POINT2021: ENDF/B-VIII.0
Temperature Dependent Cross Section Library

by
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May 15, 2021

Abstract: This report is one in the series of “POINT” reports that over the years have presented temperature dependent cross sections for the then current version of ENDF/B. In each case I have used my personal computer at home and publicly available data and codes: 1) publicly available nuclear data (the current ENDF/B data, available on-line at the National Nuclear Data Center, Brookhaven National Laboratory, http://www.nndc.bnl.gov/) and, 2) publicly available computer codes (the current PREPRO codes, available on-line at the Nuclear Data Section, IAEA, Vienna, Austria, https://www-nds.iaea.org/public/endf/prepro/) and, 3) My own personal computer located in my home. I have used these in combination to produce the temperature dependent cross sections used in applications and described in this report. I should mention that today anyone with a personal computer can produce these results: by its very nature I consider this data to be born in the public domain.
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Vienna, May 2021
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May 15, 2021
Dedication

I dedicate this report to the memory of my dear friend of more than 50 years: Said Mughabghab. During his tenure at the National Nuclear Data Center (NNDC), Brookhaven National Laboratory, Said dedicated his life to nuclear data; no one has contributed more to our understanding of the subject than he has. He will be greatly missed by all of us, as a dear friend and colleague.

Acknowledgments

I thank Said Mughabghab for his detailed explanation of the use of his published resonance parameters which were widely used in ENDF/B-VIII.0 evaluations. I thank Dave Brown and Ramon Arcilla, Jr., of the National Nuclear Data Center (NNDC), Brookhaven National Laboratory, for supplying the original ENDF/B-VIII.0, used in this project. I thank Janice Arwood and Mark Baird (RSICC, Oak Ridge) for carefully handling, checking and recommending improvements for each version of POINT. I thank Nancy Larsen, Bob MacFarlane, Maurice Greene, Mike Dunn, and Valentin Sinitsa, for their comparison of their cross section processing codes (SAMMY, NJOY, AMPX and GRUCON) against the PREPRO codes. These comparisons have led to significant improvements in the accuracy and reliability of the results produced by all codes (SAMMY, NJOY, AMPX, GRUCON, PREPRO). I thank Andrej Trkov, Bojan Zefran, Jean-Christophe Sublet (NDS, IAEA, Vienna), who contributed so many GREAT ideas for me to incorporate into my PREPRO codes. I thank Roberto Capote Noy and Kira Nathani (NDS, IAEA, Vienna) for editing my reports into a form suitable for publication by the Nuclear Data Section, IAEA.

Overview

This report is one in the series of “POINT” reports (Refs [1 – 7]) that, over the years, have presented temperature dependent cross sections for the then current version of ENDF/B [8, 9]. In each case I have used my personal computer at home and publicly available data and codes:

1) publicly available nuclear data (the current ENDF/B data, available on-line at the National Nuclear Data Center, Brookhaven National Laboratory, http://www.nndc.bnl.gov/) and,

2) publicly available computer codes (the current PREPRO codes, available on-line at the Nuclear Data Section, IAEA, Vienna, Austria, https://www-nds.iaea.org/public/endf/prepro/ and,

3) My own personal computer located in my home.

I have used these in combination to produce the temperature dependent cross sections used in applications and described in this report. I should mention that today anyone with a personal computer can produce these results: by its very nature I consider POINT data to be born in the public domain.
Introduction: POINT2021 - ENDF/B-VIII.0

The latest ENDF/B-VIII.0 [8] data library was released in 2018 and is now freely available through the National Nuclear Data Center (NNDC), Brookhaven National Laboratory. This release of ENDF/B-VIII.0 completely supersedes all preceding releases of ENDF/B. Individual files and/or complete libraries can also be downloaded from: http://www.nndc.bnl.gov/

Periodic Table

ENDF/B-VII and VIII.0 both span the periodic table of elements from Z = 1 to 100, but not all elements are represented. The below table summarizes the number of evaluations included for each element (Z) in ENDF/B-VII (7) and VIII.0 (8). 0* indicates no data for this element, e.g., ENDF/B-VIII.0 does not include any data for Z = 85, 86, and 87.

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What’s New and Old: ENDF/B-VIII.0 versus VII

ENDF/B-VIII.0 (POINT2021) includes 557 evaluations, compared to 423 evaluations in ENDF/B-VII (POINT2015). There are 135 new evaluations included in VIII.0 which were not included in VII. 422 of the 423 evaluations from VII are included in VIII.0; the only one not included is 6-C-Nat, which has been replaced by its isotopes. Note, that with 6-C-Nat replaced by its isotopes, VIII.0 does not include any elemental mixtures.

135 New Evaluations in POINT2021 (ENDF/B-VIII.0)

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423 Evaluations in POINT20115 (ENDF/B-VII) (422 in VIII.0; 6-C-Nat in RED not in VIII.0)

POINT2018 versus POINT 2015
POINT 2015 is based on ENDF/B-VII.1 and POINT2018 is based on ENDF/B-VIII.0 evaluations. The difference between them is naturally due to changes in the evaluated data, but is also due to what we have learned over the last three years and how this experience has been incorporated into the ENDF/B Pre-Processing codes (PREPRO2017), that were used to create POINT2018.

POINT2021 versus POINT 2018
POINT2018 and POINT2021 are both based on the same ENDF/B-VIII.0 data, i.e., there have been no updates to ENDF/B-VIII.0. The difference is, once again, due to experience using the data, to a major re-write of the PREPRO codes, and to the improved procedures in using the PREPRO2021 codes to produce a much more accurate POINT2021, and separation of Temperature Dependent and Independent data, as explained in detail below: separating the data into these two different parts allowed us to reduce the overall size, from POINT2018 (6.4 GB) down to POINT2021 (2.7 GB), well within the capacity of a single DVD.
Temperature Dependent and Independent Data

Doppler broadening only affects the ENDF MF=1 to 3: MF=1: temperature, MF=2: resonance parameters, MF=3: temperature dependent tabulated cross sections. Generally, these are not most of the data included in ENDF evaluations; the majority are the data used to describe secondary neutrons and other products of the interactions, e.g., photon and charged particle emission. For example, ENDF/B-VIII.0 includes 557 evaluations; in the original form that is distributed this includes roughly 83 megabytes of MF=1, 2 & 3 data (comments, resonance parameters, and tabulated background cross sections), and 1.12 gigabytes (1120 megabytes) of “other” (M = 4 to 99) data.

For past versions of ENDF POINT libraries, I have presented data reconstructed from resonance parameters, and Doppler broadened to a variety of temperatures; the result was the entire current ENDF data library as originally distributed, plus at 12 temperatures, including ALL of the data repeated 13 times, even though only a fraction of the data is actually temperature dependent. The result was that POINT2018 included almost 24 gigabytes of uncompressed data, even though only about 1/3 of these data are actually temperature dependent. The current ENDF/B-VIII.0 library has now grown to a size that may make it problematic for some potential users to be able to use it.

Starting with POINT2021 the data has been divided into Temperature Dependent Data (for simplicity ENDF MF=1,2,3) and Temperature Independent Data (ENDF MF= 4 to 99). Compared to the 24 gigabytes uncompressed in POINT2018, the result in POINT2021 is: 8.8 gigabytes of data, 1.1 gigabytes being the Temperature Independent Data (ENDF MF > 3) which is now included only once, whereas earlier this data was included 13 times (the original data and at 12 temperatures: 13 X 1.1 = 14.3 GB). In the compressed form in which it is distributed, the entire POINT2021 is only 2.7 gigabytes and easily fits onto a single DVD.

Hopefully, the decrease in size of POINT2021 will make it more accessible to potential users; again, hopefully, offsetting the inconvenience to users of having to re-combine Temperature Dependent and Independent data. For the convenience of users POINT2021 includes the PREPRO/MERGER code, to allow users to merge these data together for each isotope, and a BATCH file to allow all 557 evaluations at any one given temperature to combine ALL the Temperature Dependent and Independent data.

PREPRO 2021 Codes

Since there have not been any changes in the ENDF/B-VIII.0 evaluations between the last version of this report, where the PREPRO2017 [10] codes were used, and the current version, where the PREPRO2021 [11] codes were used, there has been a major re-write to improve the ENDF/B Pre-processing codes (PREPRO). The improvements were both in terms of improving the basic methods used by the codes and in terms of incorporating the latest ENDF-6 Formats and Procedures [9] used by the current evaluations. The result is more accurate cross section data throughout the POINT2021 library; more accurate and only about 1/3 the size of earlier POINT data libraries.
**WARNING** – due to recent changes in ENDF-6 Formats and Procedures [9] only the latest version of the ENDF/B Pre-processing codes, namely PREPRO2021 [11], can be used to accurately process all current ENDF/B-VIII.0 evaluations. If you fail to heed this warning and you use any earlier versions of these codes, the results can be inaccurate/unpredictable.

The PREPRO 2021 codes run on virtually any computer, and will soon be available FREE online from the Nuclear Data Section, IAEA, Vienna, Austria, [https://www-nds.iaea.org/public/endf/prepro/](https://www-nds.iaea.org/public/endf/prepro/)

**Data Processing**

As distributed, the original evaluated data [8, 9] includes cross sections represented in the form of a combination of resonance parameters and/or tabulated energy dependent cross sections, always at 0 Kelvin temperature. For use in applications, this data has been processed using the 2021 version of the ENDF/B Pre-processing codes (PREPRO2021) [11] to produce temperature dependent, linearly interpolable in energy, tabulated cross sections, in the ENDF-6 format.

For use in applications this library has been processed into the form of temperature dependent cross sections at seven neutron reactor like temperatures, between 0 and 1800 Kelvin, in steps of 300 Kelvin (the exception being 293.6 Kelvin, for exact room temperature at 20 Celsius). It has also been processed to five astrophysics like temperatures, 1, 10, 100 eV, 1 and 10 keV. For reference purposes, 300 Kelvin is approximately 1/40 eV, so that 1 eV is approximately 12,000 Kelvin, e.g., the 0.1 eV data is the same as the 1,200 K data. At each temperature, the cross sections are tabulated and linearly interpolable in energy.

The steps required and codes used to produce room temperature, linearly interpolable tabulated cross sections, in the ENDF-6 format [9], are described below; the name of each code is given in parenthesis; for details of each code see Refs [10, 11]. Here is a summary of the traditional PREPRO codes used to process the POINT data, in the order in which the codes were used (note, below I describe the improved order used by PREPRO2021 codes to produce POINT2021),

1) Convert all data to a FORTRAN, C and C++ compatible format (**ENDF2C**)
2) Convert to Linearly interpolable, tabulated energy dependent cross sections (**LINEAR**)
3) Add the resonance contribution to cross sections (**RECENT**)
4) Doppler broaden all cross sections to each temperature (**SIGMA1**)
5) Check data, define redundant cross sections by summation (**FIXUP**)
6) Update evaluation dictionary in MF/MT=1/451 (**DICTIN**)

For the "cold" (0 Kelvin) data steps 1), 2), 3) and 5), 6) were used (no Doppler broadening). For the data at other temperatures, after steps 1), 2), 3), the data were Doppler broadened to each temperature using step 4), and the results were then made consistent with the ENDF/B formats and conventions [9] using steps 5) and 6), to produce the final distributed data.

The result is linearly interpolable in energy, tabulated, temperature dependent cross sections, in the simple text ENDF-6 format, ready to be used in applications.
Note: This processing only involved the energy dependent neutron cross sections. All other data in the evaluations, e.g., angular and energy distributions, was not affected by this processing, and is identical in all versions of the results, i.e., it is the same in all the directories, ENDF2C, as well as K0 through K1800, and 1 eV through 10 keV. This fact has allowed us to separate the data into Temperature Dependent and Independent data, greatly reducing the distributed size of POINT2021.

Accuracy or Uncertainty of Results

WARNING: PLEASE do not confuse the OVERALL UNCERTAINTY of the nuclear data used in ENDF/B with the additional uncertainty introduced by the PREPRO codes. I judge that currently our knowledge of neutron interaction data (as reflected in current theory, measurement, and the ENDF/B cross sections) for any isotope, at any temperature and incident neutron energy is not known to better than roughly 1%; we may know integrals more accurately, but not the detailed energy dependent cross sections. As such I have defined the additional uncertainty added by the PREPRO codes to be so small that they add essentially no additional uncertainty to the OVERALL uncertainty in the ENDF/B data. This is VERY IMPORTANT if our data testing results are to have any significant validity.

Each of the codes described above that was used to process data to obtain tabulated, linearly interpolable in energy cross sections, processed the data to within a user defined accuracy, or allowable uncertainty. The ENDF/B Pre-processing codes (PREPRO) are self-documenting, in the sense that the ENDF/B formatted output data that each code produces includes comments at the beginning of each evaluation (end of comments) defining the accuracy to which the cross sections were calculated. The combination of comments added by all of the codes defines the sequence and accuracy used by all of them. For POINT2021, the accuracy is the same for all evaluations. Therefore, for exact details of the accuracy of the data, see the comments at the beginning of any evaluation.

POINT2021 Improved Accuracy

For use in earlier POINT libraries all cross sections were reconstructed to within an accuracy of 0.01% in the thermal range, and 0.1 % at all other incident neutron energies and temperatures; this is beyond the accuracy to which this data is known. In practice it has been found to be extremely difficult to achieve this degree of accuracy by consistently directly using nuclear data processing codes, such as PREPRO. For POINT2021, I took a different approach to reconstruct the data to within 0.01% at ALL temperatures and incident neutron energies, using the traditional PREPRO code sequence: LINEAR/RECENT/SIGMA1 – and I then added an additional processing step using LINEAR a second time to thin the final results back to our original goal: 0.01% thermal range, and 0.1% at all other incident neutron energies – followed by the remaining traditional sequence FIXUP/DICTION for each evaluation at each temperature.

Note: Many years of experience have shown that the number of energy points generated varies roughly as 1/sqrt(accuracy), so changing the accuracy from 0.1% to 0.01% a factor of 10 – increases the number of points by roughly 3 – subsequent thinning from 0.01% back to 0.1% actually reduces the size by more than 3, for a net gain.
Today’s computers are so much faster and cheaper than computers were even a few years ago, that we can afford to use this “overkill” approach once to invest a little more computer power to create more accurate data for later use in our many applications. The result is a POINT data file that is both more accurate, but also somewhat smaller than the direct method used earlier, i.e., by first using “overkill” to create files to within 0.01% accuracy, and then thin this back to 0.1%, we end up with somewhat SMALLER data files than we do if we try to directly create 0.1% data files.

0.01% versus 0.1% Results

Detailed comparisons of results clearly illustrate the advantage of “overkill” in reconstructing the data to be much more accurate at 0.01%, followed by thinning to 0.1% to consistently achieve our goal of limiting data processing to 0.1% ADDITIONAL PROCESSING UNCERTAINTY. For example, the below figure illustrates the same data compared to 2021 0.01% data, first comparing to the 2018 results that in 2018 I claimed was “accurate” to 0.1% (based on direct calculations to this accuracy), and next based on 2021 results first calculated to 0.01% and then thinned to within 0.1%. The later 2021 data is everywhere within 0.1% of the 0.01%, whereas the former 2018 differs by over 1.4%: 14 TIMES THE ASSUMED 0.1% ACCURACY.
Based on detailed comparisons of 0.01% and 0.1% results, I assume that the PREPRO data processing used to produce POINT2021 does not add any significant additional uncertainty to the inherent overall uncertainty of the nuclear data, i.e., we know the nuclear data to roughly 1%, and PREPRO adds only an additional 0.1%. Here I have shown that this new 2021 “overkill” approach I am using for POINT2021 is much more accurate than the earlier 2018 direct approach to 0.1% on a continuous energy convergence basis (resulting in 2018 difference of over 1.4%).

Additional comparisons to codes that claim to use integral energy convergence basis, to reduce the number of energy points required, clearly illustrate that as implemented these integral methods simply do not work, resulting in LARGE differences (factors of 100 or more larger than the claimed accuracy). These integral methods are the remains in codes from methods used decades ago when computer time was much more limited, and we were trying everything we could think of to decrease running time; they should play no role in today’s codes. Below is but one example of INTEGRAL results claiming 0.1% accuracy, but actually resulting in continuous energy differences of over 51%, i.e., OVER 510 TIMES THE CLAIMED ACCURACY.
Contents of the Library

This library contains all the evaluations in the ENDF/B-VIII.0 general purpose library. The above tables summarize the contents of the ENDF/B-VIII.0 general purpose library. This library contains evaluations for 557 materials; all are isotopes of elements Z=1 through 100, but be aware that data is not necessarily included for all elements, Z = 1 through 100; see the above table for a summary.

The POINT2021 library includes each of the 557 evaluations stored at each temperature as a separate file, i.e., 557 evaluations X 12 temperatures = 6,684 files. The data are in the simple text ENDF-6 format, which allows the data to be easily transported between computers. The entire library requires approximately 9 gigabytes of storage in uncompressed form; once compressed the data requires roughly 2 to 3 gigabytes, i.e., well within the capacity of a single DVD.

The POINT2021 webpage is compressed; when uncompressed you will find a single directory named POINT2021 containing fifteen (15) sub-directories; the 1eV data is physically the 1200K data. This includes DOCUMENT, MERGER, one directory of Temperature Independent Data (MF4to99) and 12 directories of the Original (ENDF2C) Temperature Dependent Data (ENDF MF=1 to 3).

DOCUMENT - A copy of this report in PDF formats.
MERGER - PREPRO/MERGER utility code to merge ENDF data.
MF4to99 - Temperature Independent Data
ENDF2C - The original ENDF/B data after being processed by ENDF2C.
0K - 0 Kelvin cross sections
293.6K - 293.6 Kelvin cross sections
600K - 600 Kelvin cross sections
900K - 900 Kelvin cross sections
1200K - 1200 Kelvin cross sections
1500K - 1500 Kelvin cross sections
1800K - 1800 Kelvin cross sections
1eV - 1 eV cross sections (physically the same as 1200 K data)
10eV - 10 eV cross sections
100eV - 100 eV cross sections
1keV - 1 keV cross sections
10keV - 10 keV cross sections

This POINT2021 library does not contain data from special purpose ENDF/B-VIII.0 libraries, such as fission products, thermal scattering, photon interaction data. To obtain any of these special purpose libraries contact the National Nuclear Data Center, Brookhaven National Laboratory, ENDF@bnlnnd2.dne.bnl.gov

This library contains data for some metastable materials, which are indicated by an "M" at the end of their name, e.g., ZA052131.M = 52-Te-131m

For use in applications, users MUST combine/merge the Temperature Dependent and Independent data at each temperature; The utility code PREPRO/MERGER [11] is provided to simplify this step. Most of these evaluations are complete, in the sense that they include all cross sections over the energy range $10^{-5}$ eV to at least 20 MeV.
Except for DOCUMENT and MERGER, each of these directories contains 557 files, one file for each of the 557 evaluations. Each evaluation is a simple text file, 80 characters per line, and is a complete ENDF/B "tape" [9], including a starting "tape" identification line, and ending with a "tape" end line [9]. Once the Temperature Dependent and Independent data has been combined at any temperature, this simple text form file can be used by a wide variety of available computer codes that treat data in the ENDF/B format, e.g., all the PREPRO codes.

**Requesting POINT2021 Data**

Please do not contact the author of this report to request this data; I do not have the resources necessary to directly respond to requests for this data. This data has been distributed and is internationally available from nuclear data/code centers throughout the World,

1) Within the United States: contact the National Nuclear Data Center, Brookhaven National Laboratory, Mike Herman, services@bnlnd2.dne.bnl.gov
2) Within Western Europe: contact the OECD Nuclear Energy Agency/ Data Bank (NEA/DB), Paris, France, programs@nea.fr
3) Otherwise: contact the Nuclear Data Section, International Atomic Energy Agency, Vienna, Austria, nds.contact-point@iaea.org.

**Installation and Use of POINT2021**

I recommend that you,

1) Copy the single compressed POINT2021 file to your computer.
2) Uncompress and un-tar the file; then delete the compressed and tar files.
3) You should then have one directory named POINT2021 containing all the data.
4) To randomly access the data, execute (double click) POINT2021.htm.

The main POINT2021 directory will contain the fourteen (14) sub-directories described above. These POINT2021 directories include HTML routines to allow interactive retrieval of the data for 557 evaluations at each temperature. Once uncompressed, the result will be a directory of about 9 gigabytes. To put that in perspective, today it costs less than $0.10 U.S. to purchase, install, and maintain on-line one gigabyte of disk storage. Therefore, the cost of maintaining this 9 gigabyte library on-line is trivial.

**Use of PREPRO/MERGER**

To optimize storage, POINT2021 divides each evaluation into Temperature Dependent (ENDF MF=1 to 3) and Independent (ENDF MF=4 to 99) data. To use the data, these two parts must first be merged to define one complete evaluation in the ENDF format. POINT2021 includes the PREPRO/MERGER [11] utility code that is recommended to perform this merge.

The MERGER executable is only included for IBM/Windows and MAC/OS systems. However, the code is designed to run on virtually any type of computer; for use on other systems the source code is supplied to allow users to create an executable on their system.
The MERGER directory is divided into three sub-directories:
WINDOWS = Including a MERGER executable
MACOS = Including a MERGER executable
FORTRAN = Including MERGER FORTRAN code and a Makefile to create an executable

Use whichever of these directories meets your needs. Assuming you have a MERGER executable that will run on your computer, MERGER can be used to either combine one single evaluation, or all 557 evaluations at a given temperature.

**Combine 2 parts of one evaluation**

To combine the Temperature Dependent and Independent data for one isotope, use the included MERGER.INP file – a complete copy of this file is included below. Use whatever filenames you select to define “merger.out”, “merger.in” and “merger.in2”, and run MERGER to merge the 2 parts.

merger.out

merger.in1
merger.in2
END

1 1 1 999999999

========================================================================

The above MERGER input will merge the 2 ENDF input files
merger.in1
merger.in2
Into the ENDF output file
merger.out

Next line of input defines the MAT/MF/MT range to merge
In this case it merges EVERYTHING
MAT/MF/MT = 1/1/1 to 9999/99/999
in the above case we only include one request line, but you can include up to 100 MAT/MF/MT ranges, one per input line.
Combine 2 parts of 557 evaluations

To combine the Temperature Dependent and Independent data for ALL 557 isotopes at any one temperature, use the included MERGE557.BAT file – this is a BATCH file designed to run PREPRO/MERGER 557 times, using the names defined in the included MERGER.INP file (merger.in1, merger.in2 and merger.out).

To use this batch, in one directory,

1) Download and Uncompress the entire directory of the temperature dependent data at one temperature, e.g., 293.6K, and the temperature independent data, e.g., MF4to99.
2) Create a directory named COMBINED.
3) Run the batch file MERGE557.bat – be patient as it combined all 557 evaluations.

Below is a small portion of the start of MERGE557.BAT, showing the sequence of 5 lines used to combine the two pars each evaluation – the first 5 lines here combine ZA000001 (neutron) 2 parts from the directories 293.6K\ and MF4to99\ merged into COMBINED\ - the next 5 lines do the same for ZA001001 (1-H-1) – this sequence of 5 lines is repeated 557 times.

del merger.in1 merger.in2 merger.out
copy 293.6K\ZA000001  merger.in1
copy MF4to99\ZA000001 merger.in2
merger
copy merger.out COMBINED\ZA000001
del merger.in1 merger.in2 merger.out
copy 293.6K\ZA001001  merger.in1
copy MF4to99\ZA001001 merger.in2
merger
copy merger.out COMBINED\ZA001001

If you want to use data at a different temperature (rather than 293.6K) download and uncompress the data you want to use and in MERGE557 changed ALL 293.6K to whatever temperature you want to use, e.g., 900K. At ALL temperatures, the second file to merge is always MF4to99, the Temperature Independent data.

The included MERGE555.BAT file uses Windows/DOS commands. But every computer can run BATCH files; it is merely a matter of changing a few keywords, for example on LINUX you need merely change throughout the entire MERGE557 file,

del to rm
copy to cp

The resulting BATCH file will run on your LINUX system, using the directories and filenames from the included MERGE557.BAT file. The most important point here is that the BATCH file has the filenames of ALL 557 ENDF/B-VIII.0 evaluations built into it.
FORTRAN, C   C++ Compatible ENDF results

I have added the ENDF2C code to PREPRO, to ensure that ALL PREPRO output in the simple text ENDF format are completely FORTRAN, C and C++ compatible. Currently, evaluated data even from major code centers are still not completely FORTRAN, C and C++ compatible. Therefore, when I begin pre-processing any evaluation, the first PREPRO code I run is ENDF2C to ensure that ALL ENDF formatted output in subsequent codes are completely compatible. This is a very important step: it would be such a shame if after all the effort invested to produce accurate results it cannot be accurately read and used by application codes. If, as recommended, you ALWAYS use ENDF2C first, you will be able to avoid this problem. PREPRO also uses the current ENDF convention that sequence numbers start at 1 for each section (MAT/MF/MT), instead of the older convention starting at 1 for each material (MAT); a trivial point, but it explains the difference in sequence numbers as seen in the below data.

### Before ENDF2C

<p>| | | | | | | | |</p>
<table>
<thead>
<tr>
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<td>0</td>
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<td></td>
<td></td>
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<tr>
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<td>0.0000000+0</td>
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<td>0</td>
<td>1</td>
<td>149 128 3 1 126</td>
<td></td>
<td></td>
</tr>
<tr>
<td>149 2</td>
<td></td>
<td>128 3 1 127</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.000000-5</td>
<td>3.420300+0</td>
<td>1.000000-4</td>
<td>3.403000+0</td>
<td>2.530000-2</td>
<td>3.395510+0</td>
<td>128 3 1 128</td>
<td></td>
</tr>
<tr>
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<td>1.000000+3</td>
<td>3.394900+0</td>
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<td>128 3 1 129</td>
<td></td>
</tr>
<tr>
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<td>3.394400+0</td>
<td>4.000000+3</td>
<td>3.389400+0</td>
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<td>2.000000+4</td>
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<td></td>
</tr>
<tr>
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<td>3.302000+0</td>
<td>5.000000+2+4</td>
<td>3.285000+0</td>
<td>6.000000+2+4</td>
<td>3.270000+0</td>
<td>128 3 1 132</td>
<td></td>
</tr>
</tbody>
</table>

### After ENDF2C

<p>| | | | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
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<th></th>
</tr>
</thead>
<tbody>
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<td>149 128 3 1 2</td>
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<tr>
<td>149 2</td>
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<td>1.000000E-4</td>
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<td>.025300000</td>
<td>3.39551000</td>
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<td></td>
</tr>
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<td></td>
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<tr>
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<td>3.38940000</td>
<td>5000.000000</td>
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<td></td>
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<tr>
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<td>3.32100000</td>
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<td>40000.000</td>
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<td>50000.0200</td>
<td>3.28500000</td>
<td>60000.0200</td>
<td>3.27000000</td>
<td>128 3 1 8</td>
<td></td>
</tr>
</tbody>
</table>

Note that in the above example we can see that the numerical values are EXACTLY the same in both cases. However, the ENDF2C output include 9, or even 10, digits of precision, and is completely FORTRAN, C and C++ compatible. In comparison the ENDF 7-digit, so called “E-less” data, such as 1.234567+3 (as opposed to 1234.56789) is not standard in any computer language and can lead to errors in interpretation when codes attempt to read this data.

PREPRO uses 9 or 10 digit precision for all ENDF output

As an example, consider: 9 digits: 12324.56789, versus 7 digits: 1.234567+3. Obviously the 9 digit output is a hundred times more precise compared to the 7 digit output. This is very important for narrow milli-eV wide resonances in the keV or today even in the MeV energy range. Below I show the difference between PREPRO output data using 9 or 10 digits of accuracy compared to another code using 7 digits. To see the real danger of using 7-digit output with today’s modern evaluations, let us see what happens when we run the 9-digit RECENT output through this other code and truncate it to 7-digits.
Total showing differences up to **14.3%** differences,

![Graph showing differences up to 14.3%](image)

Capture showing differences up to **21.3%** difference,

![Graph showing differences up to 21.3%](image)
Here we see that the 7-digit output is unable to accurately define the shape of these resonances – this is IMPORTANT to understand, so let me repeat: it is PHYSICALLY IMPOSSIBLE with only 7 digits. Rather than the smooth profile produced by the RECENT 9 or 10 digit output, the 7-digit output produces **Ziggurats = stepped pyramids**. To understand the problem we need merely compare the 9-digit RECENT output near the peak of the resonance,

<table>
<thead>
<tr>
<th>Energy (MeV)</th>
<th>Intensity (arb. units)</th>
</tr>
</thead>
<tbody>
<tr>
<td>122600.007</td>
<td>8.18440080</td>
</tr>
<tr>
<td>122600.018</td>
<td>8.34734256</td>
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<tr>
<td>122600.028</td>
<td>8.49343463</td>
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<tr>
<td>122600.055</td>
<td>9.86865730</td>
</tr>
<tr>
<td>122600.120</td>
<td>9.51387393</td>
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<tr>
<td>122600.131</td>
<td>9.565109362</td>
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<tr>
<td>122600.142</td>
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<td>122600.153</td>
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<td>122600.181</td>
<td>9.50582500</td>
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<td>122600.218</td>
<td>9.16076388</td>
</tr>
<tr>
<td>122600.229</td>
<td>9.01088080</td>
</tr>
</tbody>
</table>

Here the entire shape of the resonance is between 122.599 keV and 122.601 keV, and we can see that all the above tabulated points in both tables start with EXACTLY the same six digit energy 122600. This means that with 9 or 10 digit RECENT output we only have 3 or 4 digits with which to define the entire shape of the resonance, which is adequate, but with 7-digit output we only have one digit!!!!!, which is far from adequate. Compare what should be EXACTLY the same energy points that I have highlighted, and you will see smooth variation of the 9-digit RECENT energies, but **ALL OF THE HIGHLIGHTED 7-DIGIT ENERGIES ARE EXACTLY THE SAME VALUE, 1226600.2 eV**, which is what is causing the Ziggurats (stepped pyramids) that we see in the above figures = a constant X value (energy) and a range of Y values (cross sections), creating a vertical STEP in the above figure = nonsense, completely due to nothing but truncating the tabulated ENDF formatted results to 7-digit energies.
The bottom line here is to understand that due to the details included in modern evaluations it is physically impossible for 7-digit output to accurately represent the energy dependent cross sections to anywhere near our target allowable uncertainty (0.1%). In this case we find differences in the total of over 14% and in capture over 21%; see the above plots = 140 to 210 times our target uncertainty of 0.1%. Be aware that these are not isolated differences in a few resonances; we see these differences over the entire resolved resonance energy range, and this is not even the worst case, e.g., the latest Fe56 evaluation includes resonances well up into the MeV range, an order of magnitude higher in energy than the resonances shown in the above figures. Below is but one example of a capture resonance in the MeV range where truncating from 9-digits to 7-digits results in differences of up to 226% = over a factor of 2 near the peak of this resonance!!!!!
Improved BEST Input Parameters

Based on extensive use of the earlier versions of the PREPRO codes over many years, we have been able to define the BEST Input Parameters to use with these codes. Note the effect of simply decreasing the minimum cross section from $10^{-10}$ to $10^{-30}$ barns to be linearized (tabulated data below the minimum are copied, ignoring the ENDF interpolation code). This has a rather dramatic effect, particularly on (neutron, charged particle) reactions, which often have long, slowly decreasing tails toward the reaction threshold. In the below example the evaluator tabulated values of the cross sections down to below $10^{-20}$ barns using log-log interpolation (INT=5). Earlier versions of PREPRO ignored the interpolation code below $10^{-10}$ and copied the original tabulated values and indicated lin-lin interpolation (INT=2). In contrast today using the BEST input PREPRO linearized the cross sections over the entire tabulated range. Here the cross section can be quite small, but extends over a large energy range, so there might be an integral effect; in the below plot interpolated values differ by up to a factor of 1 million. Since this extension has only a minor effect on the overall size of the pre-processed ENDF data (i.e., the number of tabulated energy points), there is virtually no penalty in accurately including these data.

![Diagram showing cross section and ratio plots for different incident energies and thresholds.](image)
Doppler Broadening High Energy Cutoff

Today many modern evaluations extend to very high incident neutron energies, well above the traditional ENDF 20 MeV upper energy limit for evaluations. In these cases, the theoretical models used for the evaluations often change at or near 20 MeV, which can cause an abrupt change (a non-physical discontinuity) in cross sections. To compensate for the “intent” of the evaluators, PREPRO Doppler broadening now only extends up to 10 MeV. This has the effect of making the “discontinuities” in the cross section at or near 20 MeV temperature independent, which I judge to be the “intent” of the evaluators, i.e., this reproduces the result of the models used.

Here we are admittedly choosing between “the Devil and the deep blue sea” = both results shown in the below figures are PHYSICALLY incorrect. The discontinuities that we see in newer evaluations, to extend them above 20 MeV, are NONSENSE, e.g., no evaluator would claim these discontinuities are real. But ‘smoothing” this discontinuity due to Doppler broadening only makes the results worse and more difficult to interpret/see. As a result, at very high energy I have chosen to not Doppler broaden, and instead I keep the cross sections, including any discontinuity exactly as defined by the evaluator. This approach will at least allow us to “see” whether this discontinuity is of any importance in our calculations; and if it is, we are able to request that evaluators (rather than our codes) deal with any discontinuities.
The Effects of Temperature and Doppler Broadening

For those readers who are not familiar with the effects of temperature and Doppler broadening on neutron cross sections and transport, for details I suggest that you read Refs [12 – 16]. Here I will give a brief description of these effects. Users of neutron cross sections should be aware that there are several important effects of temperature and Doppler broadening,

First an important point to understand is that: neutron cross sections ARE NOT TEMPERATURE DEPENDENT, in the relative frame-of-reference at the same relative speed the cross sections are temperature INDEPENDENT. Unfortunately, normally we do not perform our calculations in the relative frame-of-reference; we perform our calculations in the Laboratory frame-of-reference, and it is our transformation to the LAB frame that make neutron cross sections “appear” to be temperature dependent. This problem of relative motion is quite similar to the “apparent” rotation of the Sun about the Earth, that led to mankind assuming the Earth was the center of the Universe for thousands of years. In the LAB frame-of-reference we have a similar problem in that the thermal motion of atoms within any material can change the RELATIVE speed between a neutron and a target atom, and this effect will depend on how fast the atoms within the material are moving, and this SPEED of the atoms is directly related to the TEMPERATURE of the medium. If you read references such as Refs [12 – 16], you will see that in their equations they are using exactly the same basic cross sections at all temperatures (the temperature independent, relative frame data), but in order to define the LAB frame-of-reference cross sections we need, they average over the thermal motion of the atoms in the material in order to define the average cross section “seen” (encountered) by a neutron with any given LAB speed.
Temperature Effect on Resonance Cross Sections

First, I will mention the well-known **effect of temperatures in the neutron resonance region**, where, as the temperature increases, resonances become broader, hence the name **Doppler broadening**. The below figure illustrates the effect of temperature on the $^{238}$U capture cross section for neutron-reactor-like temperatures, and the next figure illustrates this effect for astrophysical-like temperatures. These figures each contain four sub-figures, with each sub-figure comparing cross sections at two progressively higher temperatures. In both figures each sub-figure shows the same incident neutron LAB energy and cross section range. From these figures we can see that, as temperature increases, the peaks of the resonances become lower, and the minima between resonances become higher. At extremely high temperature the entire resonance structure disappears, and the cross section approaches a simple $1/V$ shape (where $v$ is the neutron speed) (see, ref. 12 for an explanation). This temperature effect will have a very important effect on resonance self-shielding in any neutron transport calculation. You should also note from these figures that due to the narrow resonance widths and large resonance spacing in $^{238}$U, the resonance structure and the effect of Doppler broadening can still be seen up to very high neutron incident energies.
To understand the importance of considering temperature we should consider reaction rates, such as captures/second, in various systems. In optically thin systems (few mean free paths dimensions), the flux will be unshielded, and our reaction rates will be defined by a simple cross section average.

Unshielded Capture = \( \int_{E_1}^{E_2} \Sigma c(E) \phi(E) dE \) = capture cross section times neutron flux

In optically thick systems (many mean free paths dimensions), the flux will be shielded (the flux is suppressed by the total cross section) and our reaction rates must include the effect of self-shielding on the cross section average.

Shielded Capture = \( \int_{E_1}^{E_2} \frac{\Sigma c(E) \phi(E)}{\Sigma t(E)} dE \) = including one over total cross section

Consider for example the \(^{238}\text{U}\) capture cross section in the incident neutron energy between 1 and 10 keV as shown in the above figures. If we calculate the unshielded and shielded average capture cross section for the energy interval over the range of temperatures shown in the above figures, we obtain the results shown in the below table.

What we see from these results is that the unshielded average capture cross section is virtually independent from temperature, being about 1 barn over the entire temperature range. In contrast, the shielded average cross section varies by over a factor of three between the 0 K average (0.293 barns) and the 10 keV average (0.939 barns). The point to learn from this is that, without including the effect of self-shielding in multi-group calculations, temperature has very little effect on the average cross sections, which is quite simply wrong for optically thick systems. So, make sure you use the POINT cross sections that are appropriate for the temperature of the media in your applications.

**Effect of Temperature on Average Cross Sections**

<table>
<thead>
<tr>
<th>Temp.</th>
<th>Unshielded (barns)</th>
<th>Shielded (barns)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 K</td>
<td>0.996</td>
<td>0.293</td>
</tr>
<tr>
<td>293.6 K</td>
<td>0.966</td>
<td>0.526</td>
</tr>
<tr>
<td>600 K</td>
<td>0.996</td>
<td>0.576</td>
</tr>
<tr>
<td>1,200 K</td>
<td>0.996</td>
<td>0.630</td>
</tr>
<tr>
<td>12,000 K (1 eV)</td>
<td>0.996</td>
<td>0.799</td>
</tr>
<tr>
<td>10 eV</td>
<td>0.998</td>
<td>0.905</td>
</tr>
<tr>
<td>100 eV</td>
<td>1.000</td>
<td>0.933</td>
</tr>
<tr>
<td>1 keV</td>
<td>1.004</td>
<td>0.935</td>
</tr>
<tr>
<td>10 keV</td>
<td>1.007</td>
<td>0.939</td>
</tr>
</tbody>
</table>
Temperature Effect on Low Energy Cross Sections

Another, less well known effect of Doppler broadening is at lower energies where, as temperature increases, the low energy constant scattering cross section increases and at very low energies approaches a simple $1/V$ shape (where $v$ is the neutron speed); this effect is explained in detail in Ref. [15]. The below figure illustrates the effect of temperature on the hydrogen total cross section. From this figure we can see that, starting from a “cold” (0 Kelvin) cross section that is constant at about 20 barns, as temperature increases the cross section increases. Compared to the “cold” 20 barn cross section, at thermal energy the Doppler broadened cross section is about 30 barns, i.e., 50% higher. Note also from this figure that this effect extends well above thermal energy. For example, at 293.6 Kelvin the thermal energy is 0.0253 eV, but we can see this effect up to about 1 eV: a factor of 40 higher in energy. From the lower half of the below figure, we can see that at very low energy the cross section approaches a simple $1/V$ shape (where $v$ is the neutron speed) and the cross sections at various temperatures become proportional to one another. This effect on the cross sections at low energy is especially important for thermal and low energy neutron systems.

Note that, as temperature increases, the lower energy cross sections approaches $1/V$. Usually the “cold” (0 Kelvin) capture and fission cross sections are already $1/V$ in shape, so that temperature may have little or no effect on these. The net effect can change the ratio of elastic to capture or fission at low incident neutron energy.
Thermal Scattering

Yet another important effect of temperature is that at lower energies neutrons do not slowdown in energy as quickly and neutron scatter can even result in the upscatter of neutrons, i.e., when neutrons scatter, they can gain, rather than lose, energy. This is a well-known effect at low energies, where thermal scattering law data, $S(a, b)$, or a free gas model, is used to model the interaction of neutrons with target atoms that are moving about with thermal motion [15].

THERMAL [15], is a routine designed to be used in conjunction with the SIGMA1 method of Doppler broadening [12], to handle neutron thermal scattering. SIGMA1 deals with Doppler broadening, which defines what happens **BEFORE** any event. THERMAL [15] defines what happens **AFTER** a thermal scatter event, i.e., it defines the new direction and energy of a scattered neutron. THERMAL is completely compatible for use with the cross sections included here, since these cross sections were Doppler broadened using the SIGMA1 method [12]. The combination of SIGMA1 [12] Doppler broadened cross sections and THERMAL [15] to handle thermal scattering, is currently used in the TART Monte Carlo transport code [16].

The below figure illustrates the effect of temperature on the neutron spectrum over a wide range of temperatures [15], e.g., THERMAL produces the Maxwellian-like energy of neutrons after scatter. This effect can also be important at higher energies, particularly near narrow resonances, where thermal motion of the target atoms can cause neutrons to slightly upscatter, but even slight upscatter can cause a neutron to scatter from below to above the energy of a very narrow resonance.
References


