THE EVALUATION OF SEVERAL ENDF/B NUCLIDE CROSS-SECTIONS BY A MONTE CARLO TECHNIQUE

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ABSTRACT

The Monte Carlo code TYCHE IV has been used to calculate with a high degree of convergence the second, fourth, and sixth spatial moments of the slowing-down density distribution at the indium resonance energy, for neutrons originating from a fission source at a point in infinitely extended light water, heavy water, graphite, aluminum/water, iron/water and zirconium/water moderators. These calculations, the results of which are compared with integral experiments, were done in support of the Phase-II data testing effort for the ENDF/B neutron cross-section files.

I. INTRODUCTION

TYCHE IV[1] is an infinite-medium slowing-down Monte Carlo program (written in Fortran IV for the IBM 360/50) which computes the first three moments of the neutron slowing-down density distribution. The moments are calculated by means of recursion relations developed by Cohen.[2]

In the calculation of neutron slowing-down, the azimuthal scattering angle is an "ignorable" coordinate in the sense that it does not appear in the description of the kinematics of a collision. Thus if we are interested in the moments rather than the precise details of the neutron slowing-down density distribution, it is possible to average each collision over the azimuthal angle and thus reduce the number of variables. Integration over path length is also easily carried out, and it is thus possible to obtain the age and higher moments of the neutron spatial distribution from a calculation which is essentially space-independent and which uses the Monte Carlo method only to follow the neutron history in energy and angle. Loss of neutrons by absorption is represented by reducing weights rather than by stochastic termination of neutron histories. Inelastic scattering is treated by the evaporation model, with the angular distribution isotropic in the center of mass.

The theoretical calculations of the neutron age and the higher moments in the moderating materials of interest were carried out in support of the ENDF/B Phase-II data testing effort. Results of these calculations are compared with experiment and the adequacy of the neutron cross-section data discussed.

II. METHOD OF ANALYSIS

As an aid to the Phase-II data testing for the ENDF/B data files, the Monte Carlo code TYCHE III(3) was converted, improved, made operational on the IBM 360/50, and christened TYCHE IV. Several areas of the program were improved. One such area deals with the method used in treating differential elastic-scattering data to determine the degree of anisotropy in neutron elastic collisions. Instead of generating and storing coefficients of a power series relating the cosine of the scattering angle, μ, to the cumulative probability distribution, ξ, the latter is stored at 21 equally spaced intervals in μ ($\Delta\mu$ = 0.1) for each energy. Another improvement, a method allowing "naive" random-number correlation, was added to assure that each neutron history will start with the same random number, given identical initial random numbers. Thus differences between results for two cases may be determined more accurately with fewer histories.

A translator program TYCHEB(1) was written to prepare ENDF/B cross-section data for use with TYCHE IV. The data translated consist of the energy and the total elastic and inelastic cross-sections for each isotope desired; the energy mesh for a given set of nuclides, i. e. hydrogen, oxygen, and iron, for calculations in iron/water mixtures was obtained by merging the individual ENDF/B total cross-section energy grids for the nuclides in that set. The energy interval is from 1.0 ev to 10.0 Mev, and up to three ENDF/B data tapes may be used.

For further assurance that results calculated by TYCHE III and IV were indeed repetitive, a cross-section library based on the hydrogen and oxygen cross-section data used to originally evaluate the neutron age in light water was prepared for TYCHE IV, and the neutron age and higher moments were recalculated. The satisfactory agreement between calculations is shown in Table 1.

The TYCHE III(4) results are based on 80,000 neutron histories while only 40,000 were sampled by TYCHE IV. The Cranberg fission spectrum is defined by:

$$f(E) = 0.453 \exp\left(\frac{-E}{0.965}\right) \sinh (2.29E)^{1/2} \quad ,$$

where

$\langle E \rangle$ = calculated mean fission energy, and

$\langle N \rangle$ = mean number of collisions to indium resonance.

TABLE 1

TYCHE-III AND -IV CALCULATIONS FOR NEUTRON AGE AND HIGHER MOMENTS IN LIGHT WATER

Density: 3.344×10^{22} molecules/cc

	τ^{φ} (cm^2)	M_4^{φ} ($10^4 cm^6$)	M_6^{φ} ($10^8 cm^6$)	$\langle E \rangle$ (Mev)	$\langle N \rangle$
TYCHE III	26.07 ± 0.09	9.55 ± 0.11	1.71 ± 0.03	1.985	15.7
TYCHE IV	26.06 ± 0.13	9.66 ± 0.13	1.72 ± 0.05	1.979	15.7

III. RESULTS

TYCHE-IV cross-section libraries were prepared for hydrogen, deuterium, carbon, oxygen, aluminum, iron, and zirconium. Differential elastic-scattering data for all nuclides were taken from the ENDF/B. Following the preparation of data libraries, Monte Carlo calculations for the neutron age and higher moments to indium resonance energy were carried out in light water, heavy water, graphite, and in metal/water mixtures of aluminum, iron, and zirconium. The calculations are based on sample sizes of 40,000 neutron histories and are believed to be adequately converged. The calculated results are compared with experiments in Tables 2 through 7.

The agreement between the calculated and measured values of the neutron age for light water leads one to conclude that the ENDF/B evaluations for hydrogen and oxygen are satisfactory; however, the discrepancy between the measured and computed higher moments for light water (Table 7) suggests that the cross-section data may not be totally satisfactory. The hydrogen cross-sections are known to be quite accurate; thus the oxygen data appear suspect. Since the higher moments generally reflect effects of high-energy neutrons,[5] we suggest that (1) the oxygen cross-section data above 1-Mev be re-evaluated and (2) the angular distribution data for oxygen be re-examined.

TABLE 2

MONTE CARLO CALCULATIONS vs MEASURED VALUES FOR NEUTRON AGE AND HIGHER MOMENTS IN WATER

Density: 3.44×10^{22} molecules/cc

	τ^{φ} (cm^2)	M_4^{φ} ($10^4 cm^4$)	M_6^{φ} ($10^8 cm^6$)
Calculation	26.06 ± 0.13	9.66 ± 0.13	1.72 ± 0.05
Experiment*	26.46 ± 0.32	9.34 ± 0.50	1.37 ± 0.20

*See Reference 5

TABLE 3

MONTE CARLO CALCULATIONS vs MEASURED VALUES FOR NEUTRON AGE AND HIGHER MOMENTS IN HEAVY WATER (99.75%)

Density (in atoms/cc):

$D = 6.604 \times 10^{22}$

$H = 0.017 \times 10^{22}$

$O = 3.309 \times 10^{22}$

	τ^{φ} (cm^2)	M_4^{φ} ($10^5 cm^4$)	M_6^{φ} ($10^9 cm^6$)
Calculation	117.6 ± 0.2	10.03 ± 0.05	2.45 ± 0.03
Experiment*	111 ± 1	-	-
Experiment†	109 ± 3	-	-

*See Reference 6
†See Reference 7

TABLE 4

MONTE CARLO CALCULATIONS vs MEASURED VALUES FOR NEUTRON AGE AND HIGHER MOMENTS IN GRAPHITE

Density: 8.023×10^{22} atoms/cc

	τ^{φ} (cm^2)	M_4^{φ} ($10^6 cm^4$)	M_6^{φ} ($10^{10} cm^6$)
Calculation	295.6 ± 0.5	6.098 ± 0.03	3.556 ± 0.05
Experiment*	307.8 ± 2.0	6.577	3.843
Experiment†	310.6 ± 3.0	6.89	4.4
Experiment§	312.6 ± 0.5	6.87	4.3

*See Reference 8
†See Reference 9
§See Reference 10

TABLE 5

MONTE CARLO CALCULATIONS vs MEASURED VALUES FOR NEUTRON AGE AND HIGHER MOMENTS IN Al/H_2O
(M/W = 1.000)

Density (in atoms/cc):

$Al = 3.026 \times 10^{22}$

$H = 3.337 \times 10^{22}$

$O = 1.668 \times 10^{22}$

	τ^{φ} (cm^2)	M_4^{φ} ($10^5 cm^4$)	M_6^{φ} ($10^8 cm^6$)
Calculation	56.7 ± 0.2	3.28 ± 0.03	7.32 ± 0.17
Experiment*	59.6 ± 0.9	3.71 ± 0.07	8.83 ± 0.23

*See Reference 11

TABLE 6

MONTE CARLO CALCULATIONS vs MEASURED VALUES FOR NEUTRON AGE AND HIGHER MOMENTS IN Fe/H_2O
(M/W = 1.737)

Density (in atoms/cc):

$Fe = 5.281 \times 10^{22}$

$H = 2.437 \times 10^{22}$

$O = 1.219 \times 10^{22}$

	τ^{φ} (cm^2)	M_4^{φ} ($10^5 cm^4$)	M_6^{φ} ($10^8 cm^6$)
Calculation	45.6 ± 0.1	1.87 ± 0.01	2.48 ± 0.03
Experiment*	46.4 ± 0.5	2.00 ± 0.03	2.90 ± 0.08

*See Reference 12

TABLE 7

MONTE CARLO CALCULATIONS vs MEASURED VALUES FOR NEUTRON AGE AND HIGHER MOMENTS IN Zr/H_2O
(M/W = 1.200)

Density (in atoms/cc):

$Zr = 2.359 \times 10^{22}$

$H = 3.281 \times 10^{22}$

$O = 1.514 \times 10^{22}$

	τ^{φ} (cm^2)	M_4^{φ} ($10^5 cm^4$)	M_6^{φ} ($10^8 cm^6$)
Calculation	47.1 ± 0.2	2.24 ± 0.02	4.0 ± 0.1
Experiment*	49.7 ± 0.9	2.71 ± 0.07	5.6 ± 0.4

*See Reference 13

From the lack of agreement between the measured and calculated moments for heavy water and graphite we conclude that the neutron cross-section data for elastic scattering in deuterium and carbon are unsatisfactory and should be re-evaluated.

It is more difficult to assess the adequacy of the ENDF/B metal-nuclide neutron cross-section data. Measurements for the neutron age and the higher moments in such homogeneous moderators as H_2O, D_2O, and C were relatively clean in the sense that the systems were essentially infinite, and corrections for neutron-streaming effects were not necessary. For the metal/water measurements the experimental systems were not homogeneous. For such systems Palmedo(14) has demonstrated that the slowing-down distributions produce significantly different results due to geometric anisotropies as compared to the homogeneous moderators. Homogeneous calculations for such heterogeneous experimental systems tend to underestimate measured-moment values. This is apparently confirmed by the results in Tables 5, 6, and 7. We simply state that the cross-section data for iron, aluminum, and zirconium are not above suspicion. Other types of data-testing are required to better resolve the adequacy of these data.

The evaluation of the ENDF/B cross-section data for hydrogen, deuterium, carbon, and oxygen was extended as follows: graphical comparisons for the several cross-sections per nuclide were prepared (Figures 1 through 10) with the ENDF/B data compared to the AIENDF data originally used to analyze the neutron-age measurements. For deuterium and carbon (Figures 2 through 6) the graphs quickly picked out the areas of difference. For ENDF/B deuterium the elastic-scattering cross-section is generally lower than the AIENDF data over the greater portion of the energy range of interest; for carbon the ENDF/B data are generally higher than the AIENDF data over the greater portion of the energy range of interest. Minor differences exist in the two data sets for oxygen above 1 Mev. The effects of these differences are illustrated in Table 8. The same sets of angular data needed to express the elastic-scattering anisotropy were used for each of the calculations.

TABLE 8

COMPARISON OF RESULTS, ENDF/B vs AIENDF vs EXPERIMENT

	τ^{φ} (cm^2)	M_4^{φ}	M_6^{φ}
H_2O		(10^4 cm^4)	(10^8 cm^6)
ENDF/B	26.1	9.66	1.72
Experiment	26.5	9.34	1.37
AIENDF	26.1	9.55	1.71
D_2O		(10^5 cm^4)	(10^9 cm^6)
ENDF/B	117.6	10.0	2.45
Experiment	111 109	-	-
AIENDF	106.6	8.3	1.86
C		(10^6 cm^4)	(10^{10} cm^6)
ENDF/B	295.6	6.10	3.56
Experiment	307.8	6.58	3.84
AIENDF	307.4	6.59	4.01

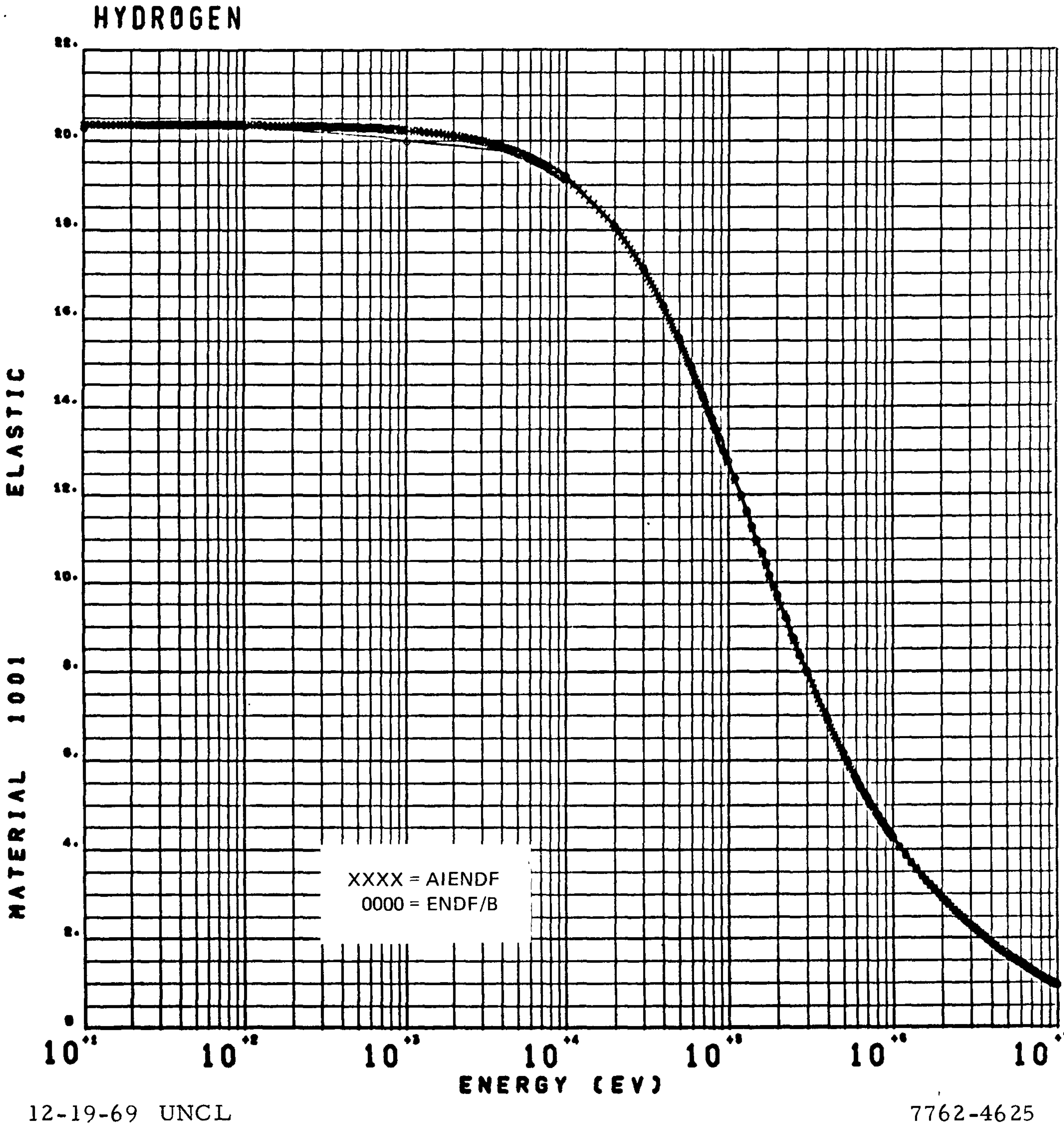

Figure 1. Comparison of Hydrogen Elastic-Scattering Cross-Section

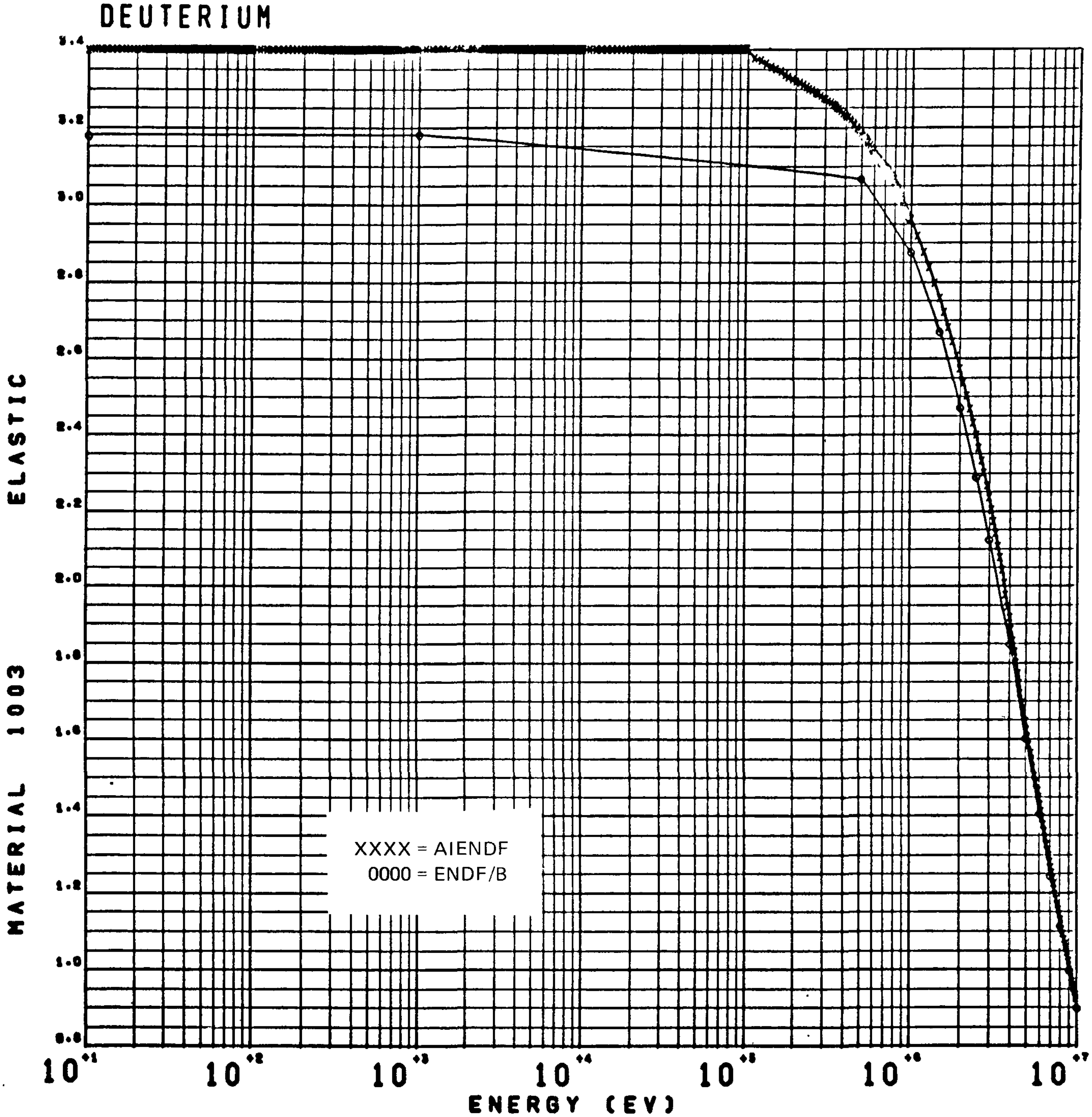

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Figure 2. Comparison of Deuterium Elastic-Scattering Cross-Section

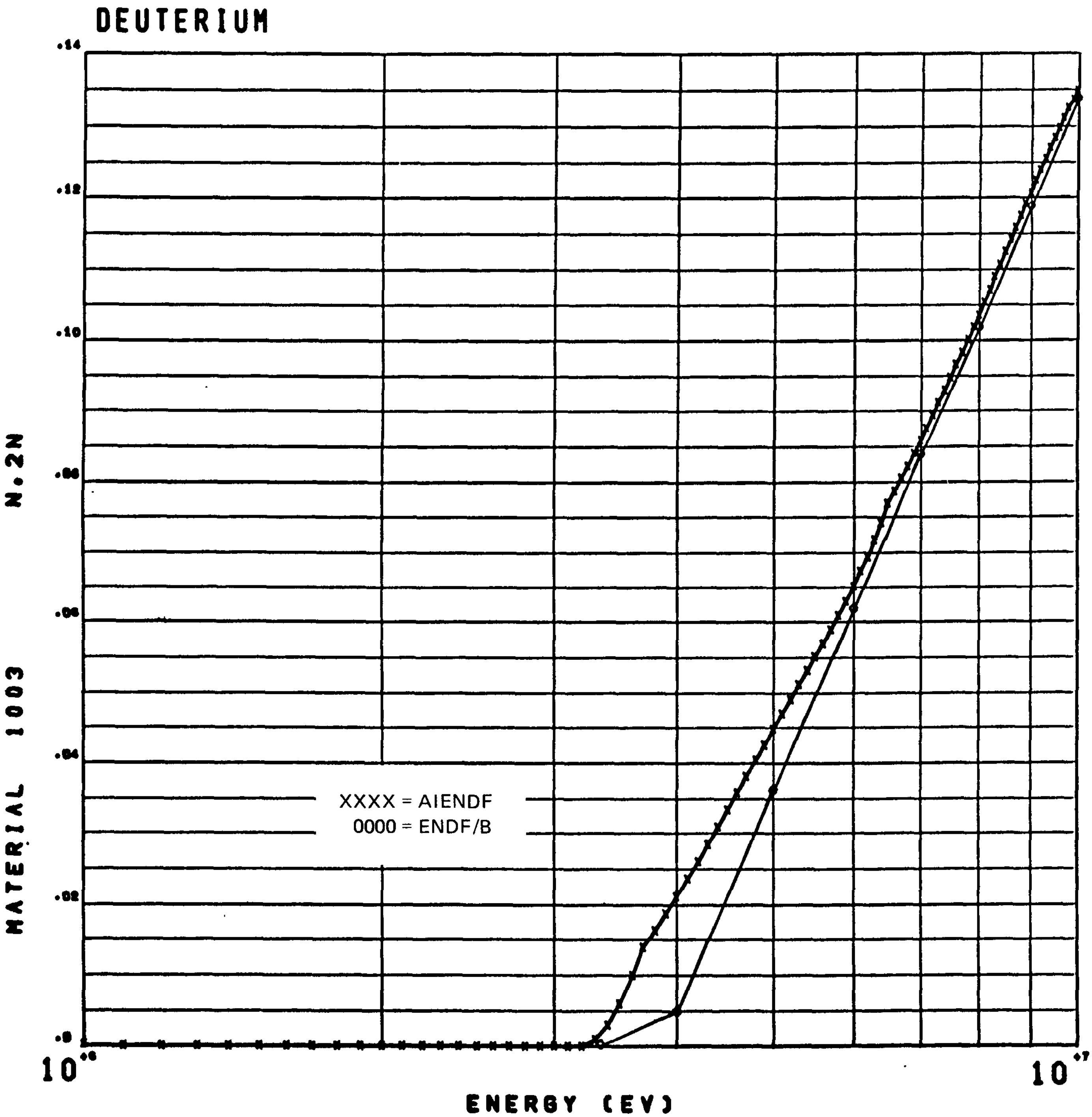

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Figure 3. Comparison of Deuterium (n,2n) Cross-Section

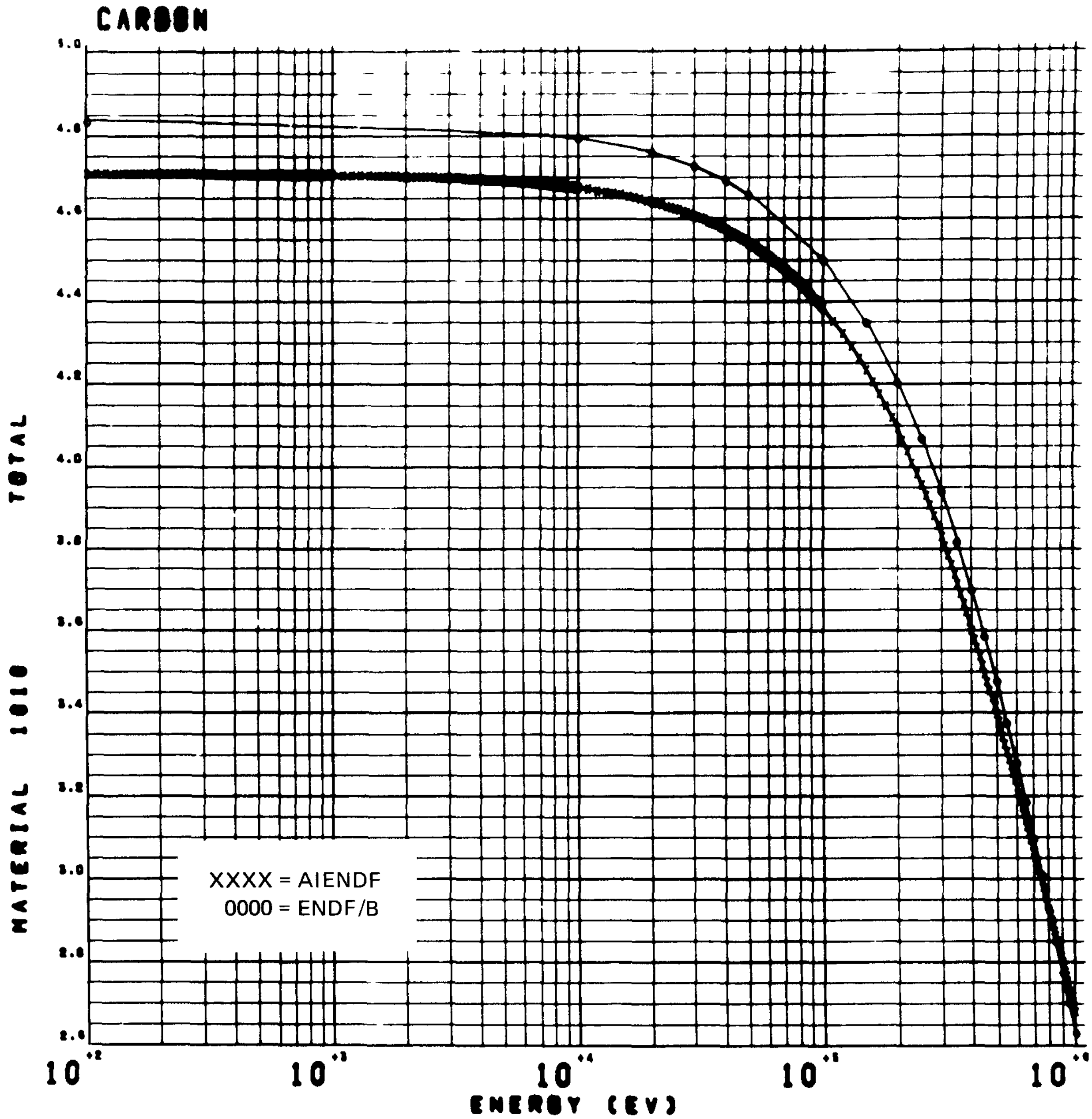

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Figure 4. Comparison of Carbon Total Cross-Section

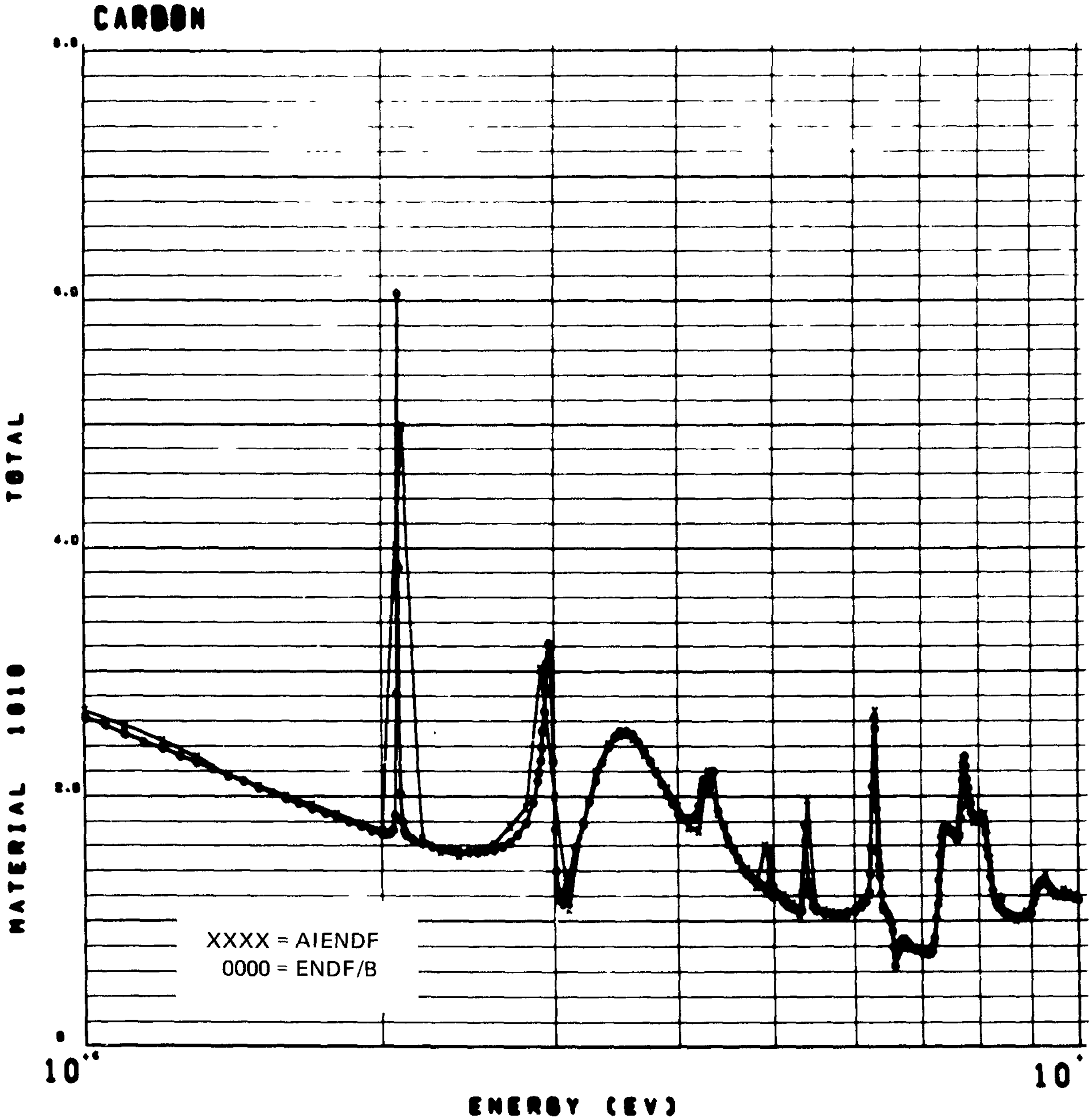

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Figure 5. Comparison of Carbon Total Cross-Section

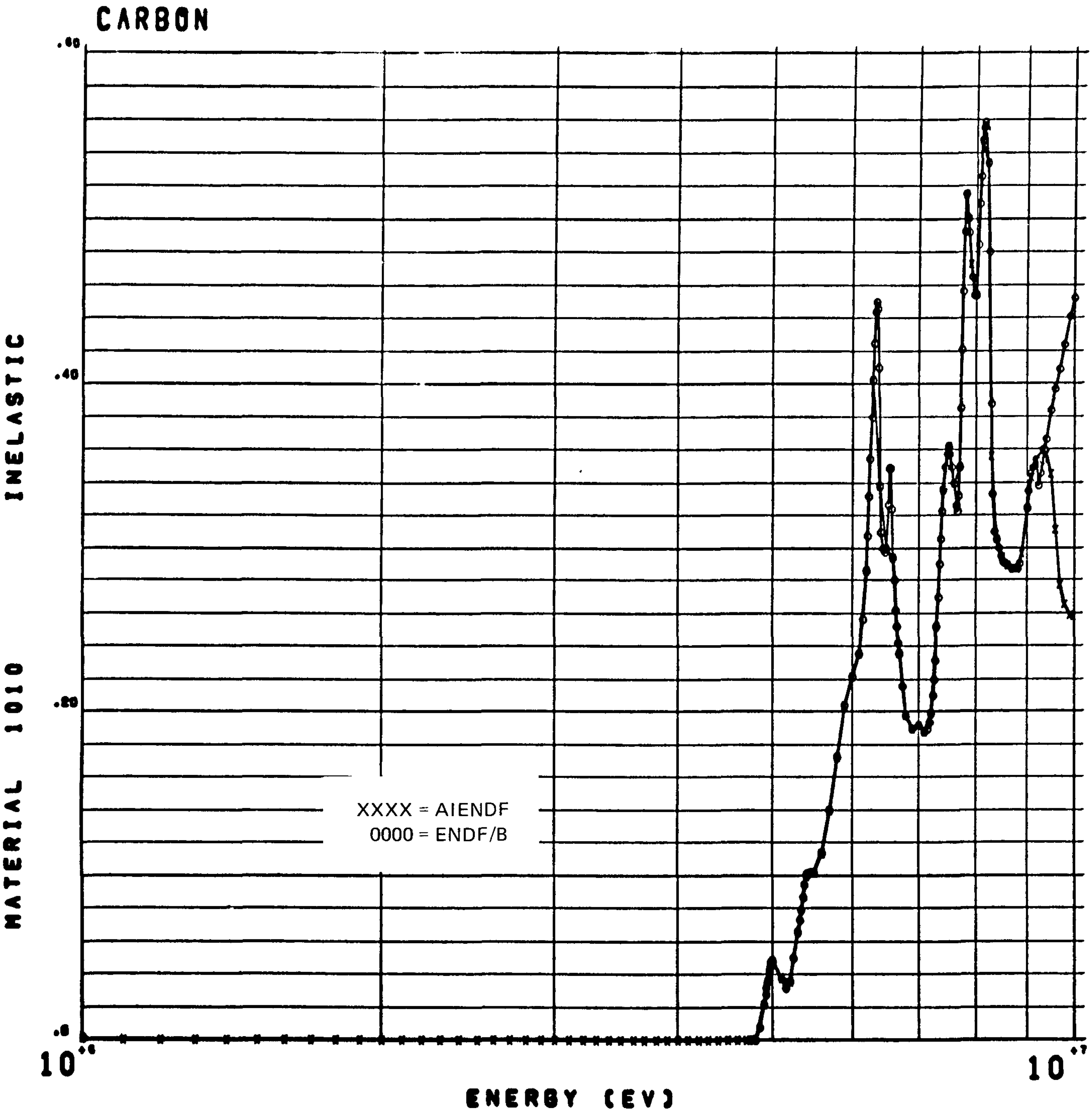

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Figure 6. Comparison of Carbon Inelastic-Scattering Cross-Section

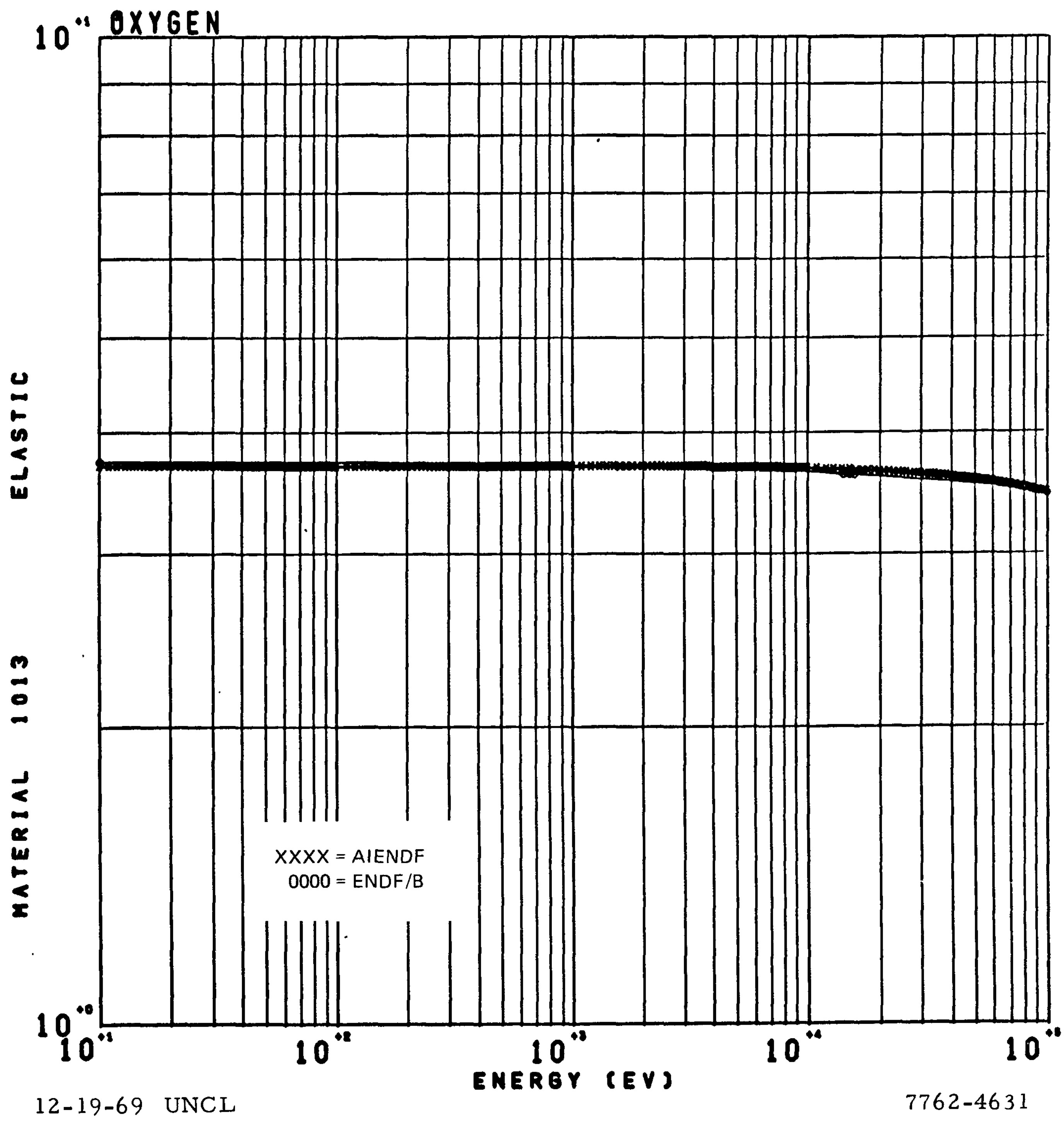

Figure 7. Comparison of Oxygen Elastic-Scattering Cross-Section

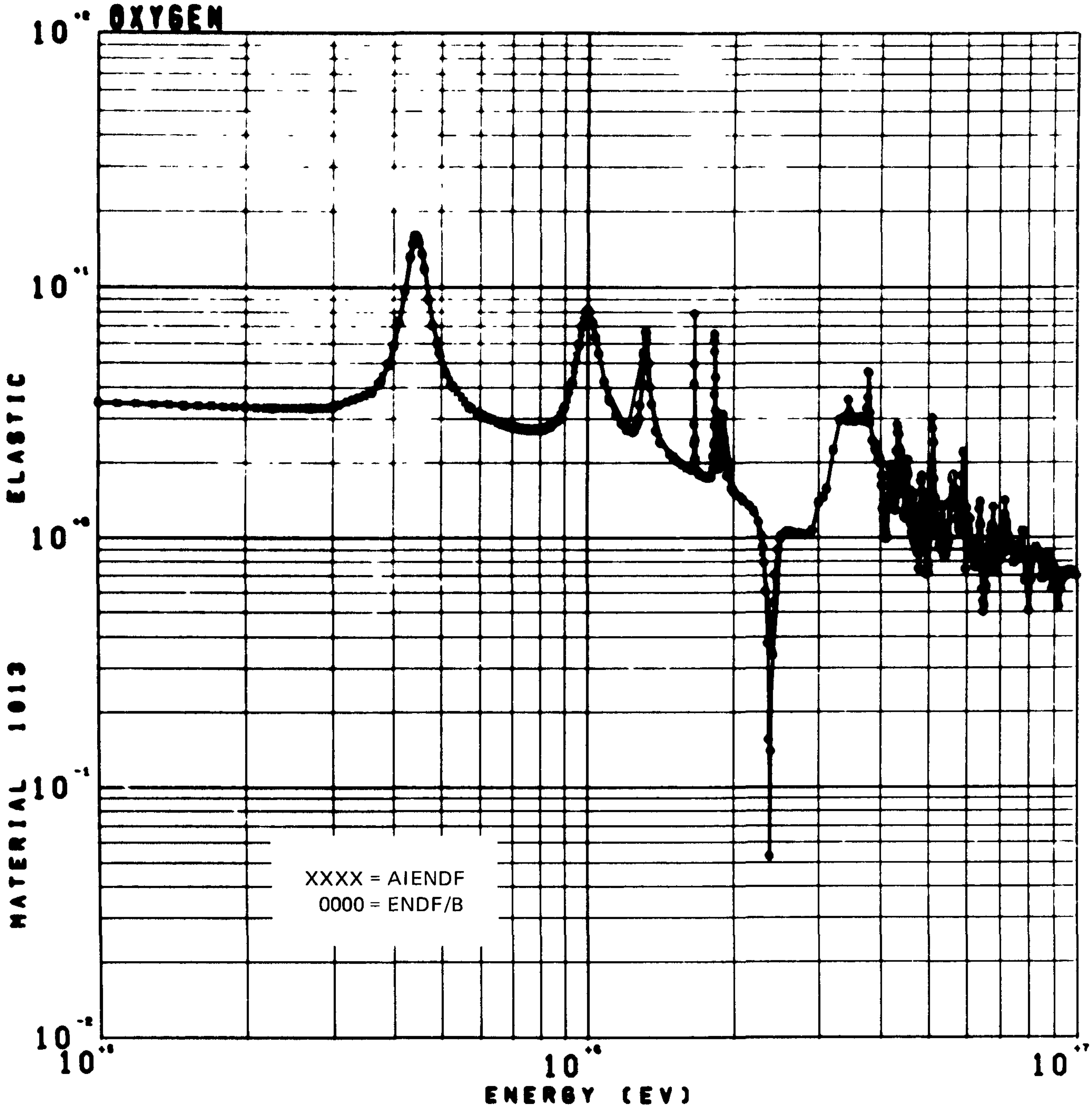

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Figure 8. Comparison of Oxygen Elastic-Scattering Cross-Section

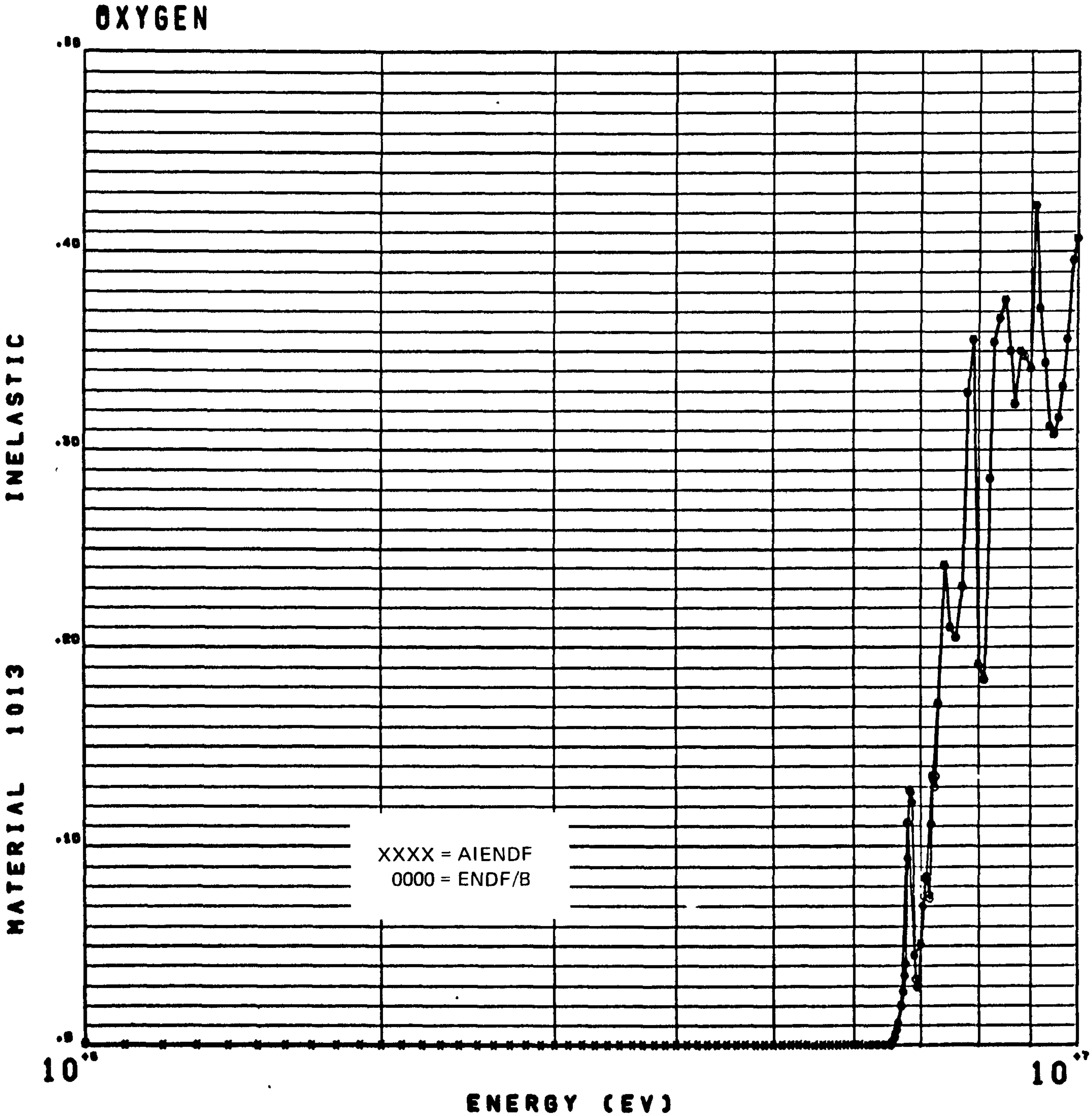

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Figure 9. Comparison of Oxygen Inelastic-Scattering Cross-Section

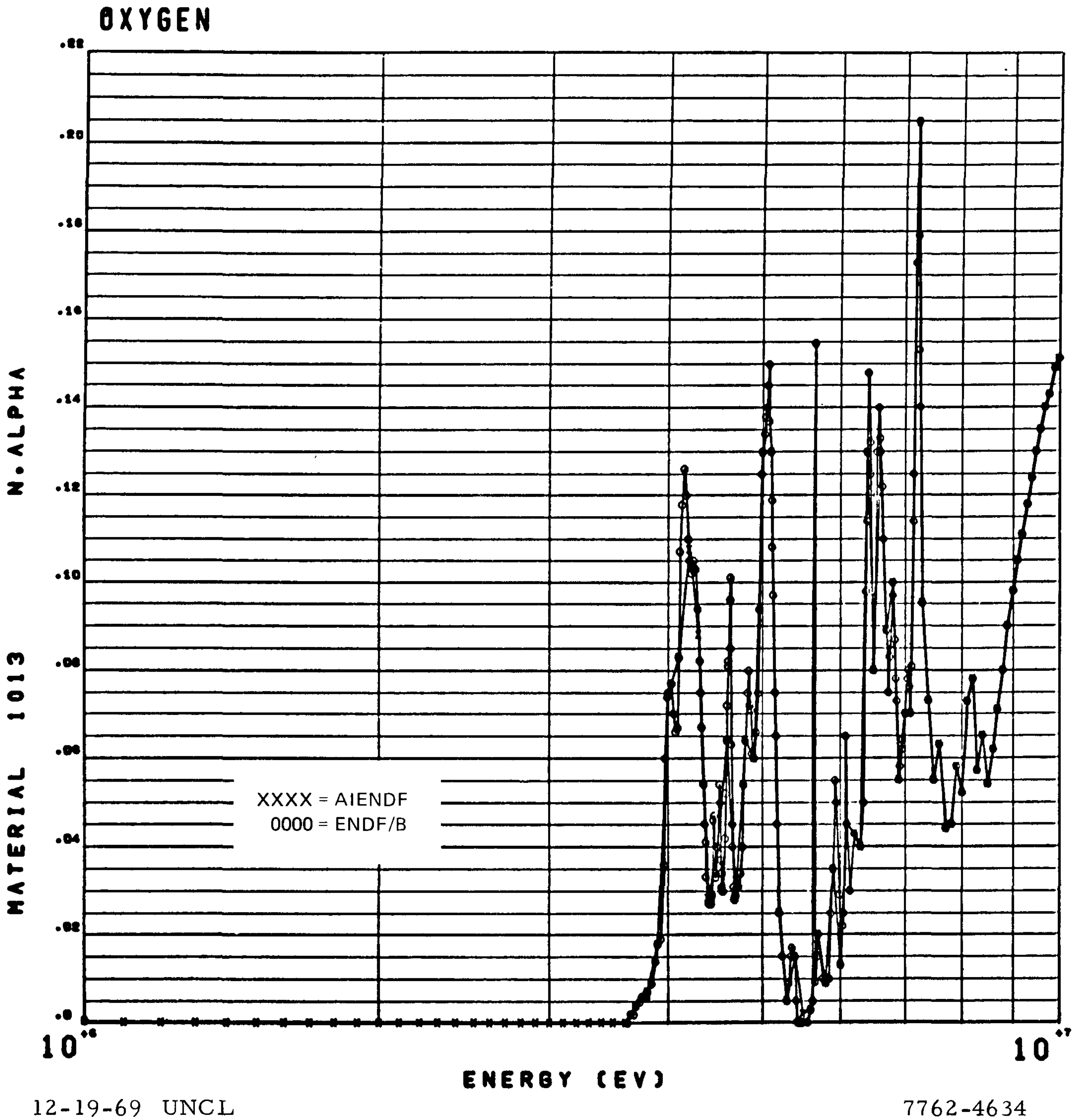

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Figure 10. Comparison of Oxygen (n,α) Cross-Section

IV. CONCLUSIONS

The applicability of the Monte Carlo code TYCHE IV to aid in the Phase-II data testing of the ENDF/B data files has been demonstrated. Comparison of calculated quantities with measured values reveals that the ENDF/B data for hydrogen and oxygen are probably satisfactory; that the elastic-scattering data for deuterium and carbon are unsatisfactory; and that determination of the validity and adequacy of the data files for aluminum, iron, and zirconium is dependent on forms of testing other than those reported here. It is recommended that the data files for deuterium and carbon be re-examined.

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