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ABSTRACT

This work considers the problem of accurately representing the temperature dependence of neutron cross-section data in neutron transport problems when there are many nuclides and when the temperature distributions vary significantly with both space and time. An approach involving interpolation between nuclear data libraries at various reference temperatures is investigated. Reference nuclear data libraries are obtained by Doppler broadening cross sections to the desired temperatures using the NJOY[1] code system. Several interpolation schemes over various temperature intervals are studied. Interpolated values at intermediate temperatures are compared to NJOY Doppler broadened results for the same temperature. Differences relative to the Doppler broadened results are calculated in order to judge the suitability of the interpolation scheme and temperature interval. The total, elastic scattering, capture, and fission (if applicable) reactions for ^{238}U, ^{235}U, natural Zr, ^{16}O, ^{10}B and ^{1}H are considered in this study, over a temperature range of 294 K to 811 K (~70 °F to ~1000 °F). The nuclides and temperature range are selected to best represent typical light water reactor calculations.

This work covers only the free-atom cross section and does not explore the many nuances of temperature treatment of nuclear data in the thermal energy range for nuclides where molecular binding effects are significant, e.g., water, beryllium, graphite. Additionally, dilute-average cross sections are used in the unresolved resonance range

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(URR) for this study. Temperature treatment of probabilistic methods used to construct cross sections in the URR are not considered for this work.

The study shows that cross sections can be interpolated within an accuracy of 0.1% over a temperature interval of 111 K (200 °F) for ^{1}H, ^{10}B, and ^{16}O. Smaller intervals are required for nuclides with more complex resonance behavior. Some values of the interpolated cross sections for natural Zr, ^{238}U and ^{235}U, remain greater than the target 0.1% relative difference even with a 28 K (50 °F) interval, suggesting a smaller interval is necessary for these nuclides.

I. INTRODUCTION

For isothermal transport problems, Doppler broadening techniques using the kernel-broadening[1,2,3] approach and Maxwellian free-gas distribution of target nuclide velocities allow for the convenient generation of point-wise, linear-linear interpolable, neutron cross-section sets at a desired temperature, prior to run time. This is the case for such popular codes as MCNP[4]. In instances where nuclides exist in a problem at many unique temperatures and/or the temperature is changing, e.g., a detailed temperature feedback model, cross-section information for many nuclides at many different temperatures may be required.

In these circumstances, it is possible to create separate Doppler broadened cross-section libraries at every possible temperature of the nuclides in the problem. However, this approach may prove problematic for cases involving more than a few nuclides and temperatures because of memory storage concerns. An additional complication to this approach is that the final temperature distribution may not be known *a priori*, as is the case in a temperature feedback problem.

An alternative to creating large sets of pre-Doppler broadened cross sections is to employ a method of approximating the cross section at various intermediate temperatures, given a set of cross-section libraries Doppler broadened at a small number of reference temperatures. The reference temperatures should be chosen to span the anticipated temperature range for a particular nuclide in the problem at some predetermined interval, e.g., 300 K to 800 K in 100 K steps. The accuracy of the interpolation is dependent not only on the size of the interval but the interpolation method used, the temperature range for the problem, and the behavior of the cross section in the resolved resonance region. Nuclides having "narrow resonances" tend to be more affected by Doppler broadening treatment and are therefore of more interest. Narrow resonances are characterized by a large Doppler width, Γ_D, relative to the total line width, Γ, where $\Gamma_D = \left(\frac{4E_0kT}{A}\right)^{1/2}$,

and

A = the atomic weight ratio of the target mass to the projectile mass,

k = Boltzmann's constant,

T = the target nuclei temperature in K,

E_0 = the energy of the resonance.

In addition to the Doppler effect on a single resonance, the presence of many close-spaced resonances can lead to interference effects. It is the combination of these effects that determine the accuracy of temperature interpolation. Therefore, nuclides with "complex" resonance behavior – many narrow and close-spaced resonances – are expected to be the most challenging for interpolation.

II. CALCULATING CROSS SECTIONS AT INTERMEDIATE TEMPERATURES USING INTERPOLATION

The well-known Doppler broadening equation in terms of energy for a Maxwellian free-gas target nuclei distribution can be derived[2]

$$\sqrt{E}\sigma(E,T) = \frac{1}{2}\left(\frac{\alpha}{\pi E}\right)^{1/2} \int_0^\infty dE_r \sqrt{E_r}\,\sigma(E_r,0) \cdot \left\{ e^{\left[-\alpha\left(\sqrt{E}-\sqrt{E_r}\right)^2\right]} - e^{\left[-\alpha\left(\sqrt{E}+\sqrt{E_r}\right)^2\right]} \right\}, \qquad (1)$$

where

$\alpha = \frac{A}{kT}$,

and

A = the atomic weight ratio of the of the target mass to the projectile mass,

k = Boltzmann's constant,

T = the target nuclei temperature in K,

E = energy of the projectile in electron volts (eV),

E_r = the relative energy of the neutron as "seen" by the target nuclei,

$\sigma(E,T)$ = Doppler broadened cross section at energy E for target nuclei temperature T,

$\sigma(E_r,0)$ = cross section at energy E_r for target nuclei temperature of 0 K.

The nature of the convoluted integral of equation (1) does not suggest a simple interpolation scheme to calculate $\sigma(E,T')$ at some intermediate temperature, T', given Doppler broadened cross sections, $\sigma(E,T_1)$ and $\sigma(E,T_2)$. For this study, five possible interpolation schemes were investigated:

"lin-lin,"

$$\sigma(E,T') = \sigma(E,T_1) + \left[\sigma(E,T_2) - \sigma(E,T_1)\right]\left[\frac{T' - T_1}{T_2 - T_1}\right], \tag{2}$$

"log-log,"

$$\ln\left(\sigma(E,T')\right) = \ln\left(\sigma(E,T_1)\right) + \left[\ln\left(\sigma(E,T_2)\right) - \ln\left(\sigma(E,T_1)\right)\right]\left[\frac{\ln(T') - \ln(T)_1}{\ln(T_2) - \ln(T_1)}\right], \tag{3}$$

"sqrt-lin,"

$$\sigma(E,T') = \sigma(E,T_1) + \left[\sigma(E,T_2) - \sigma(E,T_1)\right]\left[\frac{\sqrt{T'} - \sqrt{T_1}}{\sqrt{T_2} - \sqrt{T_1}}\right], \tag{4}$$

"lin-log,"

$$\ln\left(\sigma(E,T')\right) = \ln\left(\sigma(E,T_1)\right) + \left[\ln\left(\sigma(E,T_2)\right) - \ln\left(\sigma(E,T_1)\right)\right]\left[\frac{T' - T_1}{T_2 - T_1}\right], \tag{5}$$

and “sqrt-log,”

$$\ln\left(\sigma(E,T')\right)=\ln\left(\sigma(E,T_1)\right)+\left[\ln\left(\sigma(E,T_2)\right)-\ln\left(\sigma(E,T_1)\right)\right]\left[\frac{\sqrt{T'}-\sqrt{T_1}}{\sqrt{T_2}-\sqrt{T_1}}\right]. \tag{6}$$

II.A Generating the interpolated cross sections

A temperature range of 294 K to 811 K and energy range of 1.0 x 10-5 eV to 20.0 MeV is used for this study. The energy and temperature ranges were chosen to represent typical light water reactor applications. Doppler-broadened cross section libraries are generated over this range using the NJOY[1] code system at the following temperatures: 294 K, 367 K, 478 K, 505 K, 519 K, 533 K, 547 K, 561 K, 589 K, 700 K, and 811 K. The ENDF/B files[5] were downloaded from the National Nuclear Data Center website. Point-wise cross sections were reconstructed from resonance parameters using a tolerance of 0.1% in the RECONR module and Doppler broadened and thinned using an error tolerance of 0.1% in the BROADR module. These tolerances ensure that linear interpolation between the resulting point-wise cross sections over energy will result in cross section errors below 0.1%. Therefore, the same tolerance is adopted as the “target” for computing cross sections based on interpolation over temperature in this work. To be consistent, if larger error tolerances are allowed in RECONR and BROADR, larger error tolerances should be allowed in the evaluation of interpolated cross sections over temperature as well. The reaction types examined for this study include total (mt=1), elastic scattering (mt=2), radiative capture (mt=102) and fission (mt=18), if applicable, where the “mt” numbers designate the ENDF/B reaction type[5].

For each nuclide in the study, values of the cross sections at each temperature are mapped to a union energy mesh using linear interpolation when necessary. Five interpolation intervals of decreasing magnitude are investigated using a target temperature of 533 K: 294 K to 811 K, 367 K to 700 K, 478 K to 589 K, 505 K to 561 K, and 519 K to 547 K. For every value on the union energy mesh, an interpolated cross section, $\sigma(E,T')$, is generated at 533 K, using the reference data sets and each interpolation law (equations (2) – (6)). The resulting value of $\sigma(E,T')$ is then compared to the NJOY Doppler broadened value at 533 K, $\sigma(E,T^*)$, and a relative difference, δ_{rel}, calculated using

$$\delta_{rel} = \frac{\left|\sigma(E,T^*) - \sigma(E,T')\right|}{\sigma(E,T^*)} \quad . \tag{7}$$

III. RESULTS

Because Doppler broadening is a resonance phenomenon, it is expected that the nuclides with significant resonance behavior will be most affected by the interpolation treatment suggested – specifically, those with large numbers of narrow resonances. Figure 1 through Figure 6 show the total cross section as a function of energy for the nuclides examined in this study. The Doppler effect is clearly shown in Figure 7 for two resonances on a fine energy mesh for cross sections at 294 K and 811 K.

The comparatively large resolved resonance region and large numbers of narrow resonances in ^{238}U singles this nuclide out as the most challenging to accurately represent using an interpolation method. Other nuclide cross sections that may be difficult to accurately represent include ^{235}U, natural Zr and ^{16}O. The ^{10}B and ^{1}H cross sections are not expected to be sensitive to the effects of Doppler broadening but are included in this work for completeness in considering materials common in typical reactor calculations. The variation in the number of points required to describe the cross section behavior versus incident neutron energy shown in Tables 1 through 7 is a measure of the variation of the cross section versus energy for the various nuclides. Nuclides having many resonances and sharp resonance peaks require more points to achieve the error tolerances specified in RECONR and BROADR for linear interpolation.

III.A ^{238}U Cross Sections

Table I shows the results of the five interpolation schemes for the five temperature interpolation intervals for the total cross section of ^{238}U. Accurate representation of the complex resonance absorption characteristics of ^{238}U prove difficult using interpolation. Total cross section relative differences for the best interpolation method using the smallest interpolation temperature interval still exceed 0.2%, with an average of 0.0071% and a maximum of 0.296%. Although all the relative differences are not less than the 0.1% target, a large fraction is in this range. Depending on the desired precision of the transport calculation, this difference may be inconsequential.

Results of interpolation for the other reaction rates are provided in Table II. Unlike Table I, these results are reported at the smallest temperature interval only, since the best possible results are obtained using this temperature interval. Relative differences for the fission reaction cross section are similar to those of the total cross section, however, larger maximum relative differences are observed and a greater number of relative differences exceed the 0.1% target, with some exceeding the 0.5% maximum value bin. Of the 645 points exceeding the 0.1% relative difference target, 618 have cross-section values $\leq$ 0.001 b and the remaining 27 cross-section values are between 0.001 and 0.1 b.

Interpolating the capture cross section results in 563 relative differences exceeding the 0.5% maximum bin value, suggesting that this reaction is not approximated well with interpolation. However, the average and maximum relative differences are comparable to the fission cross section. Figure 8 shows the relative difference in the interpolated capture cross section as a function of energy using the log-log scheme. As anticipated, the largest differences occur in the resolved resonance region where Doppler effects are the greatest. Of the 4030 points exceeding the 0.1% relative difference target, 2684 have cross-section values between 0.01 b and 0.1 b, 1085 have cross-section values between 0.1 b and 1.0 b, and the remaining 264 cross-section values are > 1.0 b with two values between 10 b and 100 b.

The interpolated elastic scattering cross section results show a greater number of points in the target range of <0.1% relative difference, with maximum and average relative differences that are in a more acceptable range. Of the 332 points exceeding the 0.1% relative difference target, 276 have cross-section values between 0.1 b and 5.0 b, 21 have cross-section values between 5 and 10 b, and the remaining 35 cross-section values are between 10 b and 100 b.

III.B ^{235}U Cross Sections

Table III shows the results for interpolating the total, capture, fission, and elastic scatter cross sections over the smallest temperature interval, 519 K to 547 K. The reduction in complexity of the cross section structure in the resolved resonance range relative to ^{238}U suggests that interpolation may yield more accurate results in ^{235}U. The total cross section average and maximum relative differences are ≤ 0.1%, with the one exception of the "lin-log" interpolation scheme. The interpolated fission and capture cross sections are less accurate, however, with some relative differences exceeding the 0.1% target. Maximum relative differences for the two reactions are < 0.2%, though, and average relative differences are well below the 0.1% target. Of the 12 points exceeding the 0.1% relative difference target for fission, 5 have cross-section values between 1.0 b and 5.0 b, 4 have cross-section values between 5.0 b and 10 b, and the remaining 3 cross-section values are between 10 b and 100 b.

Figure 9 shows the relative differences for the capture cross section as a function of energy. On average, the magnitude of the relative difference is about 10 times lower than for ^{238}U over the resolved energy range. Of the 41 points exceeding the 0.1% relative difference target, 22 have cross-section values between 0.1 b and 5.0 b, 6 have cross-section values between 5.0 b and 10 b, and the remaining 13 cross-section values are between 10 b and 100 b.

The elastic scattering cross section in ^{235}U is calculated well using interpolation and all relative differences are below 0.1%.

III.C Natural Zr Cross Sections

The natural Zr cross section is dominated by scattering rather than absorption as in ^{235}U and ^{238}U. Table IV shows the results for interpolating the total, capture, and elastic scatter cross section for natural Zr over the temperature range of 519 K to 547 K. With one exception, all the relative differences for the total and elastic scattering cross section are less than 0.1%.

The interpolated capture cross sections result in higher relative differences, however, capture is a much smaller component of the total cross section than elastic scatter. Average relative differences for the interpolated capture cross sections are less than 0.1% but the maximum differences are a ~1%. Figure 10 shows that the relative differences in the capture cross section for natural Zr are of the same order as for ^{238}U.

Of the 254 points exceeding the 0.1% relative difference target, 50 have cross-section values between 0.001 b and 0.01 b, 115 have cross-section values between 0.01 b and 0.1 b, 84 have cross-section values between 0.1 b and 1.0 b and the remaining 5 cross-section values are between 1.0 b and 5.0 b.

III.D ^{16}O Cross Sections

The cross section structure in ^{16}O allows for greater accuracy of interpolated cross sections. The interpolation interval can be extended from 28 K (519 K to 547 K) to 111 K (478 K to 589 K) while maintaining the relative differences near the target of 0.1%.

Table V shows the results for interpolating the total, capture, and elastic scattering cross sections over a temperature range of 478 K to 589 K. At this temperature interval, it is possible to achieve average and maximum relative differences less than 0.1% using a "log-log" or "sqrt-lin" interpolation scheme for all the reactions. The capture cross section is less sensitive to the interpolation method and all methods result in relative differences of no consequence.

III.E ^{10}B Cross Sections

The few, wide resonances and large energy span covered by the smooth "1/*v*" behavior of the ^{10}B cross section provides a good candidate for interpolation. As is the case with ^{16}O, the interpolation interval can be extended to 111 K while maintaining the relative differences around 0.1%.

Table VI shows the results of interpolating the total, capture, and elastic scattering cross section for ^{10}B over the temperature range of 478 K to 589 K. The total and capture cross sections are well-predicted using interpolation and relative differences are well within the 0.1% target. Relative differences calculated for the elastic scattering component of the cross section are higher but, using a "log-log" interpolation scheme, are below the target.

III.F ^{1}H Cross Sections

As in the case of ^{10}B, the ^{1}H cross section is anticipated to be a good candidate for interpolation. The smooth behavior of the cross section as a function of energy, with no resonance structure, will tend to produce more accurate interpolated cross sections. The interpolation interval can be safely extended to 111 K without exceeding the 0.l% relative difference target.

Table VII shows the results for interpolating the total, capture, and elastic scatter cross sections for ^{1}H, over the range of 478 K to 589 K. Relative differences for total and elastic scatter are kept below 0.1% using either a "log-log" or "sqrt-lin" interpolation scheme. Relative differences for capture are very low and insensitive to the interpolation scheme used.

IV. CONCLUSIONS

Interpolation of cross sections provides a means to perform transport calculations on problems with complex and/or changing temperatures without prior knowledge of the final temperature distribution. By Doppler broadening to a set of cross sections at a predetermined number of temperatures spanning the temperature range of the problem, cross sections can be calculated "on the fly" for any temperature in the model.

Materials with complex resonance behavior, such as ^{238}U, require fine interpolation intervals to obtain the desired degree of accuracy. In this study, an interval of 28 K (50

°F) was not suitable to reduce the relative differences of every point in the ^{238}U cross section to less than 0.1%. Integral testing of this method is necessary to characterize whether this magnitude of relative difference is significant for reactor calculations. For nuclides that do not exhibit complex resonance behavior, interpolation intervals as large as 111 K (200 °F) were shown to produce acceptable results.

Of the five interpolation schemes examined, the "log-log" interpolation scheme performed the best. Although, in some cases other schemes predicted a lower maximum relative difference, the "log-log" scheme generally resulted in lower average relative differences and a greater number of cross section relative differences below the 0.1% target.

An alternative to the interpolation method is the *in-situ* Doppler broadening approach. This approach is to-date untested and may be viable given the increasing computational speed of computers. This method requires only a single set of cross sections, Doppler broadened to the lowest possible temperature that the nuclide will experience in the problem. In the course of particle tracking, the cross section of the constituent nuclides for the material in which the particle currently resides are Doppler broadened to the appropriate temperature, on the fly. Upon entering a new material at a different temperature, or changing the temperature of the current material, the Doppler broadening process is repeated. Integral testing of this method is necessary to determine the speed penalty for Monte Carlo codes in particular. It may very well be the most accurate approach to solve transport problems with complex and/or changing temperature distributions.

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Table I. Results of various interpolation methods over various temperature intervals for the total cross section of ^{238}U at 533 K

Temperature interval: 294 K to 811 K						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 95499)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	60.3	2.88	19323	8125	12377	55674
Log-log	46.1	2.28	21303	10594	16760	46842
Sqrt-lin	75.1	2.78	19664	8919	13611	53305
Lin-log	35.1	3.14	19432	8156	12359	55552
Sqrt-log	34.5	2.58	19789	9033	13872	52805
Temperature interval: 367 K to 700 K						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 95499)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	26.6	1.23	29717	9432	13721	42629
Log-log	19.7	0.962	35278	12839	15007	32375
Sqrt-lin	32.2	1.18	31221	10457	13938	39883
Lin-log	17.0	1.37	29799	9484	13829	42387
Sqrt-log	15.5	1.11	31544	10648	14480	38827
Temperature Interval: 478 K to 589 K						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 95499)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	3.09	0.1363	62072	11864	16089	5474
Log-log	2.24	0.1057	70486	9259	10713	5041
Sqrt-lin	3.70	0.1306	65331	13720	12312	4136
Lin-log	2.04	0.1536	62542	12794	11765	8398
Sqrt-log	1.79	0.1239	67943	10737	10154	6665
Temperature Interval: 505 K to 561 K						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 95499)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	0.825	0.0349	86876	6750	1537	336
Log-log	0.612	0.0272	88195	5634	1620	50
Sqrt-lin	0.993	0.0335	88968	3860	1954	717
Lin-log	0.562	0.0394	84723	6342	4380	54
Sqrt-log	0.500	0.0318	86207	6236	3055	1
Temperature Interval: 519 K to 547 K						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 95499)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	0.309	0.0090	94812	679	8	0
Log-log	0.296	0.0071	95268	229	2	0
Sqrt-lin	0.332	0.0087	94423	946	130	0
Lin-log	0.252	0.0101	94794	703	2	0
Sqrt-log	0.274	0.0082	95382	116	1	0

Table II. Results for interpolating the fission, capture, and elastic scattering cross sections over the temperature interval of 519 K to 547 K for ^{238}U

Fission						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 95499)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	1.68	0.0049	94462	644	342	51
Log-log	1.34	0.0038	94854	505	118	22
Sqrt-lin	1.77	0.0054	94111	892	425	71
Lin-log	1.25	0.0046	94578	800	100	21
Sqrt-log	1.29	0.0041	94842	555	80	22
Capture						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 95499)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	1.75	0.040	88038	4879	2019	563
Log-log	1.95	0.032	91466	3003	464	563
Sqrt-lin	1.70	0.042	85644	6130	3160	563
Lin-log	2.05	0.045	85413	9188	334	564
Sqrt-log	2.00	0.038	90464	4132	340	563
Elastic Scatter						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 95499)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	0.349	0.0085	94539	681	279	0
Log-log	0.314	0.0065	95167	324	8	0
Sqrt-lin	0.402	0.0085	94160	898	441	0
Lin-log	0.266	0.0094	94322	1163	14	0
Sqrt-log	0.290	0.0076	95038	454	7	0

Table III. Results for interpolating the total, fission, capture, and elastic scattering cross sections over the temperature interval of 519 K to 547 K for ^{235}U

Total						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 74549)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	0.094	0.0096	74549	0	0	0
Log-log	0.087	0.0063	74549	0	0	0
Sqrt-lin	0.082	0.0076	74549	0	0	0
Lin-log	0.112	0.0101	74546	3	0	0
Sqrt-log	0.100	0.0081	74549	0	0	0
Fission						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 74549)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	0.129	0.0156	74529	20	0	0
Log-log	0.137	0.0109	74537	12	0	0
Sqrt-lin	0.108	0.0123	74543	6	0	0
Lin-log	0.178	0.0175	74387	162	0	0
Sqrt-log	0.158	0.0141	74501	48	0	0
Capture						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 74549)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	0.169	0.0184	74490	59	0	0
Log-log	0.164	0.0134	74508	41	0	0
Sqrt-lin	0.155	0.0146	74527	22	0	0
Lin-log	0.193	0.0212	74083	466	0	0
Sqrt-log	0.179	0.0172	74469	80	0	0
Elastic Scatter						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 74549)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	0.0747	0.0028	74549	0	0	0
Log-log	0.0673	0.0018	74549	0	0	0
Sqrt-lin	0.0694	0.0023	74549	0	0	0
Lin-log	0.0780	0.0029	74549	0	0	0
Sqrt-log	0.0727	0.0023	74549	0	0	0

Table IV. Results for interpolating the total, capture, and elastic scattering cross sections over the temperature interval of 519 K to 547 K for Natural Zr

Total						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 23975)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	0.109	0.0024	23974	1	0	0
Log-log	0.108	0.0020	23974	1	0	0
Sqrt-lin	0.108	0.0020	23974	1	0	0
Lin-log	0.110	0.0024	23974	1	0	0
Sqrt-log	0.109	0.0020	23974	1	0	0
Capture						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 23975)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	1.087	0.0126	23653	188	56	78
Log-log	1.068	0.0117	23721	118	58	78
Sqrt-lin	1.132	0.0128	23561	277	59	78
Lin-log	1.093	0.0133	23723	116	58	78
Sqrt-log	1.065	0.0118	23762	77	58	78
Elastic Scatter						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 23975)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	0.106	0.0021	23974	1	0	0
Log-log	0.104	0.0018	23974	1	0	0
Sqrt-lin	0.105	0.0018	23974	1	0	0
Lin-log	0.106	0.0021	23974	1	0	0
Sqrt-log	0.105	0.0018	23974	1	0	0

Table V. Results for interpolating the total, capture, and elastic scattering cross sections over the temperature interval of 478 K to 589 K for ^{16}O

Total						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 2785)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	0.1352	0.0072	2655	130	0	0
Log-log	0.0787	0.0024	2785	0	0	0
Sqrt-lin	0.0480	0.0013	2785	0	0	0
Lin-log	0.2705	0.0146	2616	39	130	0
Sqrt-log	0.1350	0.0068	2669	116	0	0
Capture						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 2785)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	0.0421	< 0.0001	2785	0	0	0
Log-log	0.0443	0.0001	2785	0	0	0
Sqrt-lin	0.0432	< 0.0001	2785	0	0	0
Lin-log	0.0421	0.0001	2785	0	0	0
Sqrt-log	0.0432	0.0001	2785	0	0	0
Elastic Scatter						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 2785)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	0.1352	0.0072	2655	130	0	0
Log-log	0.0787	0.0024	2785	0	0	0
Sqrt-lin	0.0480	0.0013	2785	0	0	0
Lin-log	0.2706	0.0146	2616	39	130	0
Sqrt-log	0.1351	0.0068	2669	116	0	0

Table VI. Results for interpolating the total, capture, and elastic scattering cross sections over the temperature interval of 478 K to 589 K for ^{10}B

Total						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 1035)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	0.0001	< 0.0001	1035	0	0	0
Log-log	0.0001	< 0.0001	1035	0	0	0
Sqrt-lin	0.0001	< 0.0001	1035	0	0	0
Lin-log	0.0001	< 0.0001	1035	0	0	0
Sqrt-log	0.0001	< 0.0001	1035	0	0	0
Capture						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 1035)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	0.0001	< 0.0001	1035	0	0	0
Log-log	0.0002	0.0001	1035	0	0	0
Sqrt-lin	0.0001	< 0.0001	1035	0	0	0
Lin-log	0.0002	0.0001	1035	0	0	0
Sqrt-log	0.0002	0.0001	1035	0	0	0
Elastic Scatter						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 1035)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	0.1369	0.0218	889	146	0	0
Log-log	0.0754	0.0079	1035	0	0	0
Sqrt-lin	0.0415	0.0042	1035	0	0	0
Lin-log	0.2702	0.0435	852	38	145	0
Sqrt-log	0.1357	0.0209	902	133	0	0

Table VII. Results for interpolating the total, capture, and elastic scattering cross sections over the temperature interval of 478 K to 589 K for ^{1}H

Total						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 686)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	0.1342	0.0462	471	215	0	0
Log-log	0.0752	0.0121	686	0	0	0
Sqrt-lin	0.0413	0.0062	686	0	0	0
Lin-log	0.2671	0.0928	432	39	215	0
Sqrt-log	0.1328	0.0443	485	201	0	0
Capture						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 686)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	0.0001	< 0.0001	686	0	0	0
Log-log	0.0001	< 0.0001	686	0	0	0
Sqrt-lin	0.0001	< 0.0001	686	0	0	0
Lin-log	0.0001	< 0.0001	686	0	0	0
Sqrt-log	0.0001	< 0.0001	686	0	0	0
Elastic Scatter						
Method	**Max. Rel. Difference (%)**	**Avg. Rel. Difference (%)**	**Number of point-wise cross sections with Rel. Differences of (total = 686)**			
			≤ 0.1%	**0.1% - 0.2%**	**0.2% - 0.5%**	**≥ 0.5%**
Lin-lin	0.1356	0.0467	470	216	0	0
Log-log	0.0755	0.0117	686	0	0	0
Sqrt-lin	0.0416	0.0063	686	0	0	0
Lin-log	0.2714	0.0942	431	39	216	0
Sqrt-log	0.1357	0.0452	482	204	0	0

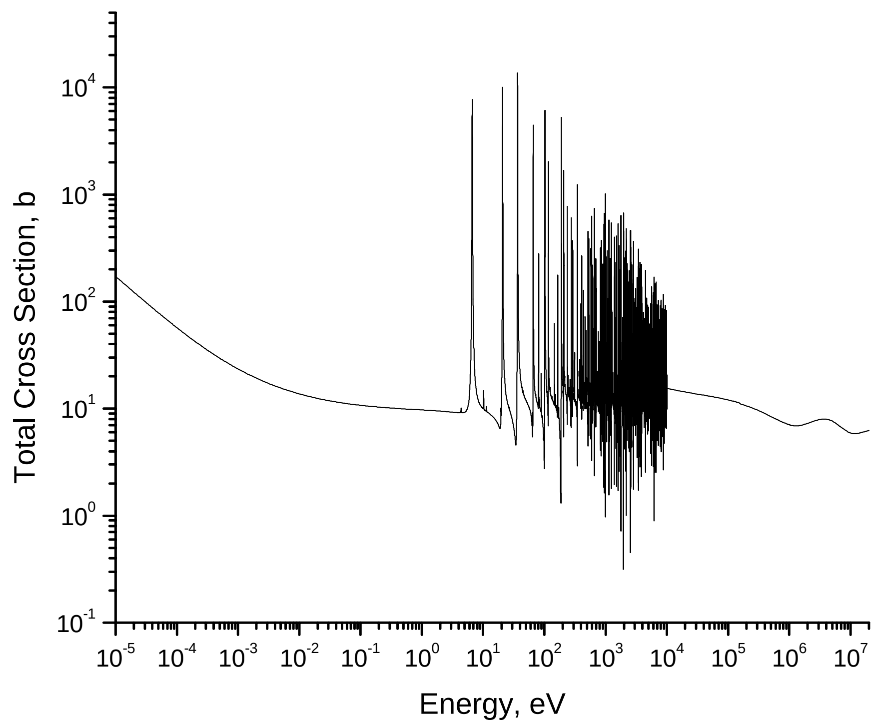

Figure 1. Total microscopic cross section for ^{238}U Doppler broadened to 294 K.

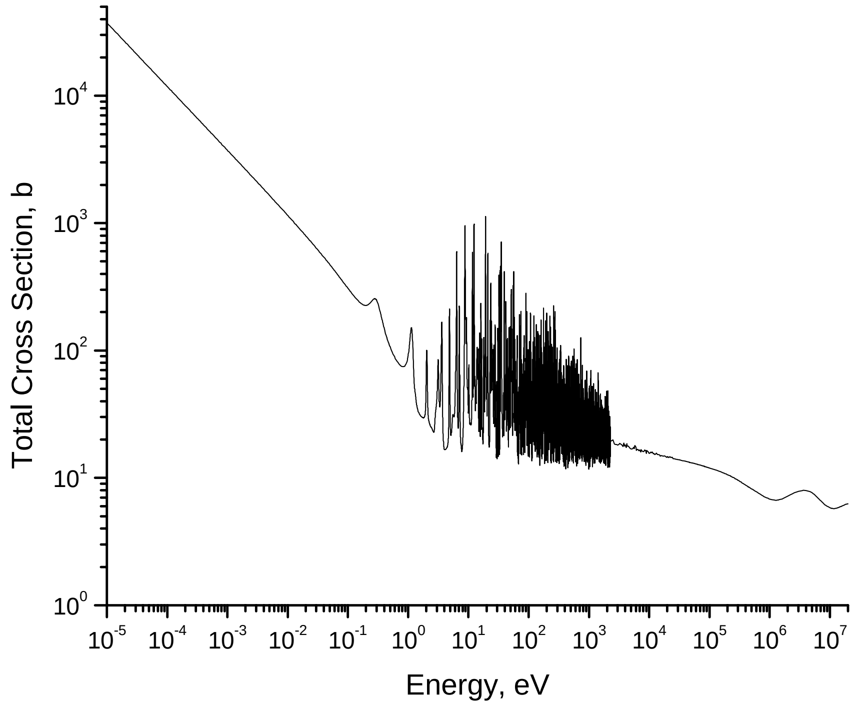

Figure 2. Total microscopic cross section for ^{235}U Doppler broadened to 294 K.

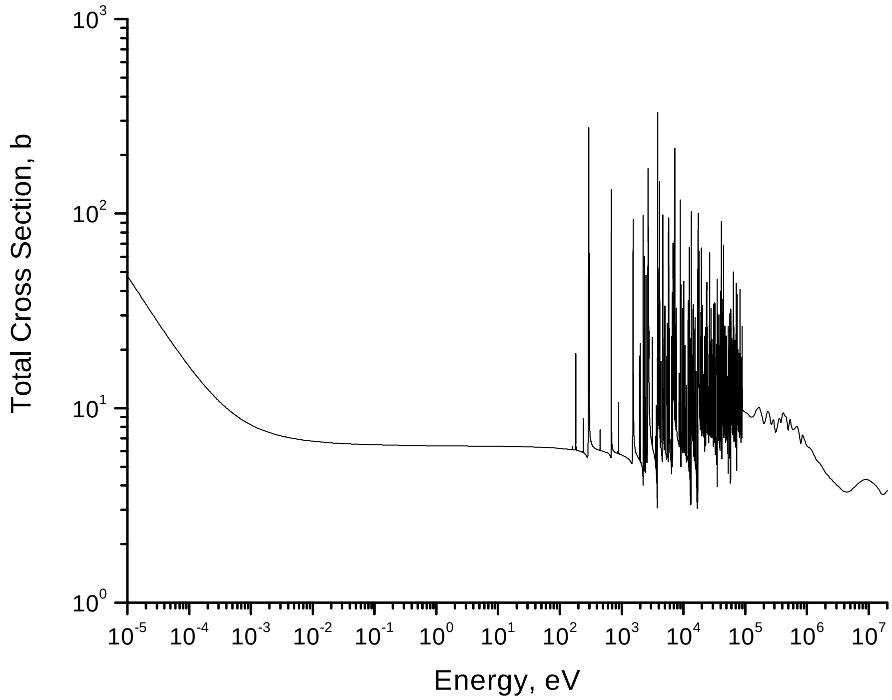

Figure 3. Total microscopic cross section for natural Zr Doppler broadened to 294 K.

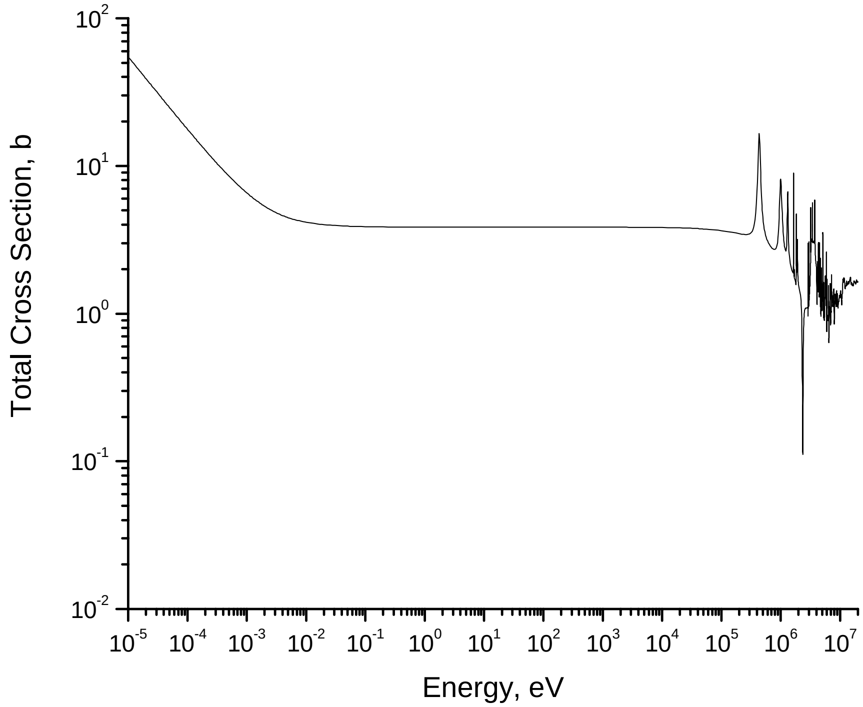

Figure 4. Total microscopic cross section for ^{16}O Doppler broadened to 294 K.

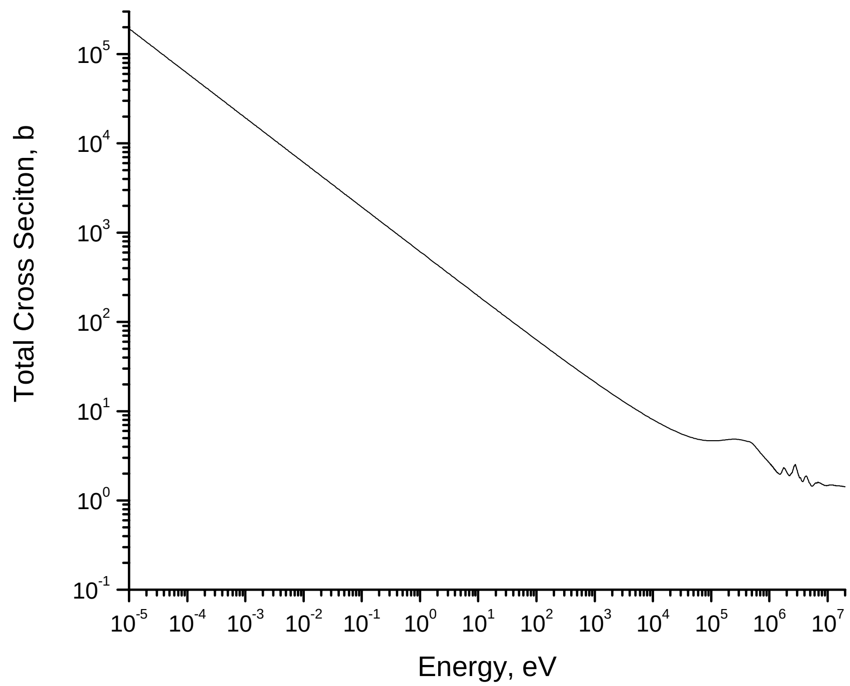

Figure 5. Total microscopic cross section for ^{10}B Doppler broadened to 294 K.

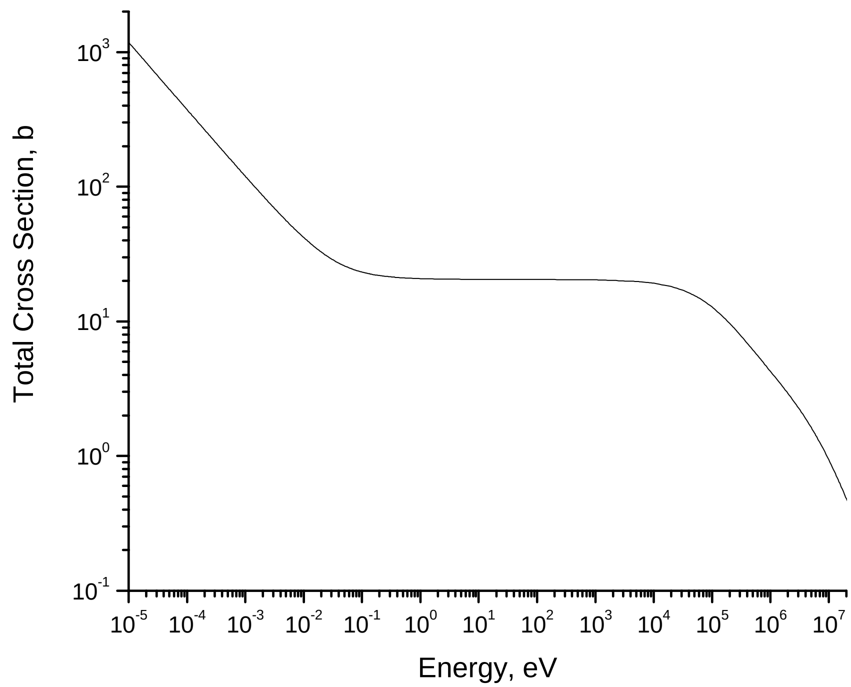

Figure 6. Total microscopic cross section for ^{1}H Doppler broadened to 294 K.

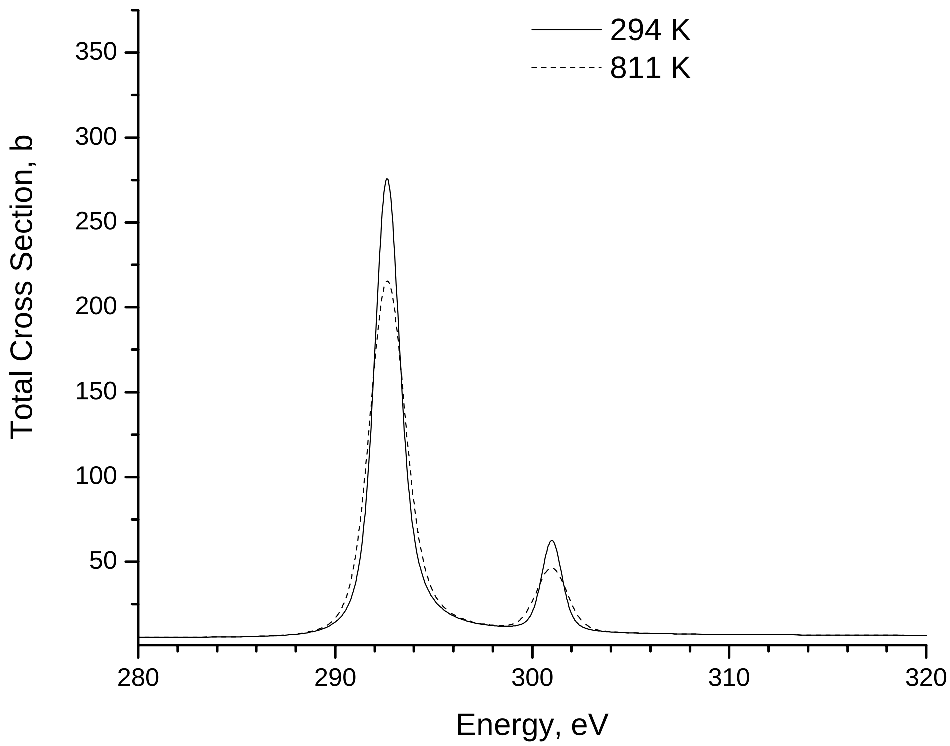

Figure 7. Effects of Doppler broadening on two resonances of the ^{238}U total microscopic cross section from 294 K to 811 K.

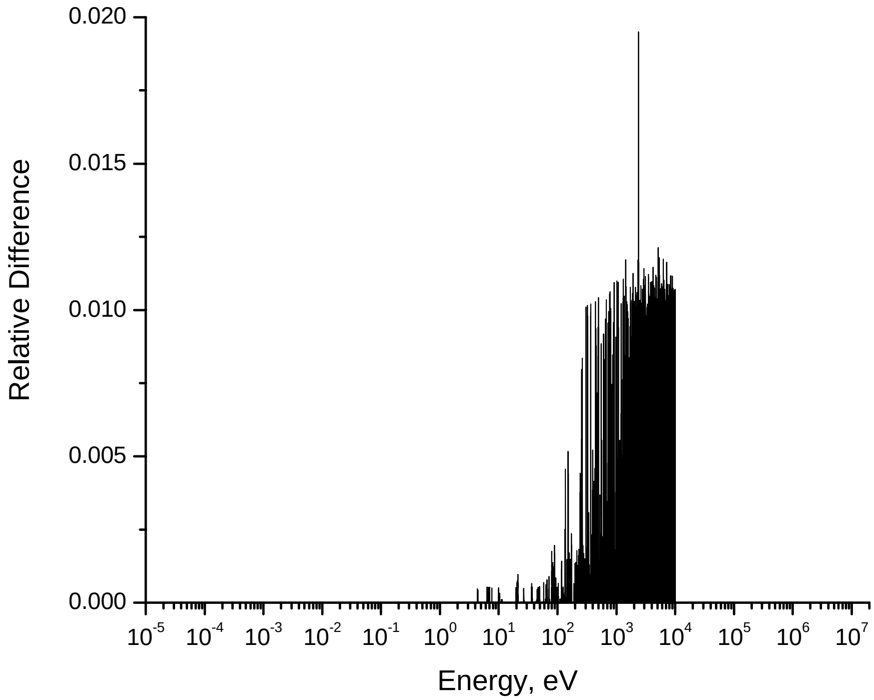

Figure 8. Absolute value of differences in the "log-log" interpolated ^{238}U capture cross section as a function of energy relative to the Doppler broadened cross section at 533 K. The interpolation interval was 28 K (519 K to 547 K).

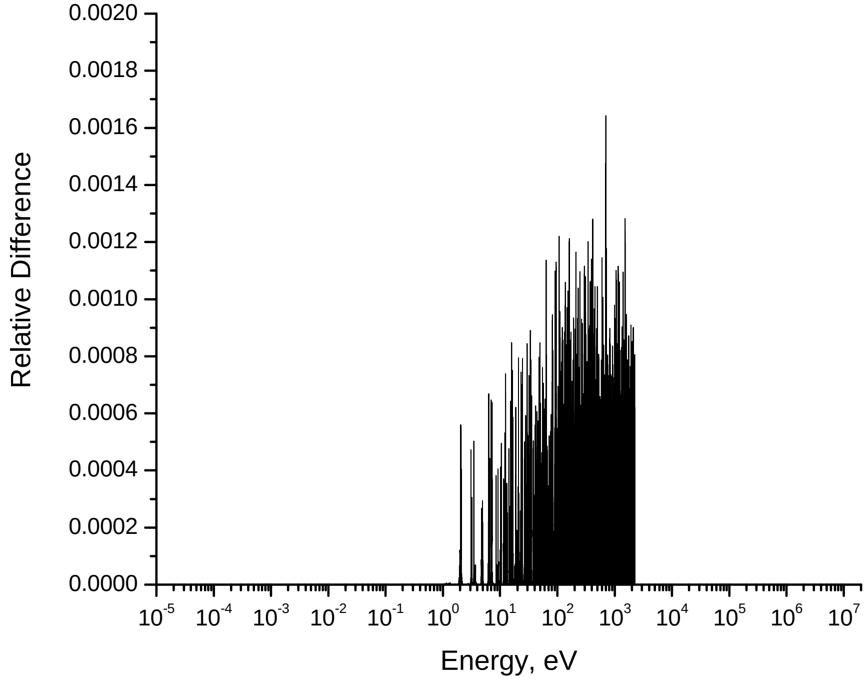

Figure 9. Absolute value of differences in the “log-log” interpolated ^{235}U capture cross section as a function of energy relative to the Doppler broadened cross section at 533 K. The interpolation interval was 28 K (519 K to 547 K).

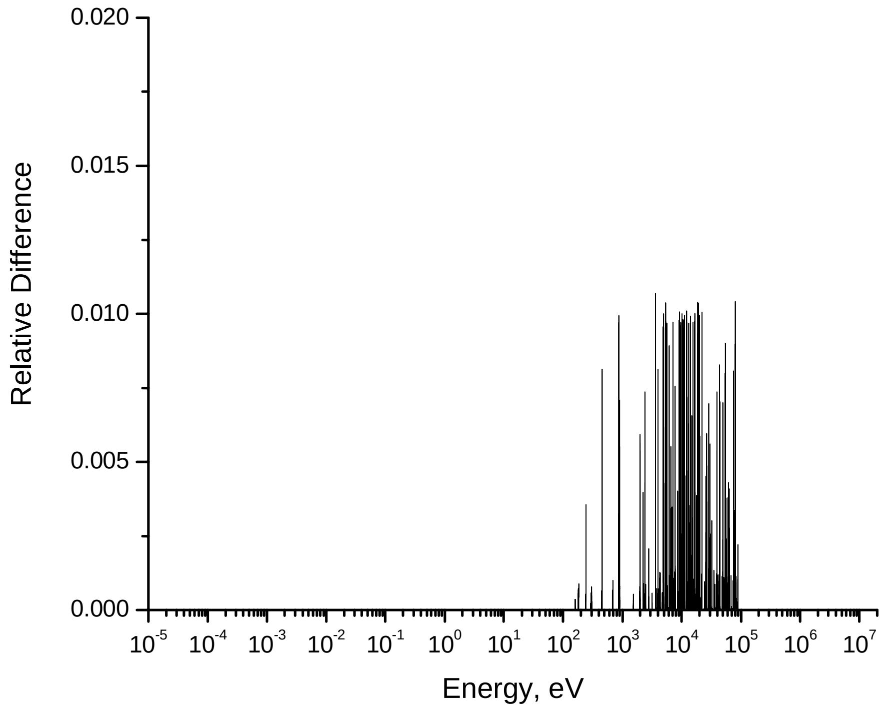

Figure 10. Absolute value of differences in the "log-log" interpolated natural Zr capture cross section as a function of energy relative to the Doppler broadened cross section at 533 K. The interpolation interval was 28 K (519 K to 547 K).