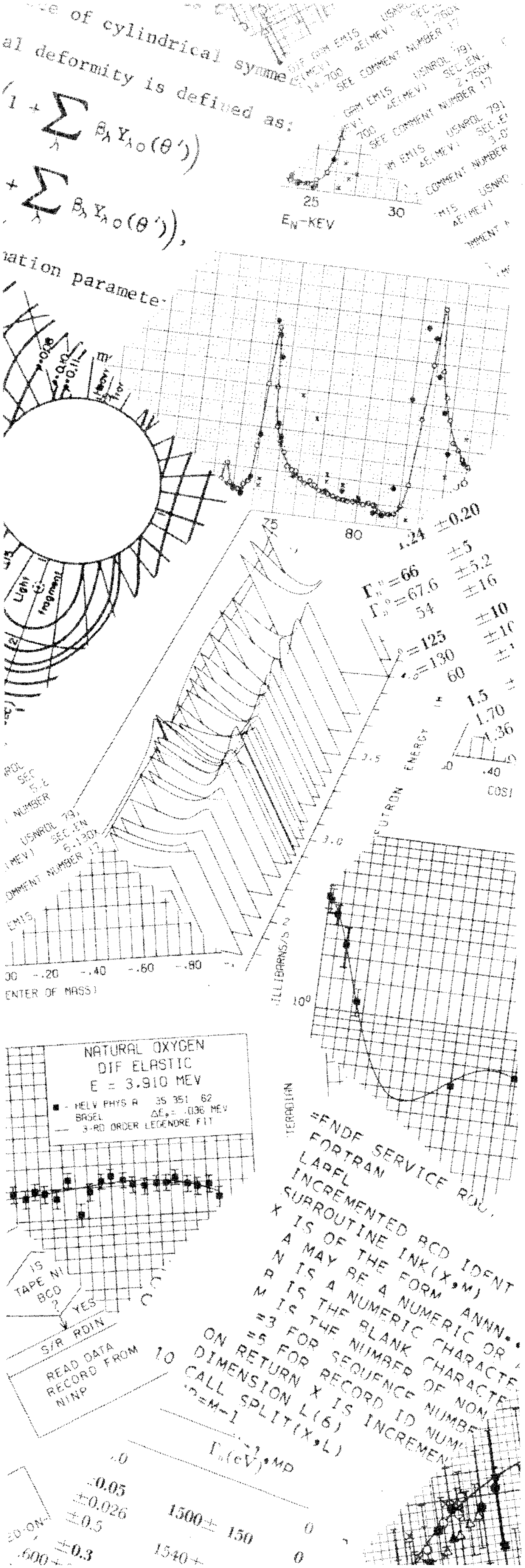

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EVALUATION OF ^{232}Th FOR ENDF/B-V

M.R. Bhat

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Abstract

This report describes the evaluation of neutron and gamma ray production cross sections of ^{232}Th from 10^{-5} eV to 20 MeV and mainly discusses the parts contributed by the author to the evaluation. All available new data have been included in this work and the procedures used to assess the experimental data and adopt recommended values are described.

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Evaluation of ^{232}Th

for

ENDF/B-V

1.0 Introduction

This report describes the evaluation of the neutron and gamma ray production data on ^{232}Th for ENDF/B-V (MAT=1390). This was a joint effort to which many persons from a number of institutions e.g., Argonne, Lawrence Livermore, Battelle-Northwest, Oak Ridge and Brookhaven contributed. Some of these partial evaluations have been described by their authors in a number of reports. Reference will be made to these reports in this section in giving an overview of the evaluation and their contents will not be discussed in detail. In assembling these partial evaluations to form the data file, some changes had to be made. These changes as well as the contributions to the evaluation by the author of this report will be discussed in detail here.

The neutron and gamma ray production cross sections given in the current evaluation of ^{232}Th (MAT=1390 of ENDF/B-V) over the neutron energy range from 1.0×10^{-5} eV to 20 MeV may be summarized as follows:

File 1: General description of the evaluation with references. This contains $\bar{\nu}_t$, $\bar{\nu}_d$ and $\bar{\nu}_p$ evaluations based on the latest available data. The $\bar{\nu}_d$ evaluation is by Kaiser and Carpenter[1] and the $\bar{\nu}_p$ data were evaluated by Gwin[2]. Energy released in fission and its partition into the different decay modes is also given[3].

File 2: Resolved resonance parameters cover a region from 5 eV to 4 keV and were evaluated by Leonard et al[4]. Various modifications to these as well as providing the background to substitute for missing p-wave resonance will be discussed in this report (Section 2.1). Unresolved resonance region extends from 4-50 keV. Procedure used to extract unresolved resonance parameters is given in Section 2.2.

<u>File 3</u>: The thermal region from 10^{-5} eV to 5 eV is mainly based on the Leonard evaluation[4] with a number of modifications discussed in Section 3.1. The continuum region extends from 50 keV and up. Evaluations of the total, capture, fission, inelastic scattering, (n,2n) and (n,3n) cross sections are by Meadows et al[5].

<u>File 4</u>: Angular distributions for elastic and inelastic scattering are based on experimental data where available supplemented by nuclear model calculations[5]. Secondary neutrons due to remaining reactions are assumed to be isotropic.

<u>File 5</u>: Secondary neutron energy distributions due to (n,2n) and (n,3n) reactions are by Meadows et al[5], and are based on the statistical model of Segev[6] with a preequilibrium component. The prompt fission neutron spectrum evaluation is discussed in Section 4. Neutron scattering into the continuum and their energy distribution was evaluated by Meadows et al[5]. Kaiser and Carpenter[1] obtained the energy distribution of delayed neutrons.

<u>File 8</u>: Fission products yield data are from the Fission Products Yields Subcommittee[7] (with T.R. England Chairman). Radioactive decay data were prepared by Reich[8].

<u>File 12</u>: Gamma ray production data were evaluated by Howerton[5,9]. For all incident energies the photon multiplicities due to fission were derived from the data of Peelle and Maienschein[10] on the prompt gamma

rays from the thermal neutron fission of ^{235}U. It was also assumed that the multiplicities are independent of incident neutron energy. Photon production from neutron capture is represented by energy dependent multiplicities and an energy independent spectrum. The spectrum used was based on undocumented data on ^{238}U with minor adjustment for small Q-value differences between ^{238}U and ^{232}Th.

File 13: Explicit representation of three photons of energy 0.04971, 0.1632 and 0.3344 MeV from inelastic scattering was derived from smooth cross section data and known branching ratios. For incident neutron energies greater than 0.7251 MeV, the Howerton formalism[11] for the calculation of continuum gamma ray production was used to obtain photon production cross sections and spectra from all reactions except photons from the above first three inelastic groups, capture and fission.

File 14: All photon angular distributions are assumed to be isotropic.

File 15: Photon spectra due to all non-elastic processes except fission and capture were derived from the formalism[11] used to calculate photon production.

For fission, the measured photon spectrum[10] was used for all incident neutron energies because of lack of experimental data.

The photon spectrum due to capture is based on an undocumented measurement of photon spectrum due to thermal capture in ^{238}U.

File 31: The covariance files on $\bar{\nu}_t$ are by Gwin[2].

File 33: The covariance files on fission and capture are discussed in Section 5.

In the following sections, the discussion will follow the above sequence of the data files rather than going from low to high incident neutron energies.

2.0 The Resonance Region

2.1 The Resolved Resonance Region

The resolved resonance region of ^{232}Th extends from 5 eV to 4 keV and was evaluated by Leonard et al[4]. In this energy region, results from the resolved resonance parameters have to be added to the background cross sections to obtain the evaluated cross sections. The evaluated resonance parameters are essentially the same as those in the third edition[12] of BNL-325 except for the inclusion of a fission width of 1.3×10^{-7} eV for s-and p-wave resonances. Leonard et al, introduced two bound levels and determined their parameters from the resonance theory fitting code SIGLEARN[4]. This code was used to perform a simultaneous least squares fitting of the low energy data on fission, capture, and scattering cross sections as well as relevant linear combinations of these such as total and absorption cross sections, alpha and eta. Adler-Adler multilevel formalism is used to determine the energy dependence of the capture and fission cross sections. Scattering cross section is described by the multilevel Breit-Wigner formalism. In using this code for ^{232}Th, the parameters of the two bound levels and the first two positive energy levels could be put in explicitly, while contributions of other positive energy resonances were included in the background terms. The parameters of the positive energy doublet at 21.8 eV and 23.4 eV were fixed at the values in BNL-325. A negative energy resonance was fixed at -22.2 eV; approximately an average level spacing from the expected location of the first negative energy resonance. The radiation width of the first negative resonance was also fixed at the average value of 21.2 meV. The remaining parameters were then determined by a least-squares fit. A 1/v background in the capture cross section was added from 5 eV to 4.0 keV corresponding to a thermal value of 1.88 b. Further details are to be found in

Ref 4. There are s and p-wave assignments to quite a few resonances in BNL-325 though the spins of the p-wave resonances are not known. The p-wave assignments are mainly based on the work of Rahn et al[13]. Leonard has arbitrarily set all the p-wave resonance spins to be 1/2; however, this is not expected to have any significant effect on the results as the p-wave resonances are in general weak. With the Leonard resonance parameters and the low energy (10^{-5} eV-5.0 eV) capture cross section, one obtains a dilute resonance capture integral of 79.9 b as compared to the recommended value of 85±3 b[12]. To obtain a higher resonance capture integral, it was decided to increase the Γ_n of the first two positive energy resonances and set them equal to those evaluated by Derrien[14]. The neutron width for the 21.78 eV and 23.43 eV resonances are respectively 2.02 and 3.88 meV and the gamma widths are 23.0 and 25.0 meV respectively. These are in good agreement with recent measurements by Chrien et al[15], who obtain 2.1±0.1 meV and 3.7±0.2 meV for the two neutron widths and 24.0±1.5 meV and 26.0±1.5 meV for the capture widths. With these modifications and other changes in the 10^{-5} eV-5.0 eV region (See Section 3.1) the dilute resonance capture integral is found to be 84.0 b in good agreement with the BNL-325 value.

In the Leonard evaluation, there are some 112 p-wave resonances from 8.35 eV to 2.932 keV. As mentioned earlier, the p-wave assignments follow from the work of Rahn et al[13]. These are all assigned to be J=1/2 resonances. A ladder plot of the p-wave resonances is shown in Fig. 1. In this plot the cumulative sum of reduced widths $\Sigma\Gamma_n^1$ of the p-wave resonances is shown plotted against the resonance energy. For comparison a straight line corresponding to the p-wave strength function $S_1 = (1.6\pm0.2)\times10^{-4}$ recommended[12] in BNL-325 is shown. This S_1 value is in good agreement with a recent measurement by Camarda using average neutron transmission data. From Fig. 1, it is evident that there are a number of missing resolved p-wave resonances. Hence, it is necessary to replace these with some contribution to the capture so that group averaged capture cross section give values in agreement with data. The following procedure similar to that used by Olsen[17] was adopted to calculate a smooth background equivalent to the missing p-wave resonances. Using the code RESEND and the p-wave resonances in the data files, the capture cross section was calculated on a fine grid from 5 eV to 4 keV. The result was averaged over 100 eV bins and the area a_{ri} under these curves in the i-th bin determined. Assuming a p-wave strength function of $S_1 = 1.6 \times 10^{-4}$ and a $\Gamma_\gamma = 21.1$ meV, capture and scattering cross sections were calculated at the same energy points at 100 eV intervals using the code UR[18]. Results of these calculations were used to calculate areas A_{ri} under these curves in 100 eV bins. The difference between these two sets of areas in effect gives the contribution of the missed p-wave resonances. A straight line ramp type of background was put in capture, scattering and total cross sections extending from 10 eV to 4 keV such that there was continuity at 10 eV and the area under the ramp was equal to the sum of the differences in A_{ri} and a_{ri}.

2.2. The Unresolved Resonance Region

The capture cross section data in the unresolved resonance region from 4 to 60 keV is shown in Fig. 2. In this figure are shown data of Macklin and Halperin[19], Miskel et al[20], Stavisskii et al[21], Chrien[22], Yamamuro et al[23], Tolstikov et al[24], Chaubey and Sehgal[25], Stavisskii et al[26] and Poenitz[27]. The continuous curve shown was calculated using the code UR[18] and the evaluated energy independent unresolved resonance region parameters of de Saussure and Macklin[28]. The dashed line extending from 35 keV to 60 keV represents an evaluation by Poenitz[29]. From this figure it is apparent that the continuous curve goes through most of the experimental points though it lies lower than the

Chrien datum. At the time of the evaluation, this value was considered preliminary and much weight could not be given to it. Macklin and Halperin data may have a normalization problem. This is indicated by the low s and p-wave strength functions obtained by them from their data. Their s-wave strength function is 0.365 ± .024 which may be compared with the generally accepted value of 0.88, and obtained by other workers using various experimental methods. It should be noted from Fig. 2, that above 30 keV, the shape of the Macklin data and the Poenitz evaluation are similar. Since the de Saussure evaluation (the continuous curve) goes through most of the experimental points up to about 40 keV, it was decided to read off the capture cross section values from the continuous curve in Fig. 2 up to 35 keV and join it smoothly to the Poenitz evaluaiton[29] above that at higher energies up to 50 keV. These values read off at 1 keV intervals are given in Table I. These input data were used along with

extract a set of unresolved resonance parameters. The s- and d-wave strength functions were kept at 0.888×10^{-4} and 0.882×10^{-4} respectively; and $\Gamma_\gamma = 21.3$ meV as given by de Saussure and Macklin[28]. For p-wave resonances a $\Gamma_\gamma = 25.2$ meV was used and the reduced neutron width varied to fit the capture data. Thus, it is possible to fit the data with p-wave strength functions which differ from the accepted value of $S_1 = (1.6\pm0.2)\times10^{-4}$ by about ±20%. A larger $\langle\Gamma_\gamma(J^-)\rangle = 25.8$ meV as opposed to $\langle\Gamma_\gamma(J^+)\rangle = 21.6$ meV was also used by Derrien[14]. These different Γ_γ values for s and p-wave resonances may be justified if one assumes that the primary transitions are E1 and the low-lying final states populated by these are mostly of one parity. The resulting parameters were run through the code RESEND to check the calculated cross sections. They were found to agree with input data to within 0.2%. In Fig. 3, the evaluated ^{232}Th capture cross sections in the region 4-60 keV are compared as given in ENDF/B-IV and V.

3.0 The Smooth Cross Sections

3.1 The Thermal Region: 10^{-5} eV to 5 eV

The evaluated capture, scattering and total cross sections in this energy region are by Leonard et al[4] with some extensive modifications. These modifications were made in stages and will be given below chronologically.

The thermal capture cross section as originally evaluated by Leonard gave a value of 7.615 b. The data available at the time of assembling the evaluated files appeared to support a value of 7.40 b at 0.0253 eV. Hence, it was decided to retain the Leonard shape and renormalize his evaluation to a thermal value of 7.40 b. This choice has also been supported by the subsequent measurements of Chrien et al[15], who obtained 7.41±.08 b and Poenitz[30], who measured $\sigma_{n\gamma}$ (0.0253 eV) = 7.33±0.17 b. Leonard's scattering cross section was added to this renormalized capture cross section to give the total cross section in the data files. After these data files had been assembled, the recent data of low energy capture by Chrien et al[15], became available. They obtained a fit to the low energy data with a thermal capture cross section of 7.41 b. This was renormalized by a small factor to give 7.40 b at 0.0253 eV and used in ENDF/B-V from 2.6×10^{-2} eV to 5 eV. From 10^{-5} eV to 2.53×10^{-2} eV the renormalized Leonard capture cross section was retained. This new capture cross section was subtracted from the modified total cross section referred to above to obtain the scattering cross section in the data files. In Fig. 4 are shown the low energy capture data of Chrien et al[15], and the ENDF/B-IV, V and Leonard evaluations. As can be seen from this figure, the Leonard evaluation based mostly on the Lundgren data[31], in the eV region is lower than the ENDF/B-V evaluation by about 30% at 5 eV. The ENDF/B-IV is lower than ENDF/B-V by about 50% at the same energy. Between 5 eV and 15 eV, the background cross sections in file 3 were adjusted to obtain a smooth transition between the energy region below 5 eV and the resolved resonance region above 5 eV.

3.2 Capture Cross Section 50 keV - 20 MeV

This evaluation is by Poenitz who will be publishing details of this work. A comparison of ENDF/B-IV and V capture cross sections is shown in Fig. 5. The experimental data in this region are discrepant and new measurements are needed to resolve this discrepancy.

4.0 Prompt Fission Neutron Spectrum

There are very few data on the fission neutron spectrum of ^{232}Th. The only measurement that is available is due to Vasil'ev et al[32], at 14.3 MeV who obtained a mean energy of 2.255 MeV for the fission spectrum. The procedure adopted to calculate the fission spectrum is as follows:

Gwin's evaluation[2] of $\bar{\nu}_p$ (E) and the ratios $\sigma_{nn'f}/\sigma_{nf}$, $\sigma_{n,2nf}/\sigma_{nf}$ $\sigma_{n,3nf}/\sigma_{nf}$ from Poenitz[33] were used to calculate $\bar{\nu}_f$ (E)-the average number of neutrons from the fission process excluding any prefission neutrons from the (n,n'f), (n,2nf) and (n,3nf) reactions. Howerton and Doyas[34] have given an expression for the mean energy $\bar{E}$ of fission spectrum and $\bar{\nu}_f$ as:

$\bar{E} = 3/2\ T_m = 1.4955 + 0.1875\ \bar{\nu}_f$. This expression was used to calculate the mean energy of the fission spectrum as a function of incident neutron energy. The resulting functional dependance was normalized to the experimental value $\bar{E} = 2.255$ MeV by Vasel'ev at 14.3 MeV. From these values of $\bar{E}$ at different incident neutron energies, one could calculate the energy dependent parameters a and b of the Watt Spectrum:

$$f(E \rightarrow E') = \frac{e^{-E'/a}}{I} \text{ Sinh } (\sqrt{bE'})$$

since $\bar{E} = 0.5 + 1.5\ T_f$ where $T_f = a$ in the ENDF/B notation. The resulting parameters and $\bar{E}$ are given at a few energies in Table II.

5.0 The Error Files

The error files for ^{232}Th give estimated errors for $\bar{\nu}_t, \sigma_{nf}$ and $\sigma_{n\gamma}$ only. The variance-covariance matrices for $\bar{\nu}_t$ was evaluated by Gwin[2]. The variance-covariance matrices for σ_{nf} and $\sigma_{n\gamma}$ do not give any off-diagonal elements or correlations with other evaluations such as the ^{235}U(n,f) and other standards used in the evaluation. These files are a simplified representation of some of the error estimates for σ_{nf}, given in Table V-5, and $\sigma_{n\gamma}$, in the ^{232}Th evaluation report by the Argonne Group[5]. Further, it is estimated that the thermal capture cross section is known to about 1%. The Chrien data from 0.035 eV to about 15eV have errors from 3% to 14% and are estimated to be uncertain by about 8% in the energy band from thermal to 15 eV. Uncertainties in the capture cross section are estimated to be 10% from 15 eV to 1 MeV and about 20% above 1 MeV.

Table I

^{232}Th Capture Cross Section 4 to 50 keV

E_n(keV)	$\sigma_{n\gamma}$(b)	E_n(keV)	$\sigma_{n\gamma}$(b)
4	1.130	28	0.465
5	0.982	29	0.459
6	0.908	30	0.452
7	0.850	31	0.448
8	0.803	32	0.443
9	0.764	33	0.439
10	0.730	34	0.435
11	0.702	35	0.431
12	0.677	36	0.429
13	0.655	37	0.426
14	0.636	38	0.424
15	0.618	39	0.422
16	0.601	40	0.420
17	0.585	41	0.420
18	0.571	42	0.420
19	0.557	43	0.420
20	0.545	44	0.417
21	0.533	45	0.414
22	0.521	46	0.411
23	0.511	47	0.407
24	0.500	48	0.401
25	0.491	49	0.395
26	0.482	50	0.390
27	0.473		

Table II

^{232}Th Fission Spectrum Parameters.

E_n (MeV)	$\bar{E}$ (MeV)	a (MeV)	b (MeV^{-1})
10^{-11}	2.133	1.0888	1.6871
7.0	2.210	1.140	1.5389
14.0	2.255	1.170	1.4610
20.0	2.320	1.2131	1.3591

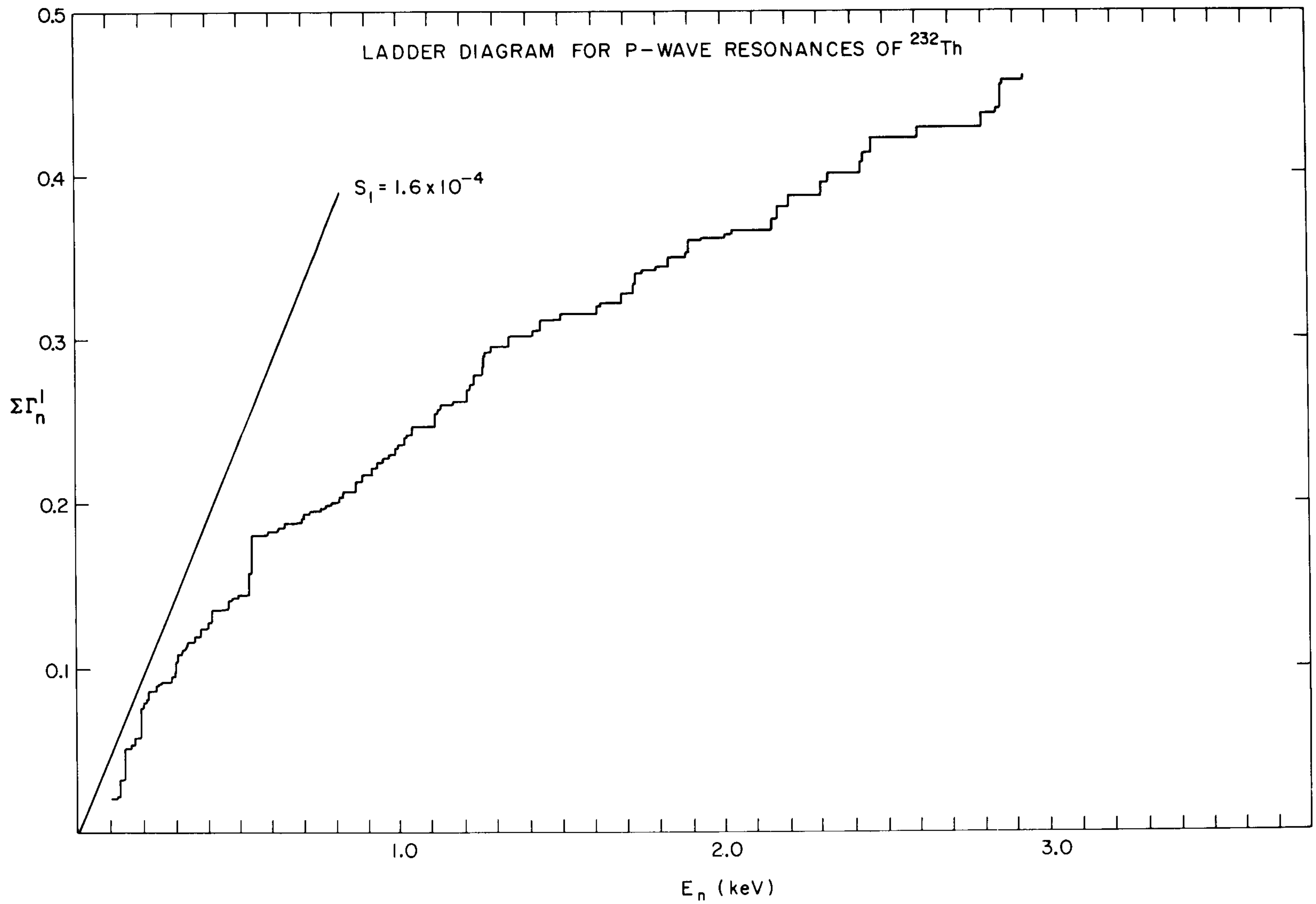

Figure 1. Ladder Diagram for P-wave Resonances of ^{232}Th.

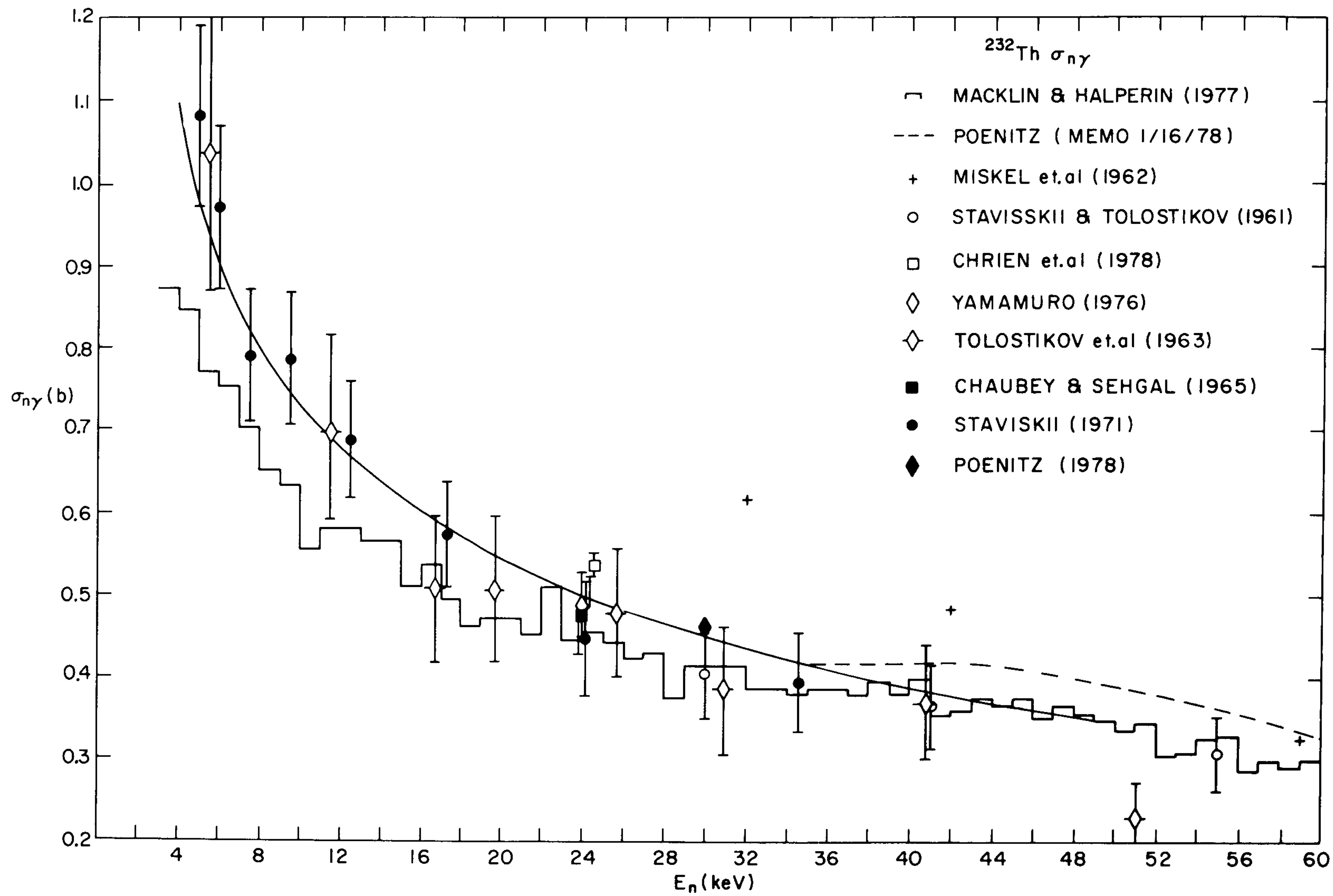

Figure 2. ^{232}Th Capture Cross Section 4-60 keV.

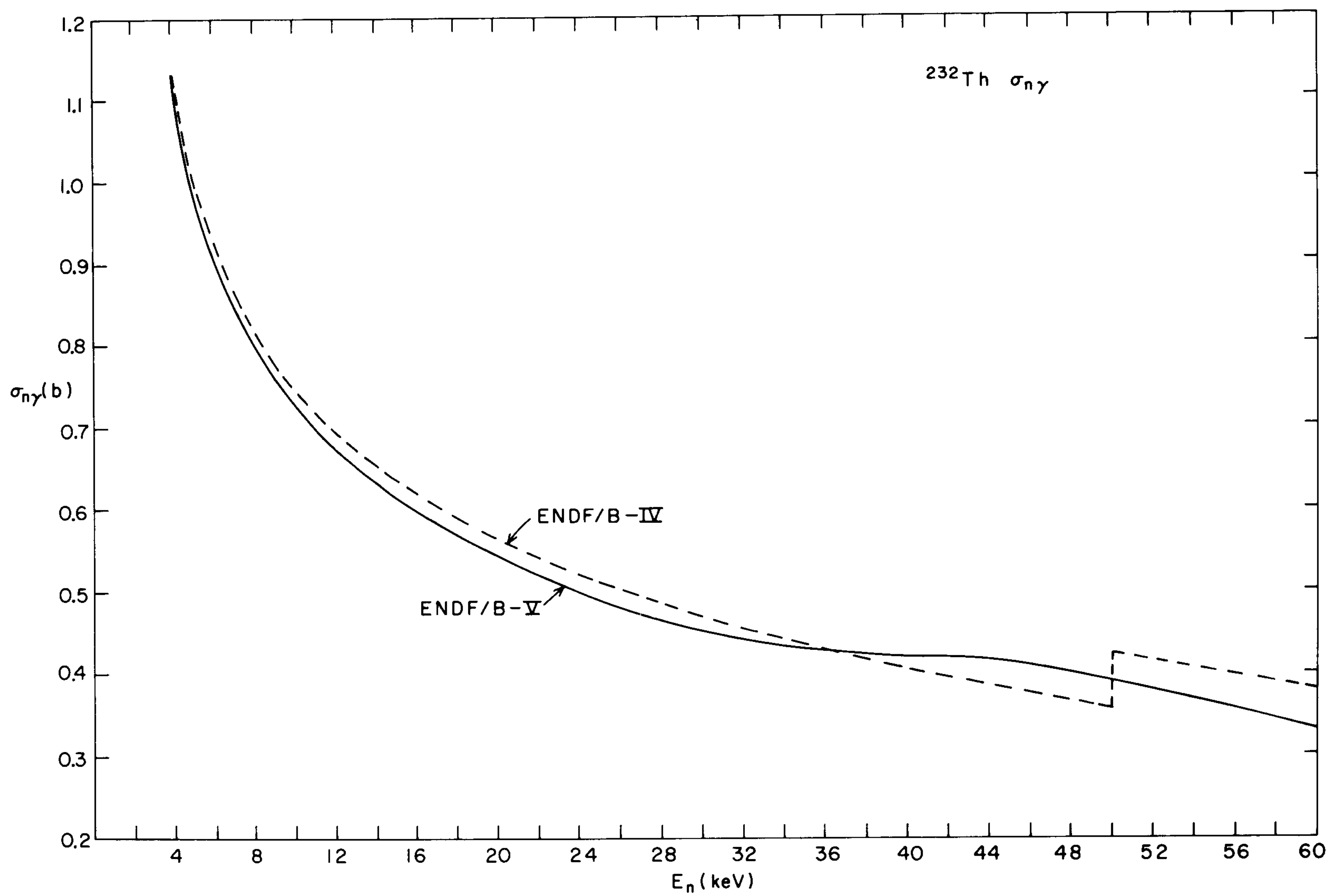

Figure 3. Comparison of ^{232}Th Capture Cross Section in ENDF/B-IV and V from 4-60 keV.

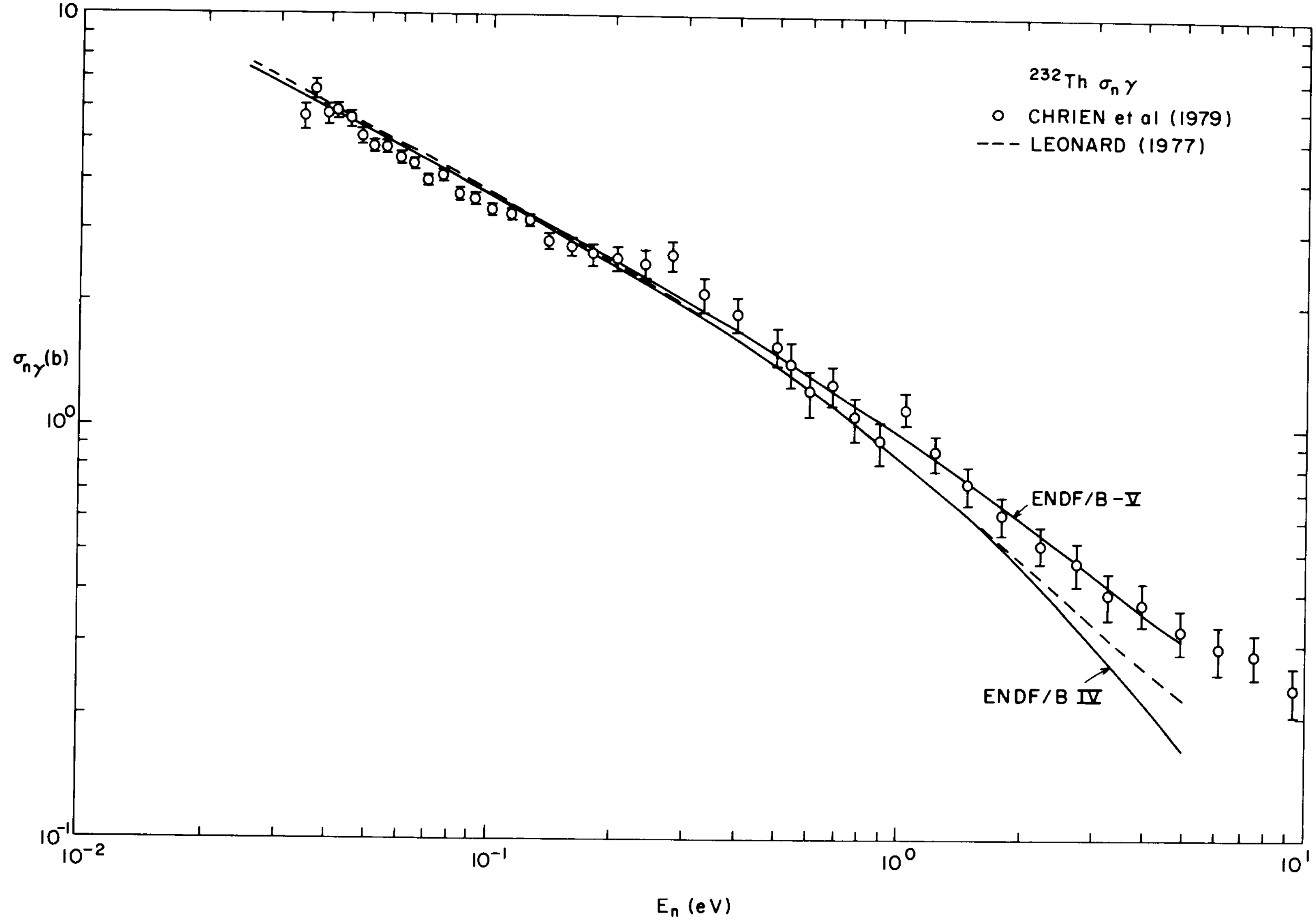

Figure 4. Low Energy Capture Data of Chrien et. al. with ENDF/B-IV, V and Leonard Evaluations.

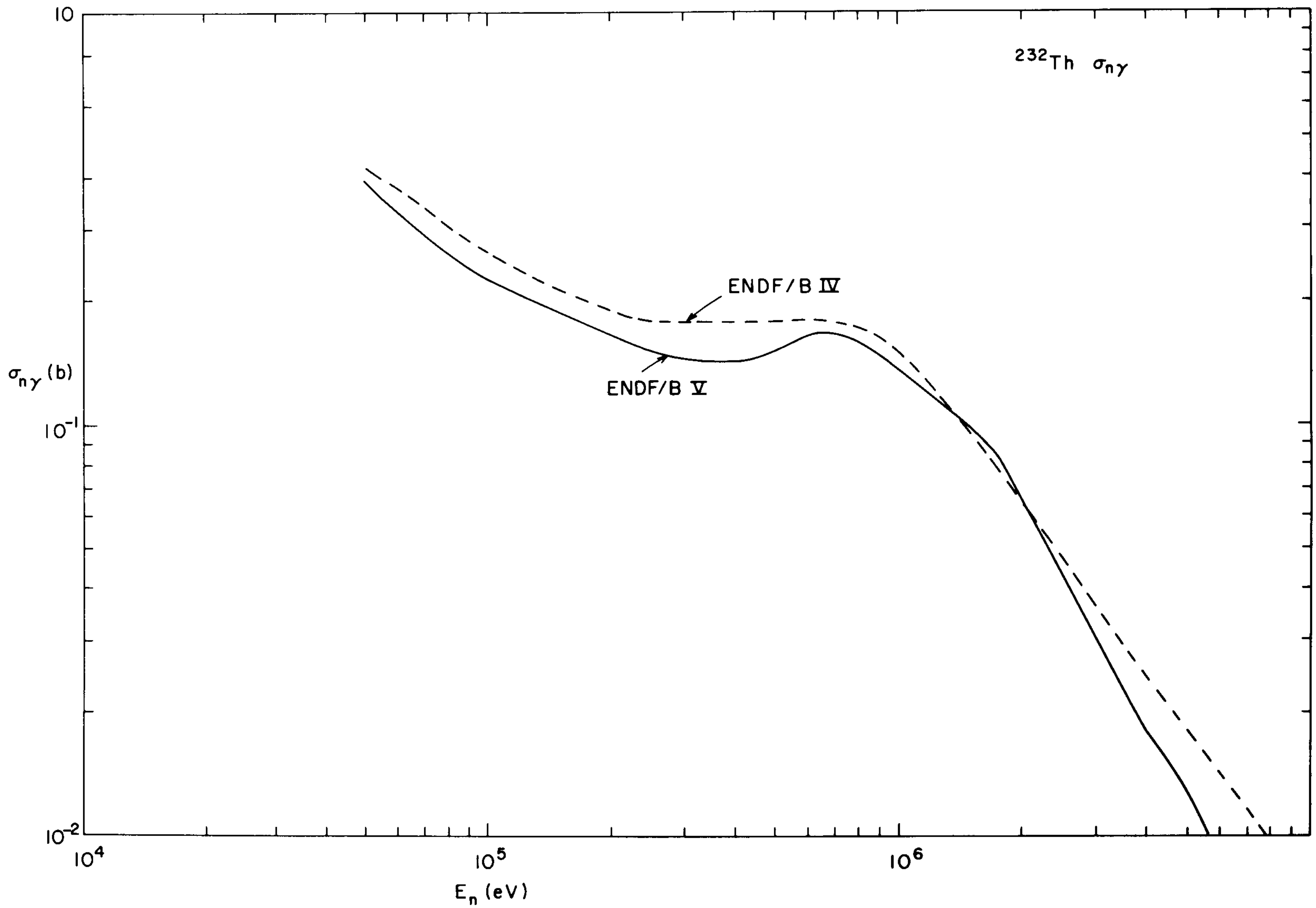

Figure 5. Comparison of ^{232}Th Capture Cross Section in ENDF/B-IV and V from 50 keV - 8MeV.

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