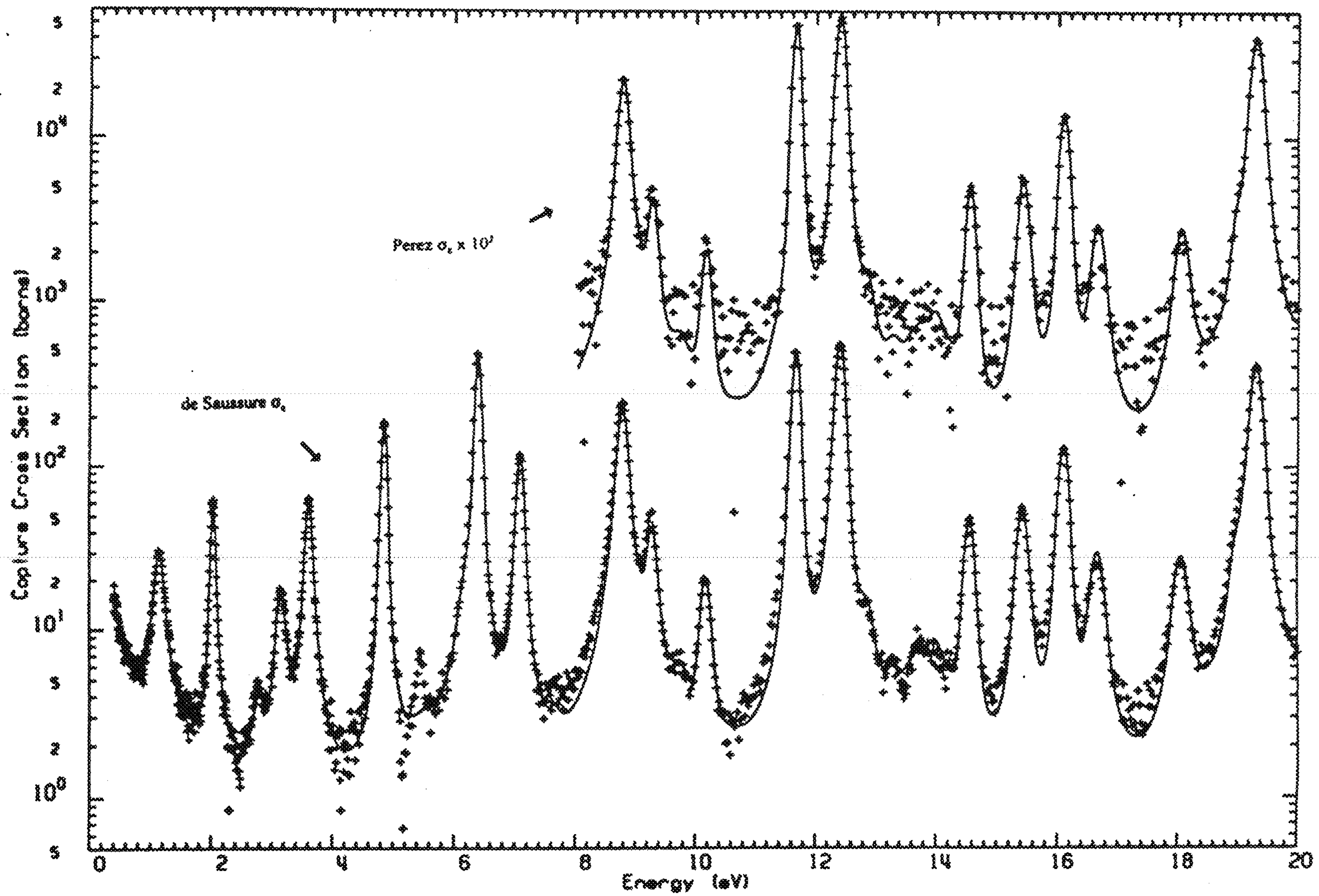

Figure 9. Capture cross section data (symbols) and calculated values (solid curves) from 0 to 20 eV.

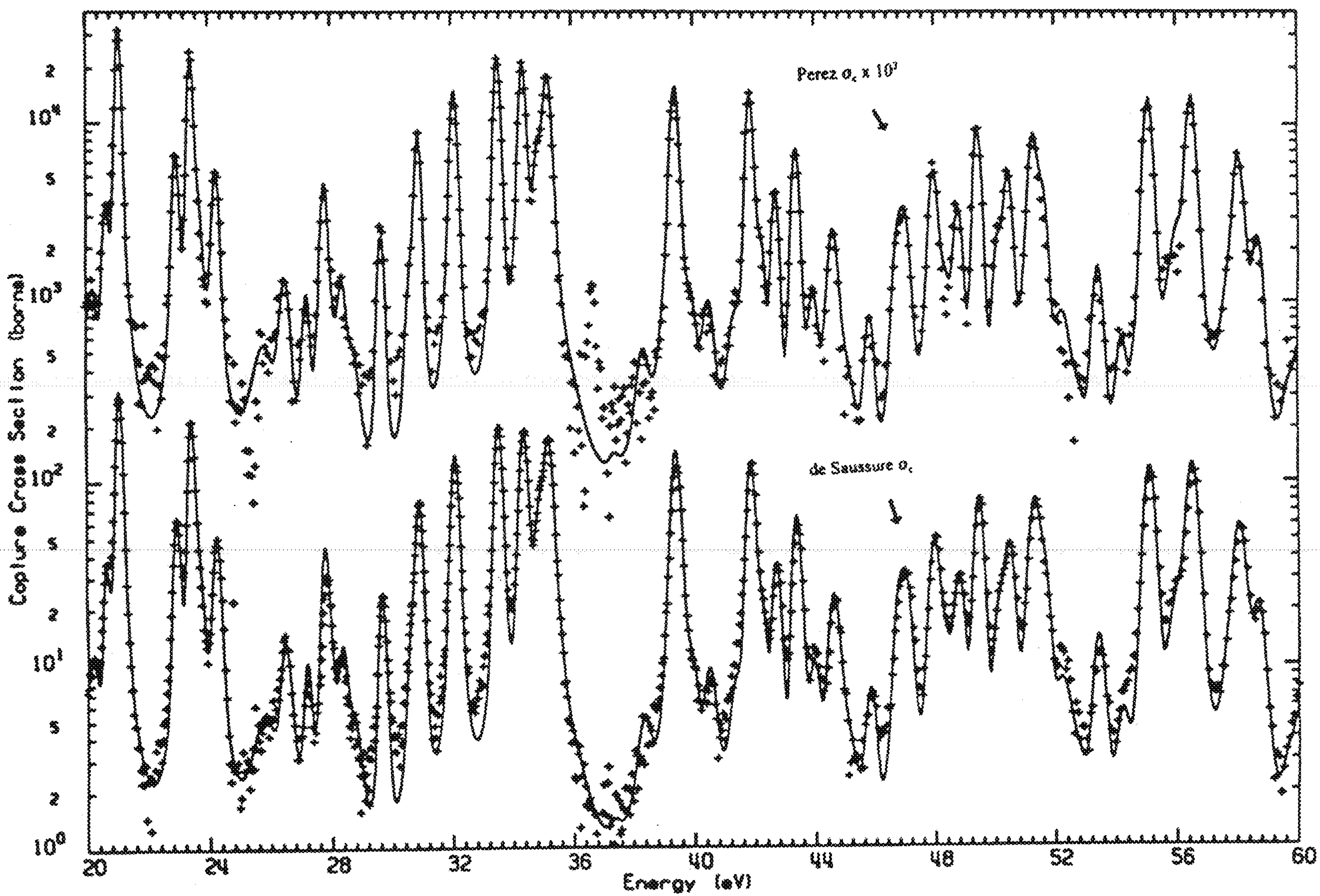

Figure 10. Capture cross section data (symbols) and calculated values (solid curve) from 20 to 60 eV.

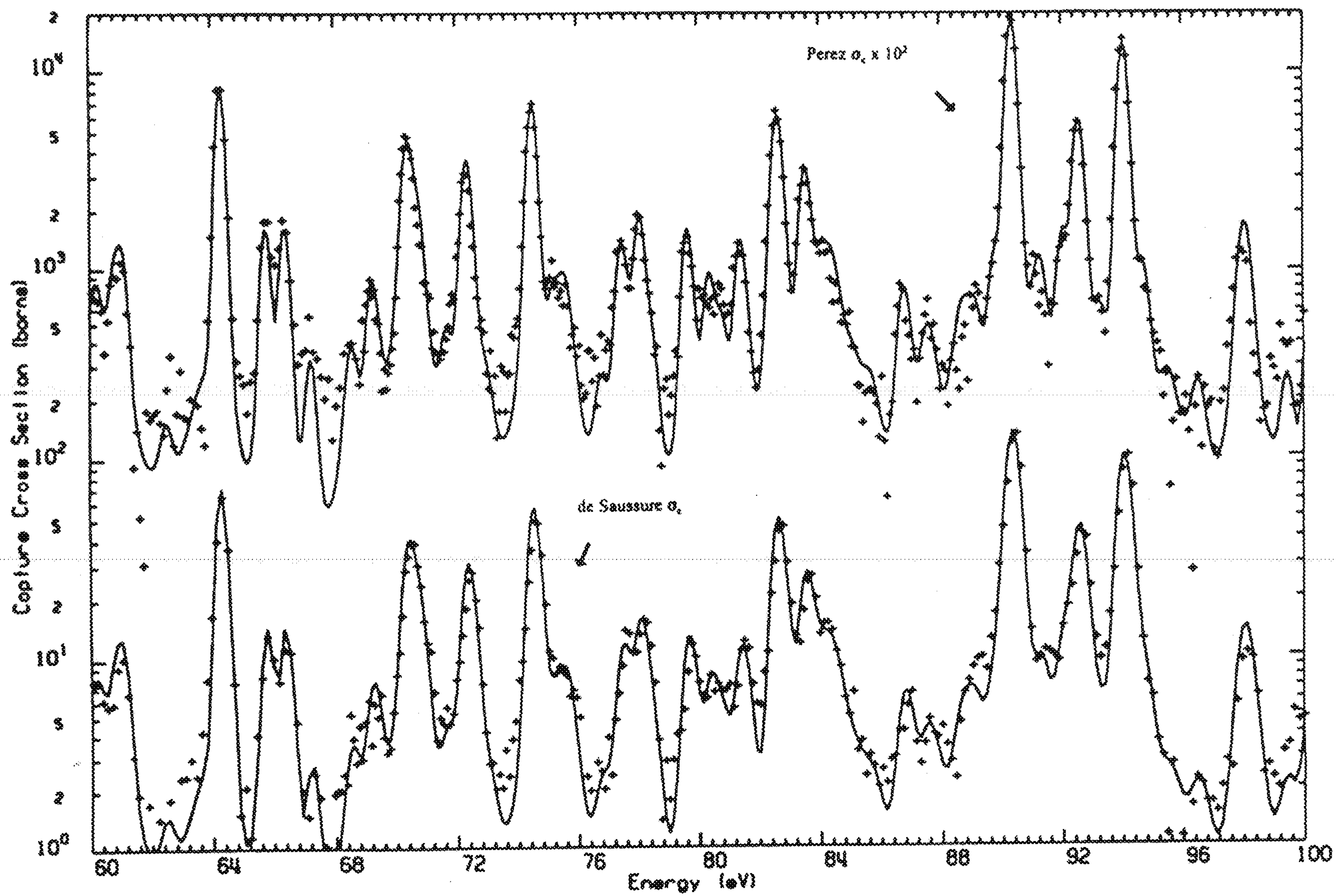

Figure 11. Capture cross section data (symbols) and calculated values (solid curves) from 60 to 100 eV.

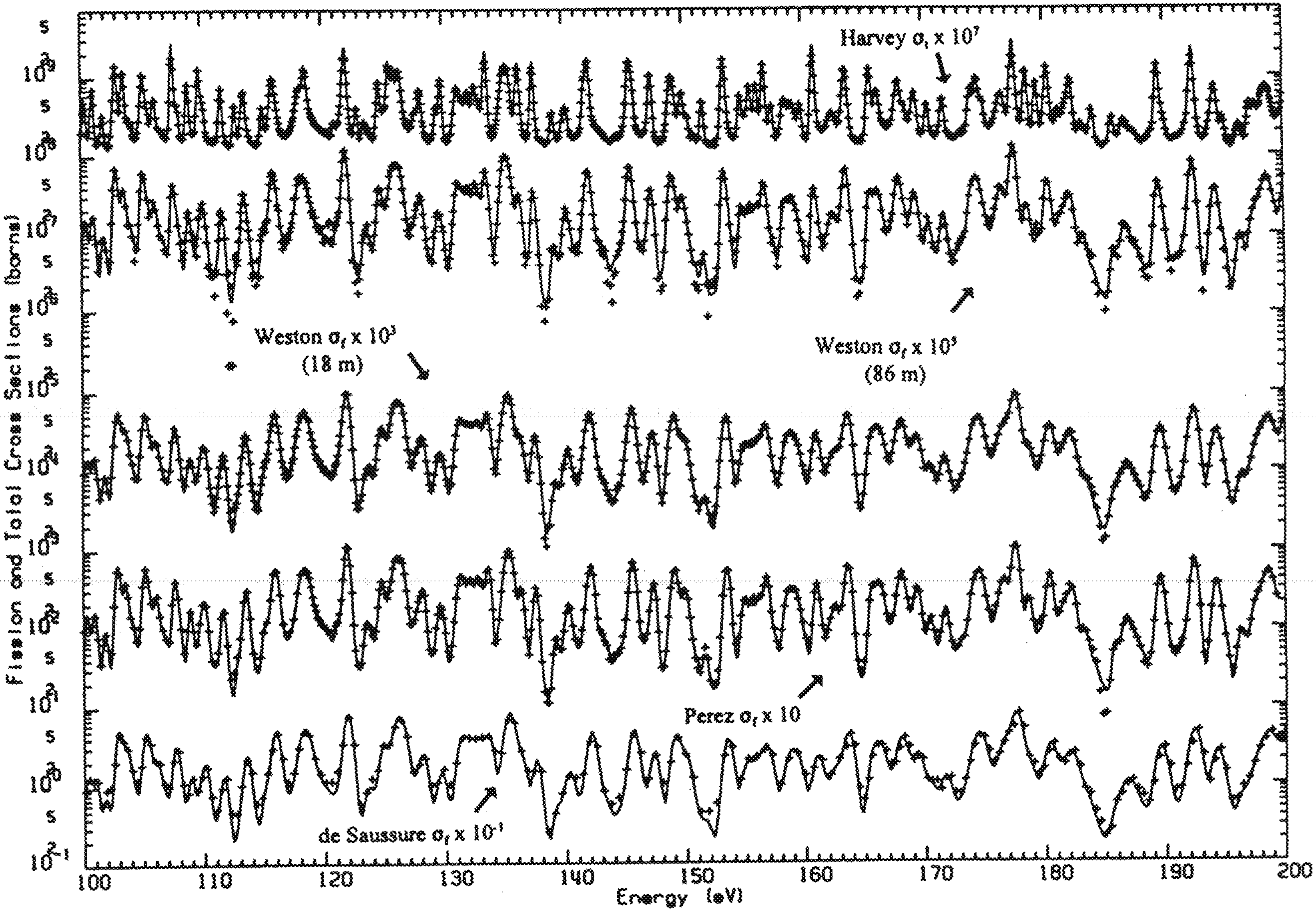

Figure 12. Fission (lower three curves) and total (upper two curves) cross section data (symbols) and calculated values (solid curves) from 100 to 200 eV.

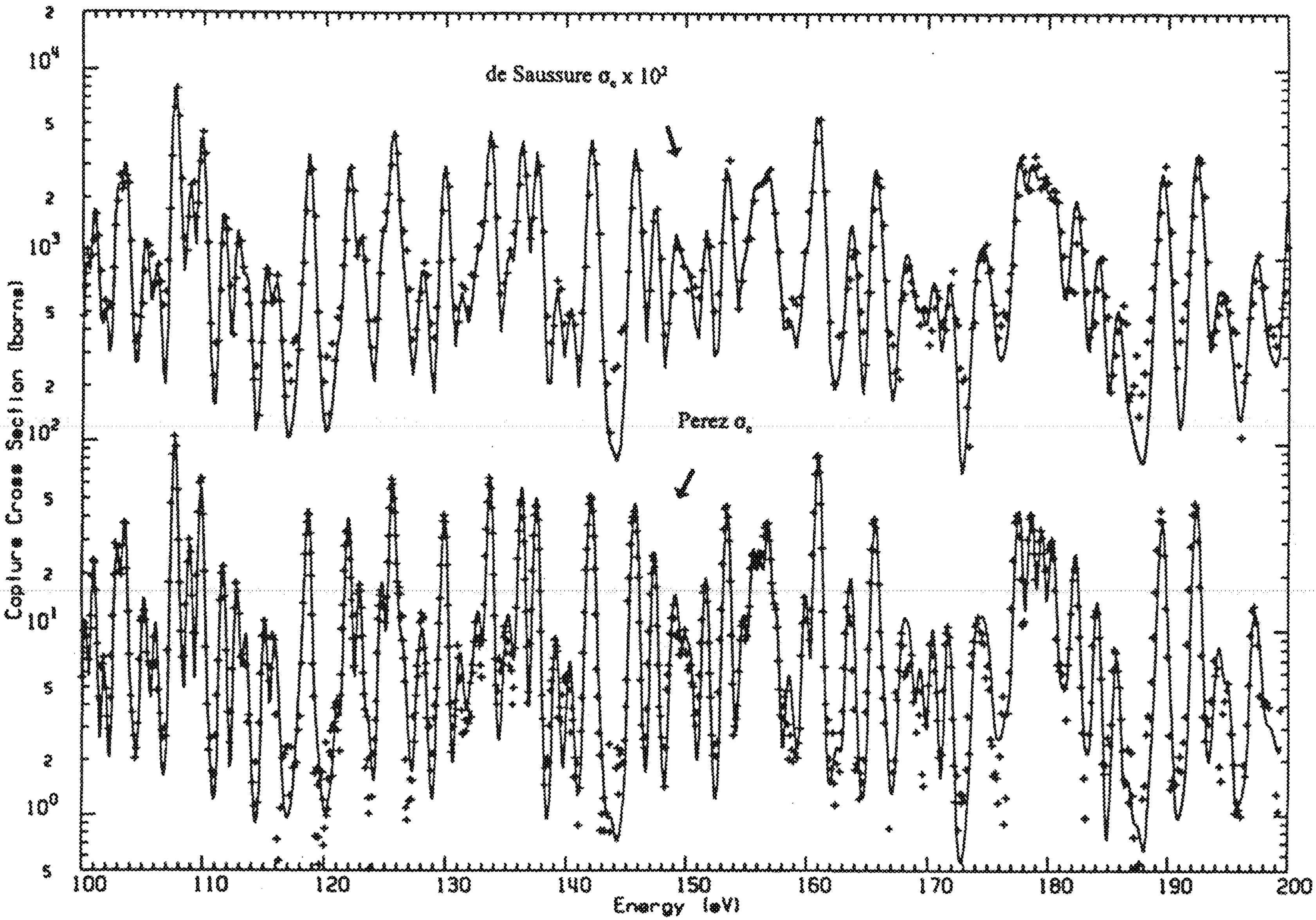

Figure 13. Capture cross section data (symbols) and calculated values (solid curves) from 100 to 200 eV.

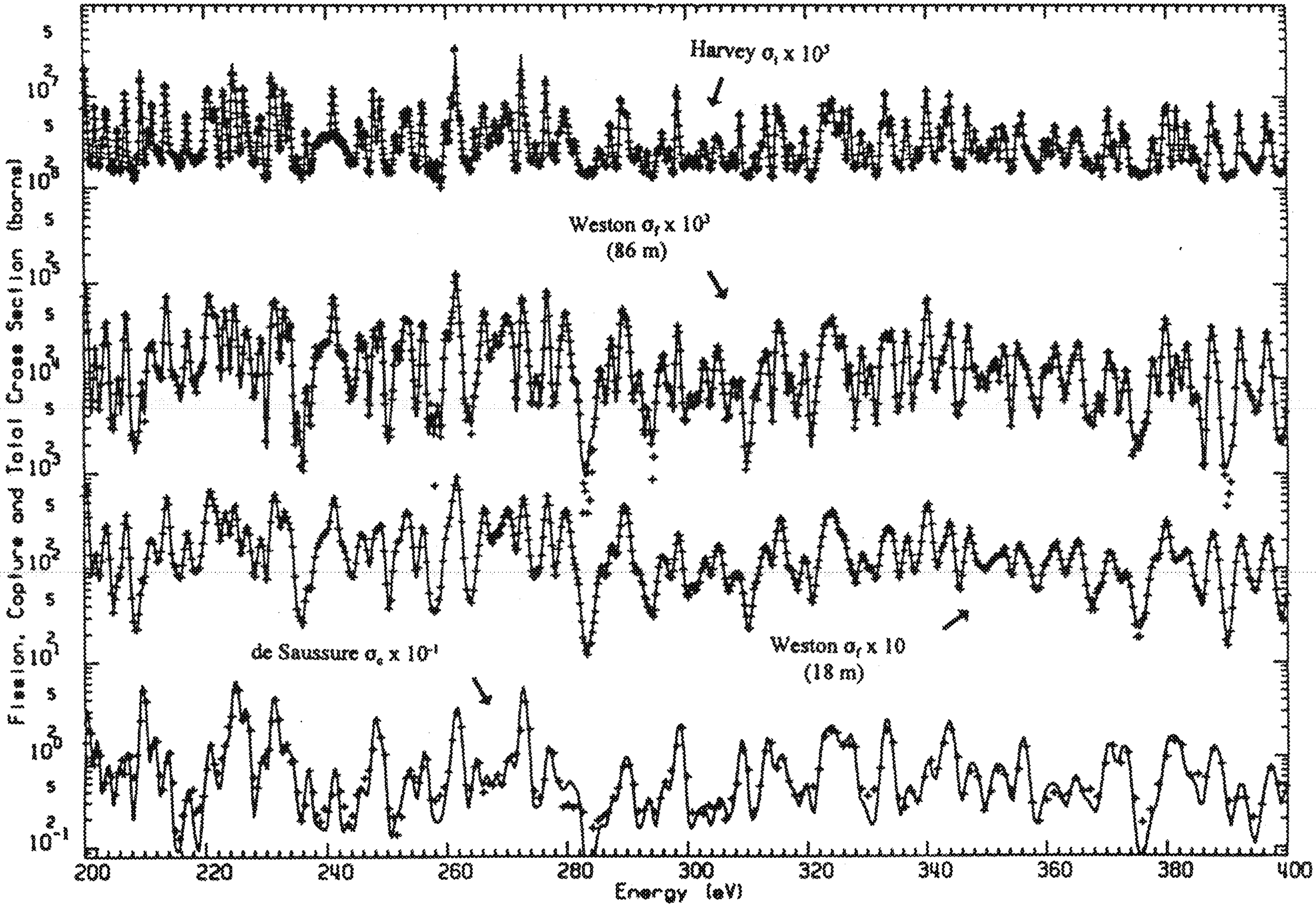

Figure 14. Total (upper curve), fission (two center curves), and capture (bottom curve) cross section data (symbols) and calculated values (solid curve) from 200 to 400 eV.

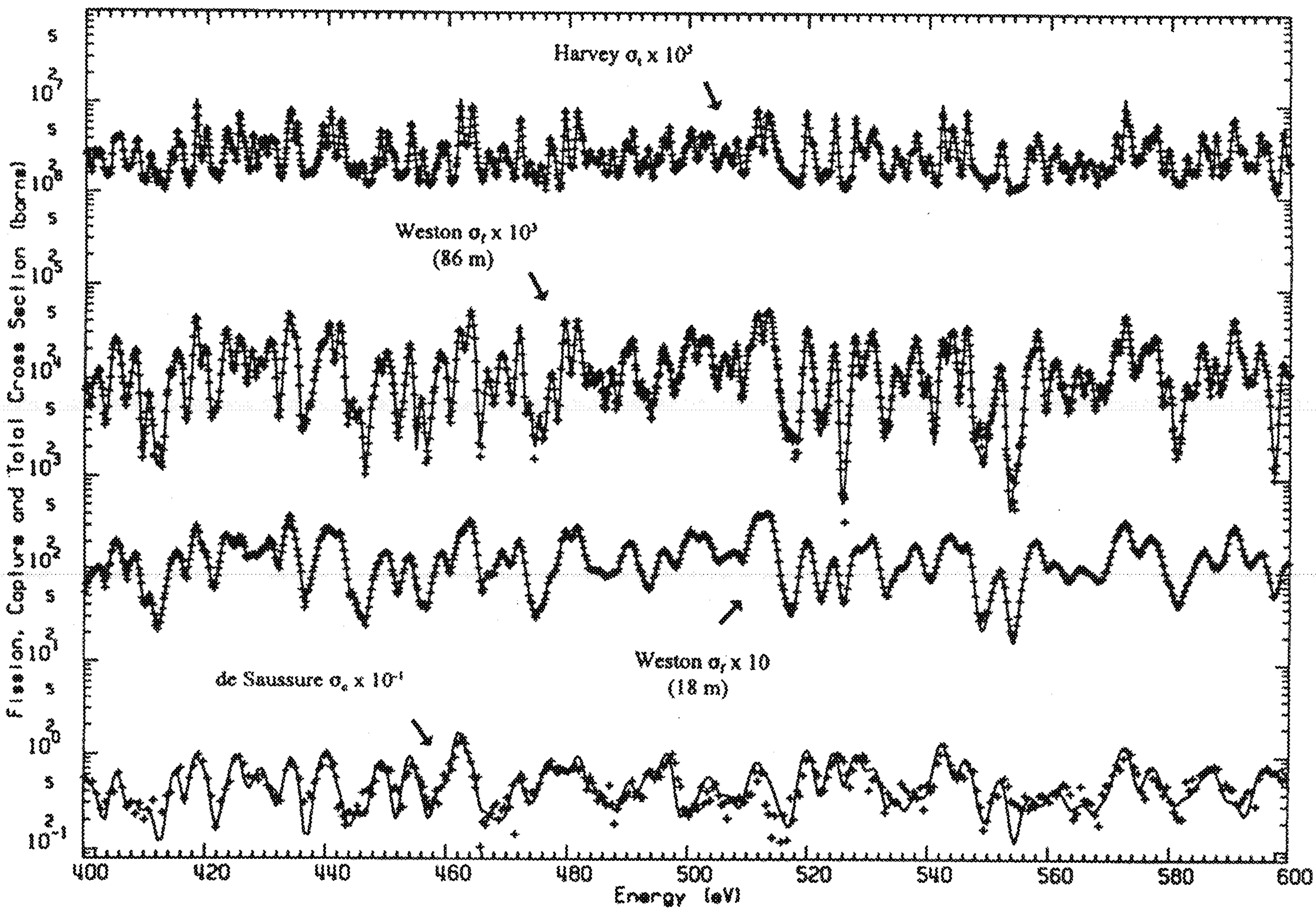

Figure 15. Total (upper curve), fission (two center curves), and capture (bottom curve) cross section data (symbols) and calculated values (solid curve) from 400 to 600 eV.

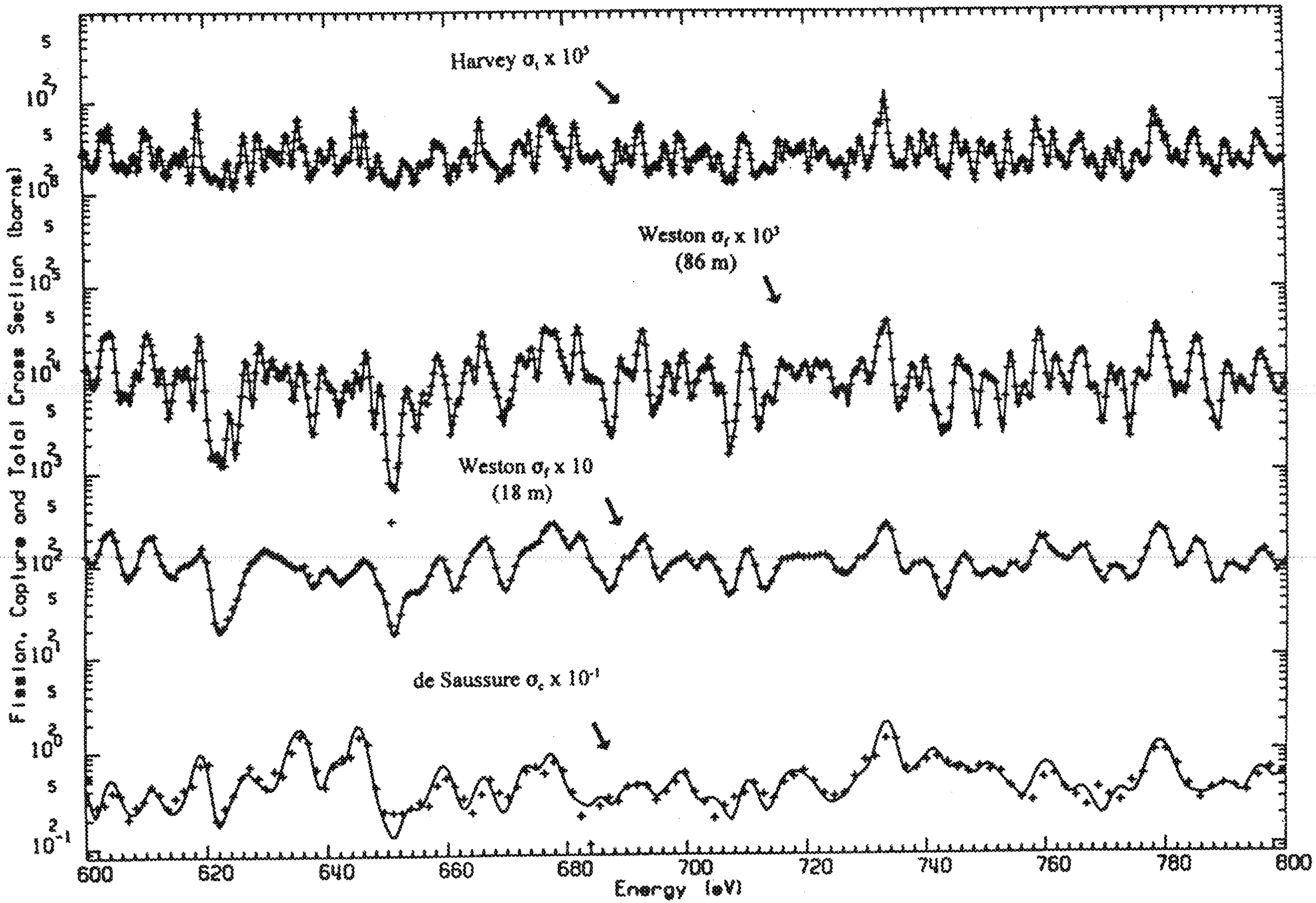

Figure 16. Total (upper curve), fission (two center curves), and capture (bottom curve) cross section data (symbols) and calculated values (solid curve) from 600 to 800 eV.

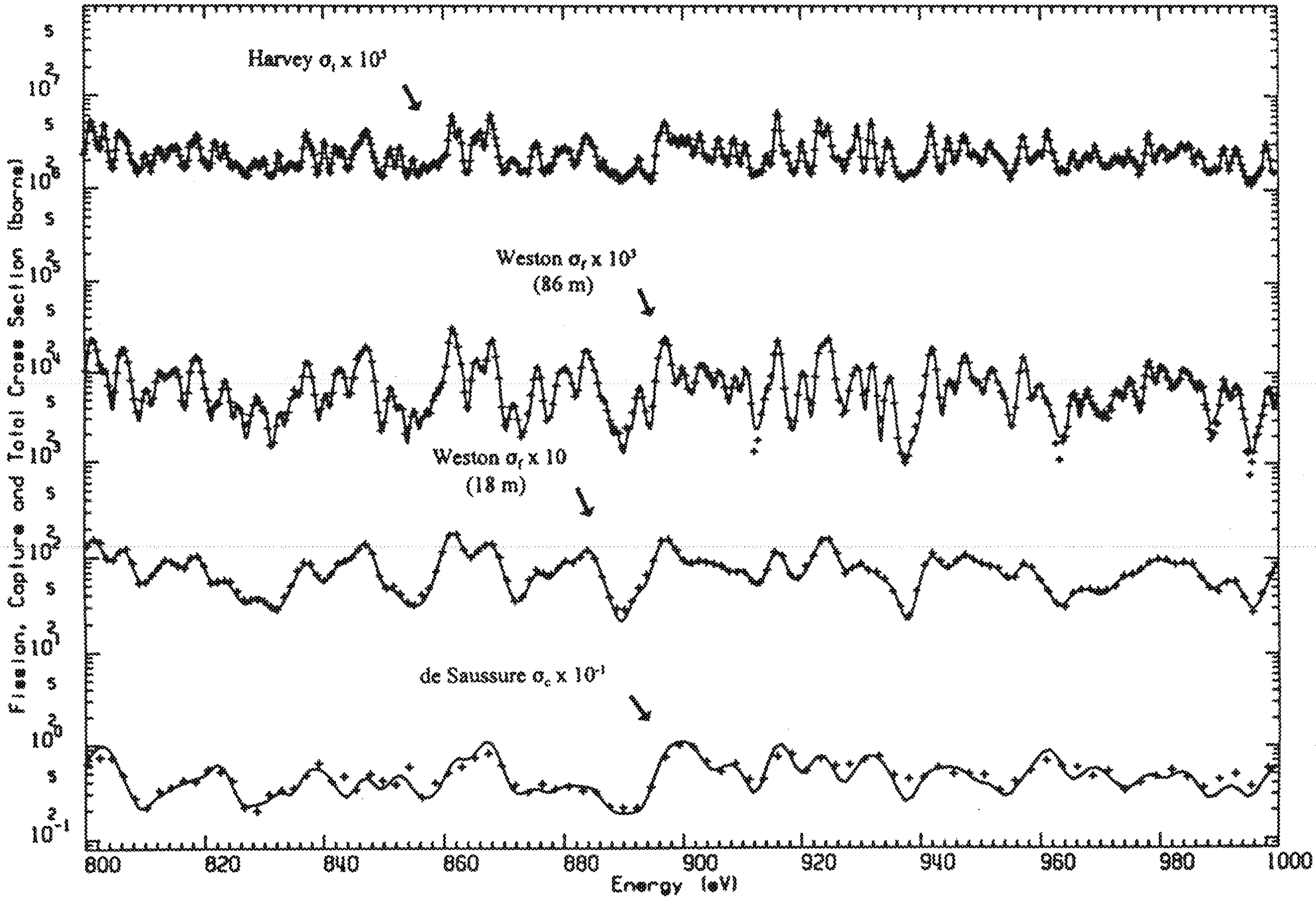

Figure 17. Total (upper curve), fission (two center curves), and capture (bottom curve) cross section data (symbols) and calculated values (solid curve) from 800 to 1000 eV.

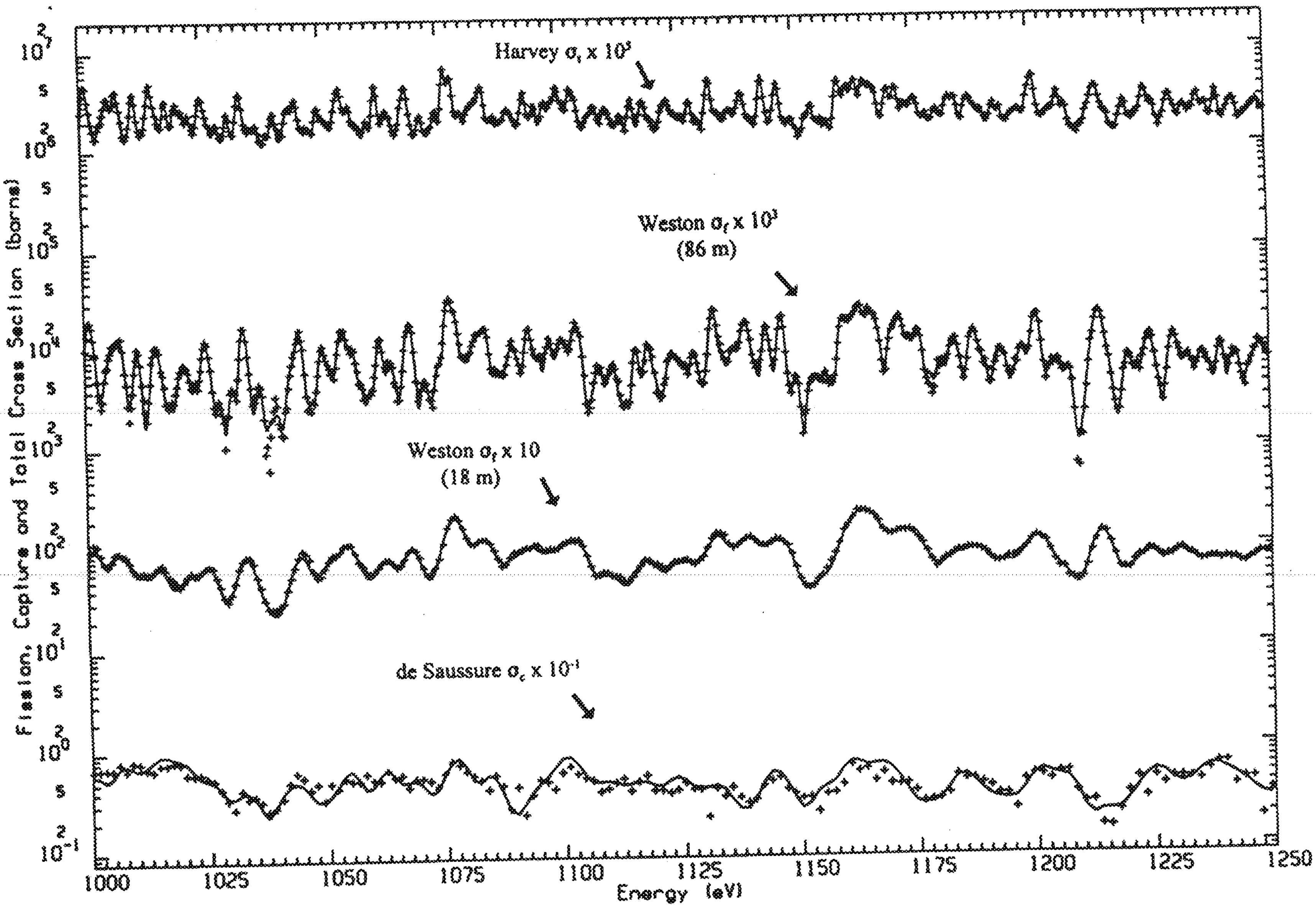

Figure 18. Total (upper curve), fission (two center curves), and capture (bottom curve) cross section data (symbols) and calculated values (solid curve) from 1000 to 1250 eV.

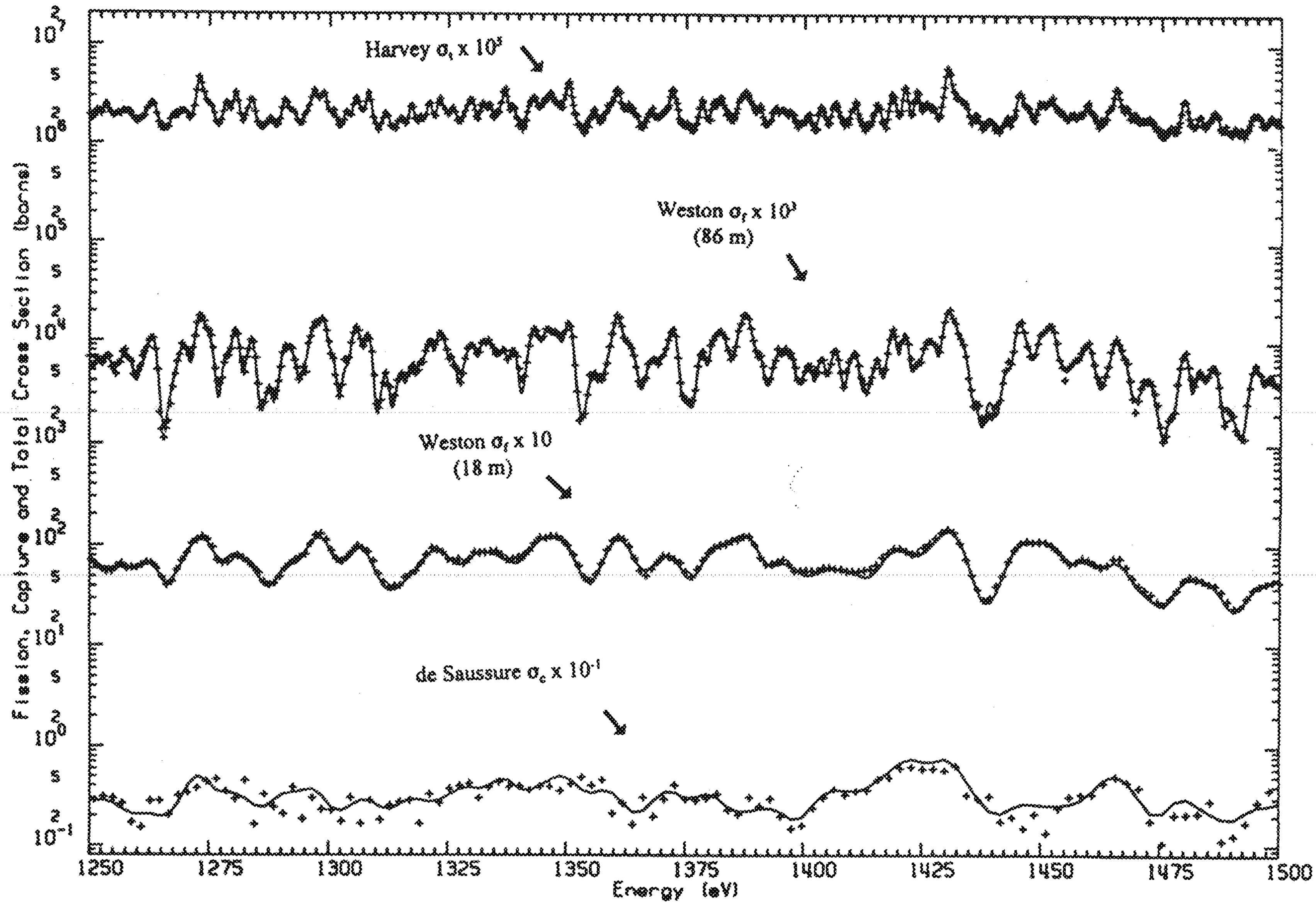

Figure 19. Total (upper curve), fission (two center curves), and capture (bottom curve) cross section data (symbols) and calculated values (solid curve) from 1250 to 1500 eV.

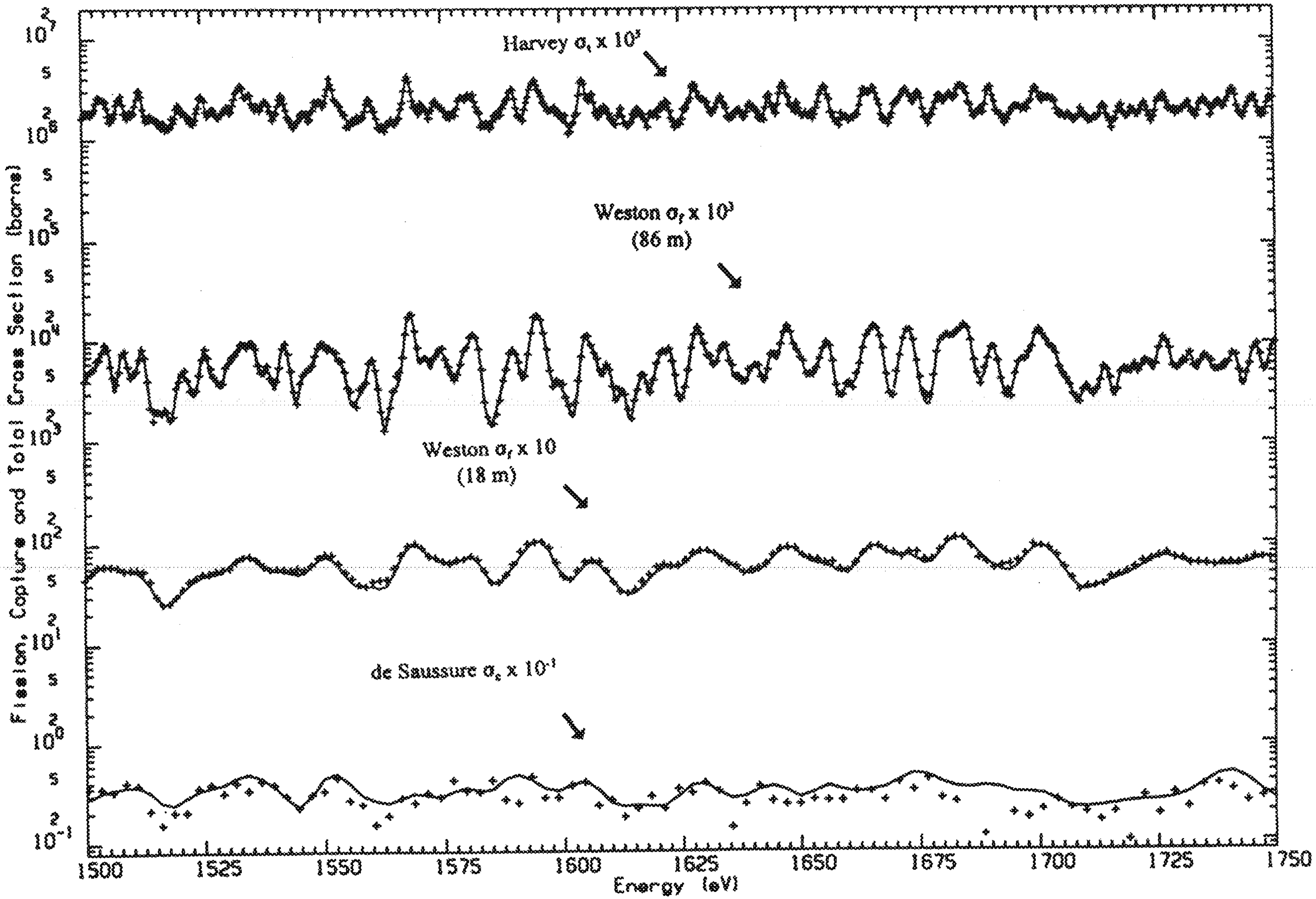

Figure 20. Total (upper curve), fission (two center curves), and capture (bottom curve) cross section data (symbols) and calculated values (solid curve) from 1500 to 1750 eV.

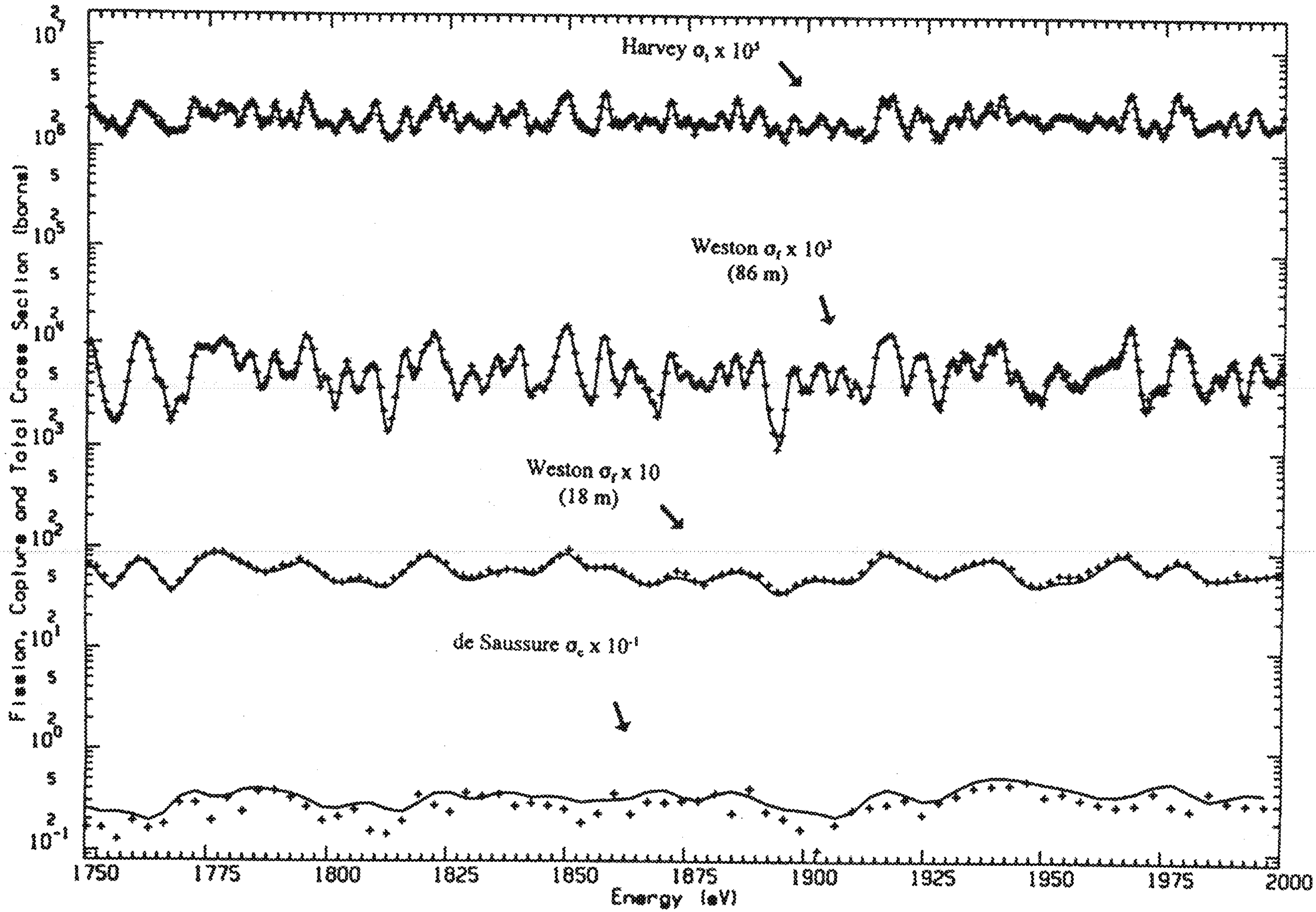

Figure 21. Total (upper curve), fission (two center curves), and capture (bottom curve) cross section data (symbols) and calculated values (solid curve) from 1750 to 2000 eV.

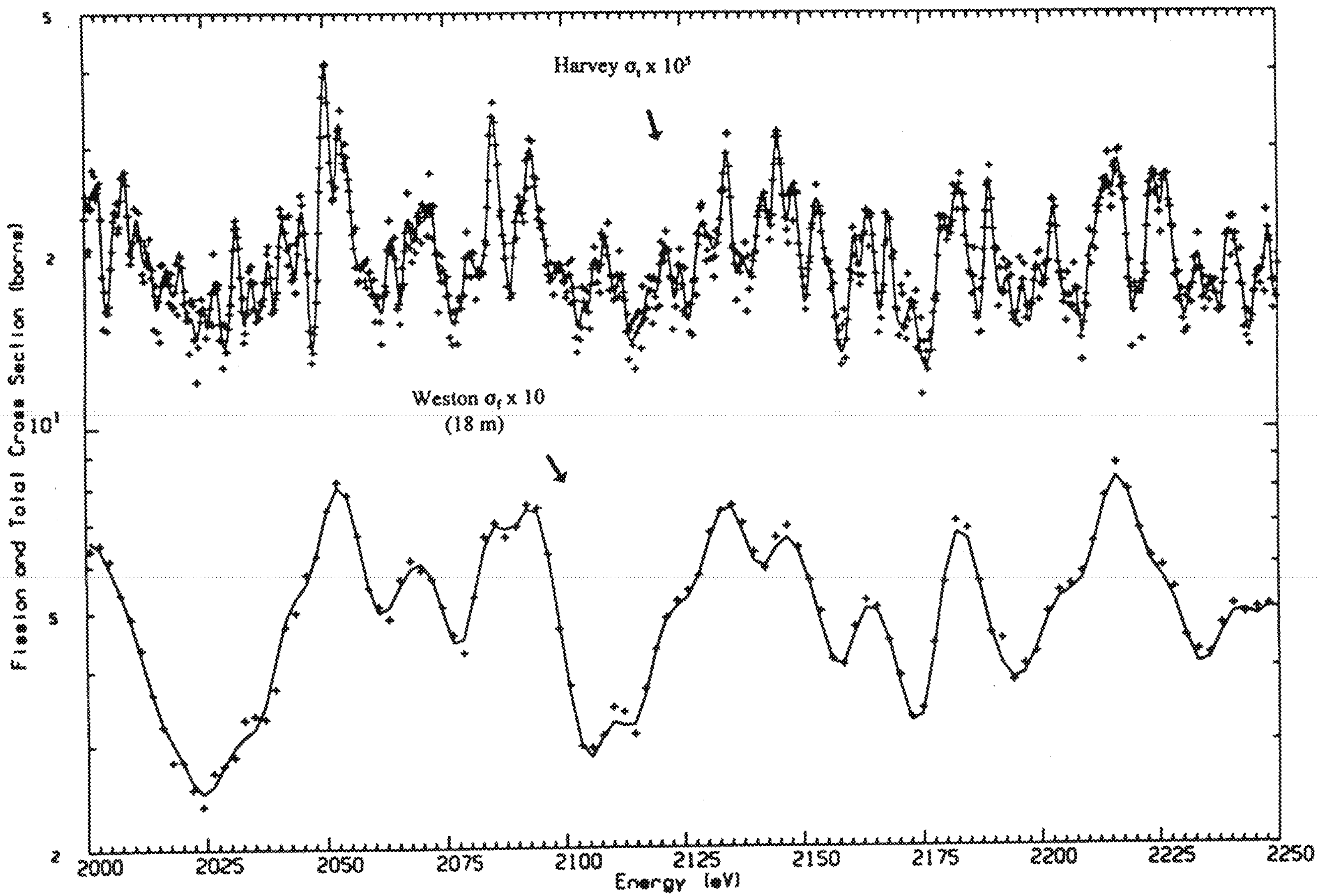

Figure 22. Total (upper plot) and fission (lower plot) cross section data (symbols) and calculated values (solid curve) from 2000 to 2250 eV.

MARTIN MARIETTA

MARTIN MARIETTA ENERGY SYSTEMS, INC.
OAK RIDGE, TENNESSEE 37831

Acting Under U.S. Government Contract DE-AC05-84OR21400 With the U.S. D.O.E.

SHIPPING ORDER

MATERIAL TO BE SHIPPED LOCATION	CONTACT (PERSON) NAME AND PHONE	OUR PURCHASE ORDER NO.	RELEASE NO.	R. R. NO.	DATE ISSUED	SHIPPING ORDER NO.
6011, 6370	Luiz C. Leal (4-5281)				1/11/96	

SHIPPED BY
MARTIN MARIETTA ENERGY SYSTEMS, INC.

POST OFFICE BOX 2008 . ORNL PLANT, OAK RIDGE, TENNESSEE 37831

SHIP VIA (AS CODED): A. MOTOR FREIGHT; B. RAIL FREIGHT; E. PREMIUM TRANSPORT (AS SHOWN); F. NON-PREMIUM PARCEL (AS SHOWN); H. CONSIGNEE'S TRUCK; J. CARTAGE CONTRACTOR; K. BUS; L. OTHER (AS SHOWN); M. COMPANY TRUCK

E | Federal Express

DELIVER BY DATE: 01/12/96

DATE SHIPPED: JAN 11 1996

SHIPPING ORDER ORIGINATED BY: Janice Helton (4-5267)

PARCEL POST DATA: ZONE; POSTAGE; WEIGHT; INSURANCE FEE; TOTAL

140 3392 374

VENDOR/PAYEE CODE:

SHIP TO:
Dr. Dennis Cabrilla
Chairman, EM Criticality Working Group
EM-23 (Quince Orchard, Room 487)
US Department of Energy
1000 Independence Avenue
Washington DC 20585-0002

TRANSPORTATION ACCOUNT CHARGE: 3350-0010

TRANSPORTATION TERMS (AS CODED): 2 — 1. COLLECT; 2. PREPAID; 3. GOVERNMENT B/L; 4. DEADHEAD; 5. PREPAID/DEBIT SELLER'S ACCOUNT

INSURANCE: 1. ACCOUNT OF GOV'T. DO NOT INSURE; 2. ACCOUNT OF CONSIGNEE; 3. OTHER (SEE BELOW)

VALUATION (FOR SHIPPING PURPOSES ONLY): $0.00

NUMBER AND KIND OF CONTAINERS: env

GROSS WEIGHT: 1

PURPOSE: Being sent to Dennis Cabrilla by L.C. Leal, Nucl. Engg. (CPED) in connection with collaborative research. Will not be returned to ORNL.

AUTHORITY (PURCHASE ORDER, CONTRACT NUMBER, OR OTHER OFFICIAL DOCUMENT):

HAZARDOUS MATERIAL: ☐ YES ☒ NO

INSTRUCTIONS:

ESTIMATED DATE OF RETURN:

S. O. ITEM NO.	STORES CATALOG NO. OR PROPERTY NO.	DESCRIPTION OF MATERIAL, SERIAL NO., MODEL NO., ETC.	QUANTITY	UNIT	UNIT VALUE	TOTAL VALUE
1		Printed Material - Paper "Final Report on Evaluation of the 235U Cross..."	1	lot		$0.00

HAZARDOUS SHIPMENT CHECKLIST: SEE FEDERAL REGULATIONS CODES 49 AND 49

1. MATERIALS PROPER SHIPPING DESCRIPTION
2. FLASH POINT, IF APPLICABLE
3. HAZARD CLASS
4. MANUFACTURER'S BRAND NAME
5. PHYSICAL AND CHEMICAL FORM
6. WEIGHT OF CONTENTS
7. CONTAINER TYPE
8. CONTAINER NUMBER
9. PACKAGING NOTATION
10. TYPE LABELS REQUIRED
11. TYPE PLACARD REQUIRED
12. SPECIAL NOTATION/ INSTRUCTIONS
13. GREEN TAG APPLIED ☐ Yes ☐ No

	ACCOUNT	AMOUNT		ACCOUNT	AMOUNT
DEBIT		$0.00	CREDIT		$0.00
DEBIT			CREDIT		
DEBIT			CREDIT		
DEBIT			CREDIT		

NOTICE TO CONSIGNEE: PLEASE USE ABOVE SHIPPING ORDER NO. AND PURCHASE ORDER NO. IN CORRESPONDENCE OR QUESTIONS REGARDING THIS SHIPMENT. ALSO USE THEM TO IDENTIFY RETURN OF ABOVE MATERIAL TO MARTIN MARIETTA ENERGY SYSTEMS, INC.

AUTHORIZED SIGNATURE AND DIVISION: Computational Physics & Engineering, R. M. Westfall — R M Westfall (10)

SHIPPING DEPT. APPROVAL: [signature]

PAGE 1 OF 1

UCN-2160
(12350M 6-86)

2/20/69M