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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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Contents

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.

Z	7	8	Z	7	8	Z	7	8	Z	7	8	Z	7	8
1	3	3	21	1	1	41	3	3	61	5	10	81	2	3
2	2	2	22	5	5	42	8	9	62	9	11	82	4	5
3	2	2	23	2	3	43	1	2	63	7	7	83	1	2
4	2	2	24	4	5	44	10	11	64	8	9	84	0*	3
5	2	2	25	1	2	45	2	3	65	2	4	85	0*	0*
6	1	2	26	4	5	46	7	9	66	7	11	86	0*	0*
7	2	2	27	3	3	47	4	12	67	2	2	87	0*	0*
8	2	3	28	6	7	48	9	11	68	6	9	88	4	4
9	1	1	29	2	3	49	2	3	69	3	4	89	3	3
10	0*	3	30	6	7	50	14	15	70	0*	9	90	8	8
11	2	2	31	2	3	51	5	6	71	2	2	91	5	5
12	3	3	32	5	7	52	11	15	72	6	9	92	12	12
13	1	2	33	2	3	53	5	10	73	3	3	93	6	7
14	3	5	34	7	9	54	12	14	74	5	7	94	10	11
15	1	1	35	2	3	55	5	5	75	2	3	95	7	7
16	4	5	36	7	9	56	9	11	76	0*	9	96	11	11
17	2	3	37	3	3	57	3	3	77	2	4	97	6	6
18	3	6	38	6	7	58	8	10	78	0*	9	98	8	9
19	3	3	39	3	3	59	3	3	79	1	1	99	6	6
20	6	9	40	7	7	60	8	9	80	7	10	100	1	1

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)

Neutron	18-Ar-41	33-As-73	47-Ag-112	52-Te-131	61-Pm-143	68-Er-163	72-Hf-181	77-Ir-192	81-Tl-204
6-C -12	20-Ca-41	34-Se-75	47-Ag-113	52-Te-131m	61-Pm-144	68-Er-165	72-Hf-182	77-Ir-194m	82-Pb-205
6-C -13	20-Ca-45	34-Se-81	47-Ag-114	53-I -128	61-Pm-145	68-Er-169	74-W -181	78-Pt-190	83-Bi-210m
8-O -18	20-Ca-47	35-Br-80	47-Ag-115	53-I -132	61-Pm-146	69-Tm-171	74-W -185	78-Pt-191	84-Po-208
10-Ne-20	23-V -49	36-Kr-79	47-Ag-116	53-I -132m	61-Pm-150	70-Yb-168	75-Re-186m	78-Pt-192	84-Po-209
10-Ne-21	24-Cr-51	36-Kr-81	47-Ag-117	53-I -133	62-Sm-145	70-Yb-169	76-Os-184	78-Pt-193	84-Po-210
10-Ne-22	25-Mn-54	38-Sr-85	47-Ag-118m	53-I -134	62-Sm-146	70-Yb-170	76-Os-185	78-Pt-194	93-Np-236m
13-Al-26m	26-Fe-55	42-Mo-93	48-Cd-107	54-Xe-125	64-Gd-159	70-Yb-171	76-Os-186	78-Pt-195	94-Pu-245
14-Si-31	28-Ni-63	43-Tc-98	48-Cd-109	54-Xe-127	65-Tb-158	70-Yb-172	76-Os-187	78-Pt-196	98-Cf-247
14-Si-32	29-Cu-64	44-Ru-97	49-In-114	56-Ba-131	65-Tb-161	70-Yb-173	76-Os-188	78-Pt-197	
16-S -35	30-Zn-69	45-Rh-104	50-Sn-121m	56-Ba-139	66-Dy-154	70-Yb-174	76-Os-189	78-Pt-198	
17-Cl-36	31-Ga-70	46-Pd-103	51-Sb-122	58-Ce-137	66-Dy-155	70-Yb-175	76-Os-190	80-Hg-197	
18-Ar-37	32-Ge-71	46-Pd-109	52-Te-121	58-Ce-137m	66-Dy-157	70-Yb-176	76-Os-191	80-Hg-197m	
18-Ar-39	32-Ge-75	47-Ag-108	52-Te-121m	60-Nd-149	66-Dy-159	72-Hf-175	76-Os-192	80-Hg-203	

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

1-H -1	20-Ca-44	32-Ge-74	42-Mo-92	49-In-115	54-Xe-131	61-Pm-147	68-Er-166	88-Ra-224	94-Pu-242
1-H -2	20-Ca-46	32-Ge-76	42-Mo-94	50-Sn-112	54-Xe-132	61-Pm-148	68-Er-167	88-Ra-225	94-Pu-243
1-H -3	20-Ca-48	33-As-74	42-Mo-95	50-Sn-113	54-Xe-133	61-Pm-148m	68-Er-168	88-Ra-226	94-Pu-244
2-He-3	21-Sc-45	33-As-75	42-Mo-96	50-Sn-114	54-Xe-134	61-Pm-149	68-Er-170	89-Ac-225	94-Pu-246
2-He-4	22-Ti-46	34-Se-74	42-Mo-97	50-Sn-115	54-Xe-135	61-Pm-151	69-Tm-168	89-Ac-226	95-Am-240
3-Li-6	22-Ti-47	34-Se-76	42-Mo-98	50-Sn-116	54-Xe-136	62-Sm-144	69-Tm-169	89-Ac-227	95-Am-241
3-Li-7	22-Ti-48	34-Se-77	42-Mo-99	50-Sn-117	55-Cs-133	62-Sm-147	69-Tm-170	90-Th-227	95-Am-242
4-Be-7	22-Ti-49	34-Se-78	42-Mo-100	50-Sn-118	55-Cs-134	62-Sm-148	71-Lu-175	90-Th-228	95-Am-242m
4-Be-9	22-Ti-50	34-Se-79	43-Tc-99	50-Sn-119	55-Cs-135	62-Sm-149	71-Lu-176	90-Th-229	95-Am-243
5-B -10	23-V -50	34-Se-80	44-Ru-96	50-Sn-120	55-Cs-136	62-Sm-150	72-Hf-174	90-Th-230	95-Am-244
5-B -11	23-V -51	34-Se-82	44-Ru-98	50-Sn-122	55-Cs-137	62-Sm-151	72-Hf-176	90-Th-231	95-Am-244m
6-C -Nat	24-Cr-50	35-Br-79	44-Ru-99	50-Sn-123	56-Ba-130	62-Sm-152	72-Hf-177	90-Th-232	96-Cm-240
7-N -14	24-Cr-52	35-Br-81	44-Ru-100	50-Sn-124	56-Ba-132	62-Sm-153	72-Hf-178	90-Th-233	96-Cm-241
7-N -15	24-Cr-53	36-Kr-78	44-Ru-101	50-Sn-125	56-Ba-133	62-Sm-154	72-Hf-179	90-Th-234	96-Cm-242
8-O -16	24-Cr-54	36-Kr-80	44-Ru-102	50-Sn-126	56-Ba-134	63-Eu-151	72-Hf-180	91-Pa-229	96-Cm-243
8-O -17	25-Mn-55	36-Kr-82	44-Ru-103	51-Sb-121	56-Ba-135	63-Eu-152	73-Ta-180	91-Pa-230	96-Cm-244
9-F -19	26-Fe-54	36-Kr-83	44-Ru-104	51-Sb-123	56-Ba-136	63-Eu-153	73-Ta-181	91-Pa-231	96-Cm-245
11-Na-22	26-Fe-56	36-Kr-84	44-Ru-105	51-Sb-124	56-Ba-137	63-Eu-154	73-Ta-182	91-Pa-232	96-Cm-246
11-Na-23	26-Fe-57	36-Kr-85	44-Ru-106	51-Sb-125	56-Ba-138	63-Eu-155	74-W -180	91-Pa-233	96-Cm-247
12-Mg-24	26-Fe-58	36-Kr-86	45-Rh-103	51-Sb-126	56-Ba-140	63-Eu-156	74-W -182	92-U -230	96-Cm-248
12-Mg-25	27-Co-58	37-Rb-85	45-Rh-105	52-Te-120	57-La-138	63-Eu-157	74-W -183	92-U -231	96-Cm-249
12-Mg-26	27-Co-58m	37-Rb-86	46-Pd-102	52-Te-122	57-La-139	64-Gd-152	74-W -184	92-U -232	96-Cm-250
13-Al-27	27-Co-59	37-Rb-87	46-Pd-104	52-Te-123	57-La-140	64-Gd-153	74-W -186	92-U -233	97-Bk-245
14-Si-28	28-Ni-58	38-Sr-84	46-Pd-105	52-Te-124	58-Ce-136	64-Gd-154	75-Re-185	92-U -234	97-Bk-246
14-Si-29	28-Ni-59	38-Sr-86	46-Pd-106	52-Te-125	58-Ce-138	64-Gd-155	75-Re-187	92-U -235	97-Bk-247
14-Si-30	28-Ni-60	38-Sr-87	46-Pd-107	52-Te-126	58-Ce-139	64-Gd-156	77-Ir-191	92-U -236	97-Bk-248
15-P -31	28-Ni-61	38-Sr-88	46-Pd-108	52-Te-127m	58-Ce-140	64-Gd-157	77-Ir-193	92-U -237	97-Bk-249
16-S -32	28-Ni-62	38-Sr-89	46-Pd-110	52-Te-128	58-Ce-141	64-Gd-158	79-Au-197	92-U -238	97-Bk-250
16-S -33	28-Ni-64	38-Sr-90	47-Ag-107	52-Te-129m	58-Ce-142	64-Gd-160	80-Hg-196	92-U -239	98-Cf-246
16-S -34	29-Cu-63	39-Y -89	47-Ag-109	52-Te-130	58-Ce-143	65-Tb-159	80-Hg-198	92-U -240	98-Cf-248
16-S -36	29-Cu-65	39-Y -90	47-Ag-110m	52-Te-132	58-Ce-144	65-Tb-160	80-Hg-199	92-U -241	98-Cf-249
17-Cl-35	30-Zn-64	39-Y -91	47-Ag-111	53-I -127	59-Pr-141	66-Dy-156	80-Hg-200	93-Np-234	98-Cf-250
17-Cl-37	30-Zn-65	40-Zr-90	48-Cd-106	53-I -129	59-Pr-142	66-Dy-158	80-Hg-201	93-Np-235	98-Cf-251
18-Ar-36	30-Zn-66	40-Zr-91	48-Cd-108	53-I -130	59-Pr-143	66-Dy-160	80-Hg-202	93-Np-236	98-Cf-252
18-Ar-38	30-Zn-67	40-Zr-92	48-Cd-110	53-I -131	60-Nd-142	66-Dy-161	80-Hg-204	93-Np-237	98-Cf-253
18-Ar-40	30-Zn-68	40-Zr-93	48-Cd-111	53-I -135	60-Nd-143	66-Dy-162	81-Tl-203	93-Np-238	98-Cf-254
19-K -39	30-Zn-70	40-Zr-94	48-Cd-112	54-Xe-123	60-Nd-144	66-Dy-163	81-Tl-205	93-Np-239	99-Es-251
19-K -40	31-Ga-69	40-Zr-95	48-Cd-113	54-Xe-124	60-Nd-145	66-Dy-164	82-Pb-204	94-Pu-236	99-Es-252
19-K -41	31-Ga-71	40-Zr-96	48-Cd-114	54-Xe-126	60-Nd-146	67-Ho-165	82-Pb-206	94-Pu-237	99-Es-253
20-Ca-40	32-Ge-70	41-Nb-93	48-Cd-115m	54-Xe-128	60-Nd-147	67-Ho-166m	82-Pb-207	94-Pu-238	99-Es-254
20-Ca-42	32-Ge-72	41-Nb-94	48-Cd-116	54-Xe-129	60-Nd-148	68-Er-162	82-Pb-208	94-Pu-239	99-Es-254m
20-Ca-43	32-Ge-73	41-Nb-95	49-In-113	54-Xe-130	60-Nd-150	68-Er-164	83-Bi-209	94-Pu-240	99-Es-255
							88-Ra-223	94-Pu-241	100-Fm-255

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 PREEPRO/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 on-line from the Nuclear Data Section, IAEA, Vienna, Austria,
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

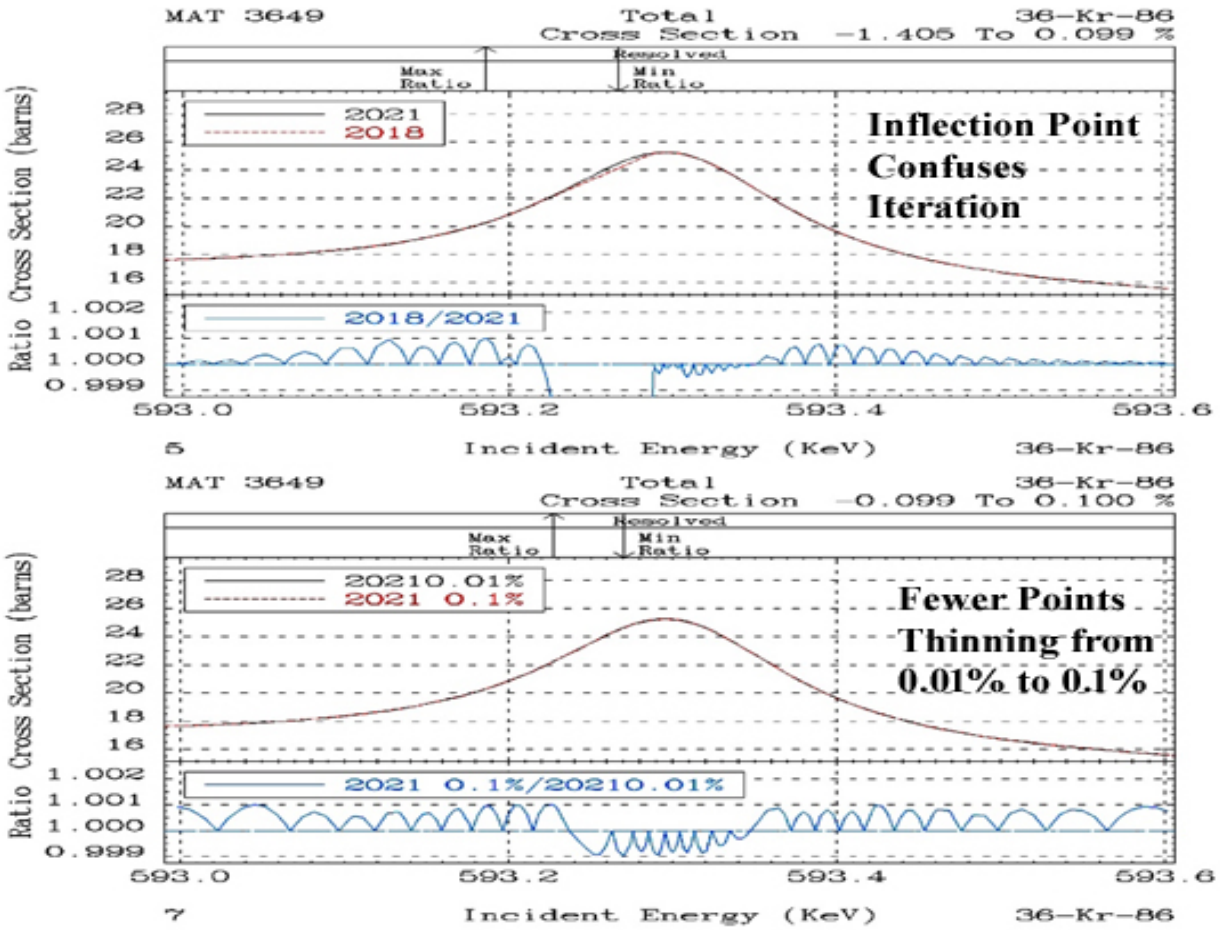
For use in earlier POINT libraries all cross sections were reconstructed to within an accuracy of 0.01% in the thermal range, and 0.1 % at all other incident neutron energies and temperatures; this is beyond the accuracy to which this data in known. **In practice it has been found to be extremely difficult 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.

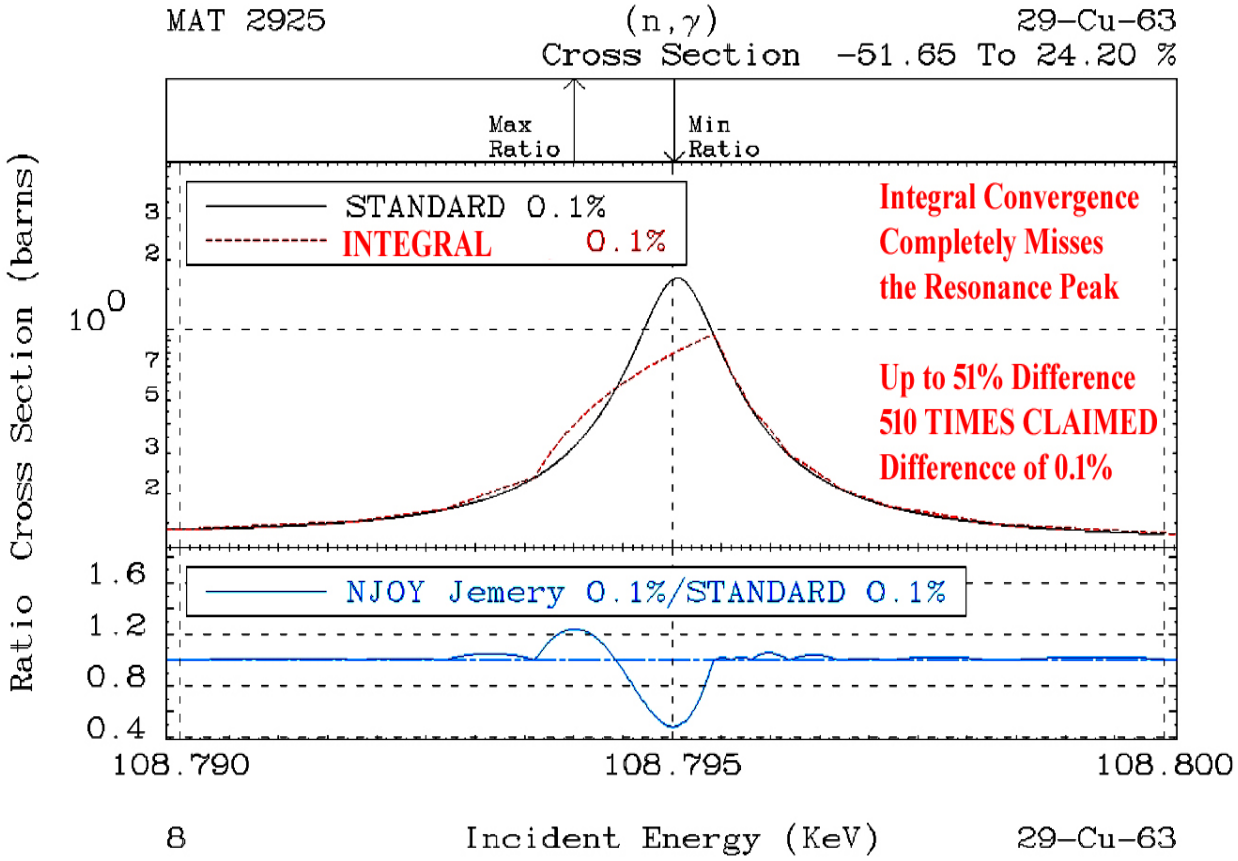
0.01% versus 0.1% Results

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 POINT2021library 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@bnlnd2.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 ZA00001 (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

```
1.002000+3 1.996800+0          0          0          0          0 128 3  1  125
0.000000+0 0.000000+0          0          0          1        149 128 3  1  126
       149          2                                              128 3  1  127
1.000000-5 3.420300+0 1.000000-4 3.403000+0 2.530000-2 3.395510+0 128 3  1  128
1.000000+2 3.395010+0 1.000000+3 3.394900+0 2.000000+3 3.394800+0 128 3  1  129
3.000000+3 3.394400+0 4.000000+3 3.389400+0 5.000000+3 3.385000+0 128 3  1  130
1.000000+4 3.367000+0 2.000000+4 3.342000+0 3.000000+4 3.321000+0 128 3  1  131
4.000000+4 3.302000+0 5.000002+4 3.285000+0 6.000002+4 3.270000+0 128 3  1  132
```

After ENDF2C

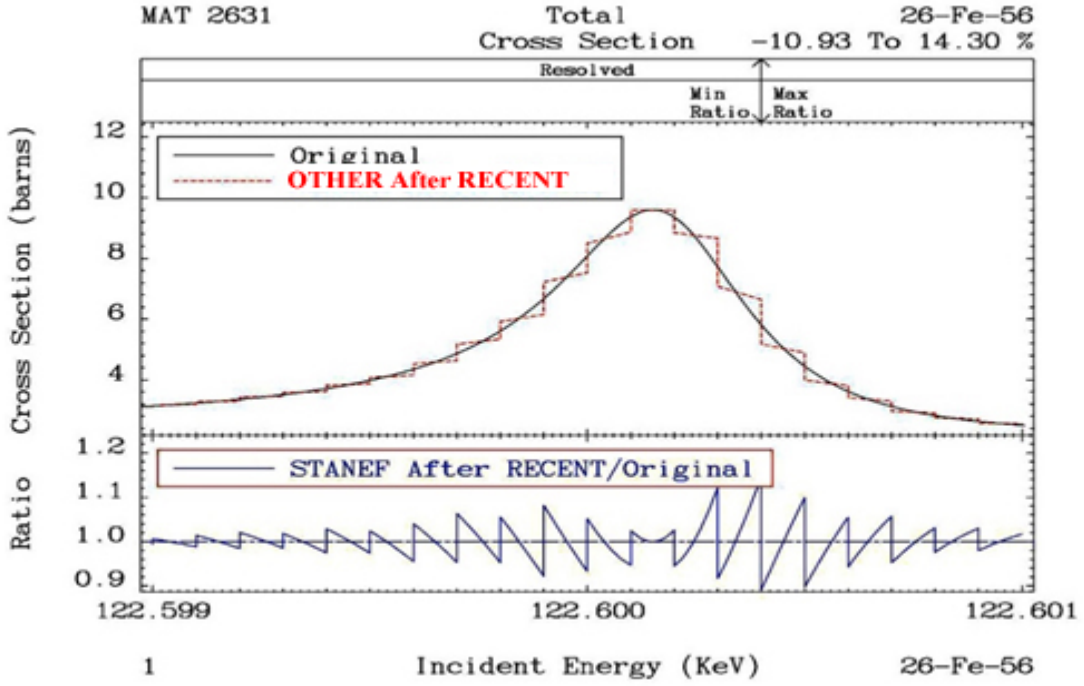
```
1002.00000 1.99680000          0          0          0          0 128 3  1    1
0.0        0.0                 0          0          1        149 128 3  1    2
       149          2                                              128 3  1    3
1.00000E-5 3.42030000 1.00000E-4 3.40300000 .025300000 3.39551000 128 3  1    4
100.000000 3.39501000 1000.00000 3.39490000 2000.00000 3.39480000 128 3  1    5
3000.00000 3.39440000 4000.00000 3.38940000 5000.00000 3.38500000 128 3  1    6
10000.0000 3.36700000 20000.0000 3.34200000 30000.0000 3.32100000 128 3  1    7
40000.0000 3.30200000 50000.0200 3.28500000 60000.0200 3.27000000 128 3  1    8
```

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.

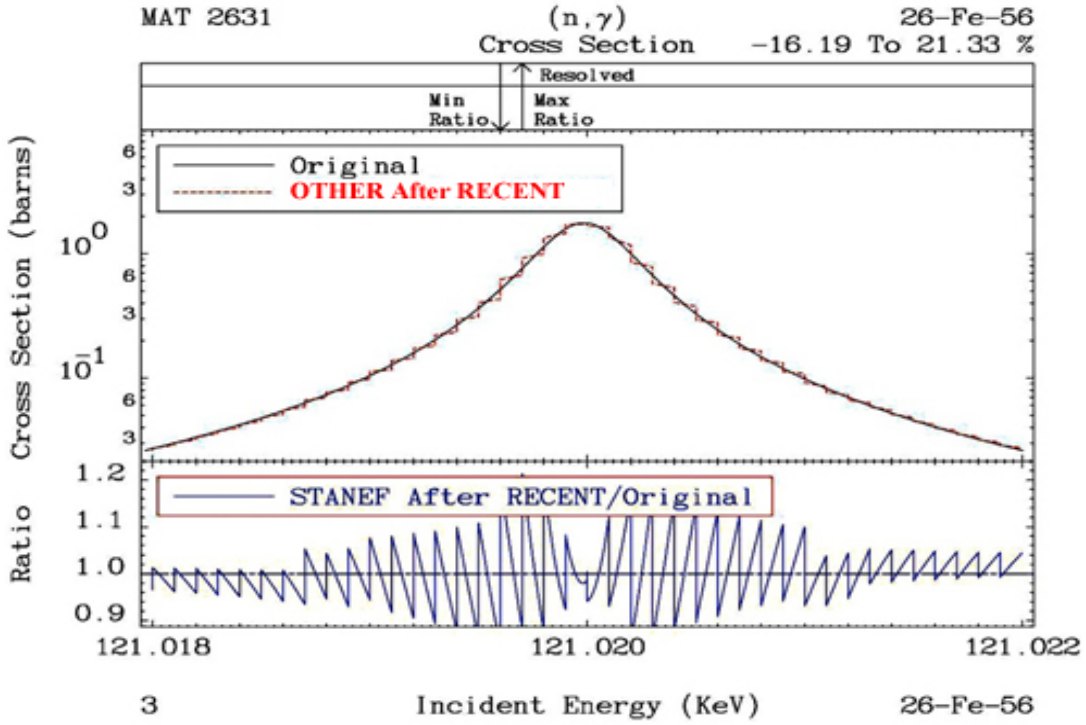
PREPRO uses 9 or 10 digit precision for all ENDF output

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,



Capture showing differences up to 21.3% difference,



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,

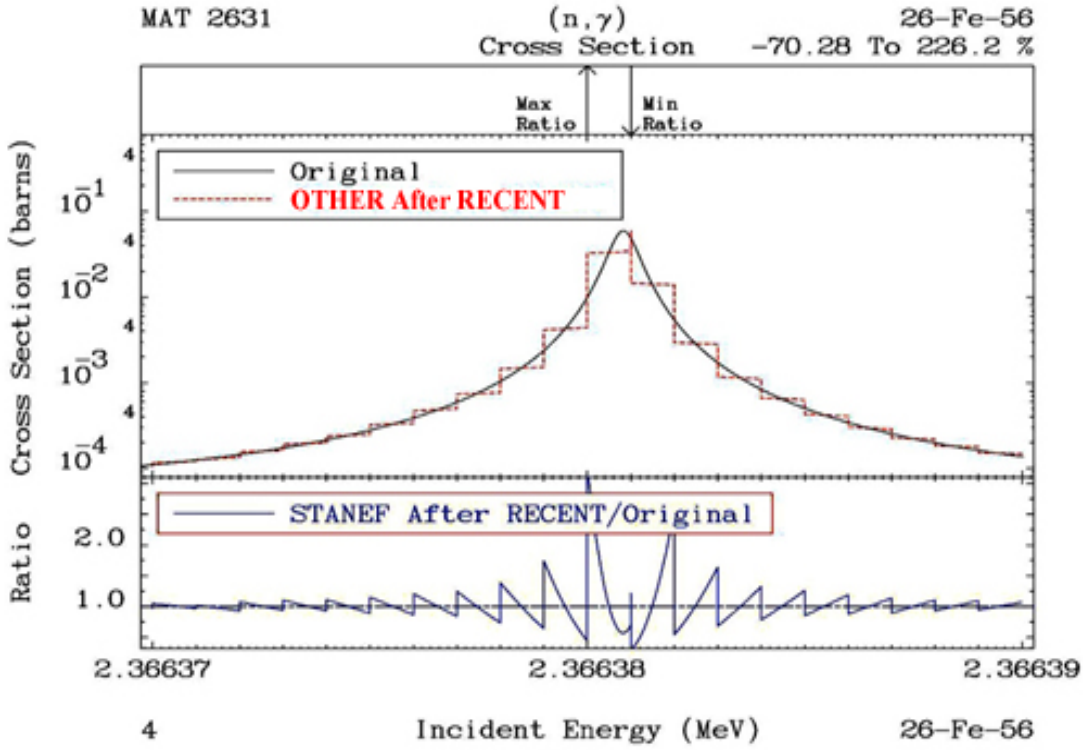
```
122600.007 8.18440080 122600.018 8.34734256 122600.021 8.391426722631 3  1 6030
122600.028 8.49343634 122600.055 8.86885730 122600.077 9.139853322631 3  1 6031
122600.099 9.36221564 122600.120 9.51387393 122600.131 9.565109362631 3  1 6032
122600.142 9.59483076 122600.153 9.60178112 122600.164 9.585085692631 3  1 6033
122600.176 9.53939892 122600.178 9.52899291 122600.180 9.517793222631 3  1 6034
122600.182 9.50580250 122600.184 9.49302393 122600.196 9.400050502631 3  1 6035
122600.207 9.29106975 122600.218 9.16076388 122600.229 9.010880802631 3  1 6036
122600.240 8.84348060 122600.251 8.66085453 122600.261 8.483667022631 3  1 6037
122600.283 8.06587838 122600.305 7.62540465 122600.319 7.341331292631 3  1 6038
122600.332 7.07896654 122600.354 6.64519685 122600.375 6.250366772631 3  1 6039
122600.397 5.86278292 122600.419 5.50514627 122600.441 5.178659552631 3  1 6040
122600.462 4.89577103 122600.484 4.62825344 122600.505 4.398676332631 3  1 6041
122600.527 4.18301692 122600.549 3.99047205 122600.571 3.818722112631 3  1 6042
122600.592 3.67214930 122600.614 3.53482178 122600.625 3.471802962631 3  1 6043
122600.636 3.41225491 122600.658 3.30276311 122600.679 3.209061382631 3  1 6044
122600.701 3.12093801 122600.722 3.04533219 122600.744 2.974035832631 3  1 6045
122600.766 2.90992540 122600.788 2.85219006 122600.809 2.802371112631 3  1 6046
122600.831 2.75512041 122600.853 2.71238188 122600.875 2.673669622631 3  1 6047
122600.896 2.64007944 122600.918 2.60804847 122600.939 2.580185982631 3  1 6048
122600.961 2.55355301 122600.983 2.52927697 122601.005 2.507124522631 3  1 6049
```

To the 7-digit output over the same energy range,

```
 1.226000+5 8.184401+0 1.226000+5 8.347343+0 1.226000+5 8.391427+02631 3  1 4518
 1.226000+5 8.493436+0 1.226001+5 8.868857+0 1.226001+5 9.139853+02631 3  1 4519
 1.226001+5 9.362216+0 1.226001+5 9.513874+0 1.226001+5 9.565109+02631 3  1 4520
 1.226001+5 9.594831+0 1.226002+5 9.601781+0 1.226002+5 9.585086+02631 3  1 4521
 1.226002+5 9.539399+0 1.226002+5 9.528993+0 1.226002+5 9.517793+02631 3  1 4522
 1.226002+5 9.505802+0 1.226002+5 9.493024+0 1.226002+5 9.400051+02631 3  1 4523
 1.226002+5 9.291070+0 1.226002+5 9.160764+0 1.226002+5 9.010881+02631 3  1 4524
 1.226002+5 8.843481+0 1.226003+5 8.660855+0 1.226003+5 8.483667+02631 3  1 4525
 1.226003+5 8.065878+0 1.226003+5 7.625405+0 1.226003+5 7.341331+02631 3  1 4526
 1.226003+5 7.078967+0 1.226004+5 6.645197+0 1.226004+5 6.250367+02631 3  1 4527
 1.226004+5 5.862783+0 1.226004+5 5.505146+0 1.226004+5 5.178660+02631 3  1 4528
 1.226005+5 4.895771+0 1.226005+5 4.628253+0 1.226005+5 4.398676+02631 3  1 4529
 1.226005+5 4.183017+0 1.226005+5 3.990472+0 1.226006+5 3.818722+02631 3  1 4530
 1.226006+5 3.672149+0 1.226006+5 3.534822+0 1.226006+5 3.471803+02631 3  1 4531
 1.226006+5 3.412255+0 1.226007+5 3.302763+0 1.226007+5 3.209061+02631 3  1 4532
 1.226007+5 3.120938+0 1.226007+5 3.045332+0 1.226007+5 2.974036+02631 3  1 4533
 1.226008+5 2.909925+0 1.226008+5 2.852190+0 1.226008+5 2.802371+02631 3  1 4534
 1.226008+5 2.755120+0 1.226009+5 2.712382+0 1.226009+5 2.673670+02631 3  1 4535
 1.226009+5 2.640079+0 1.226009+5 2.608048+0 1.226009+5 2.580186+02631 3  1 4536
 1.226010+5 2.553553+0 1.226010+5 2.529277+0 1.226010+5 2.507125+02631 3  1 4537
```

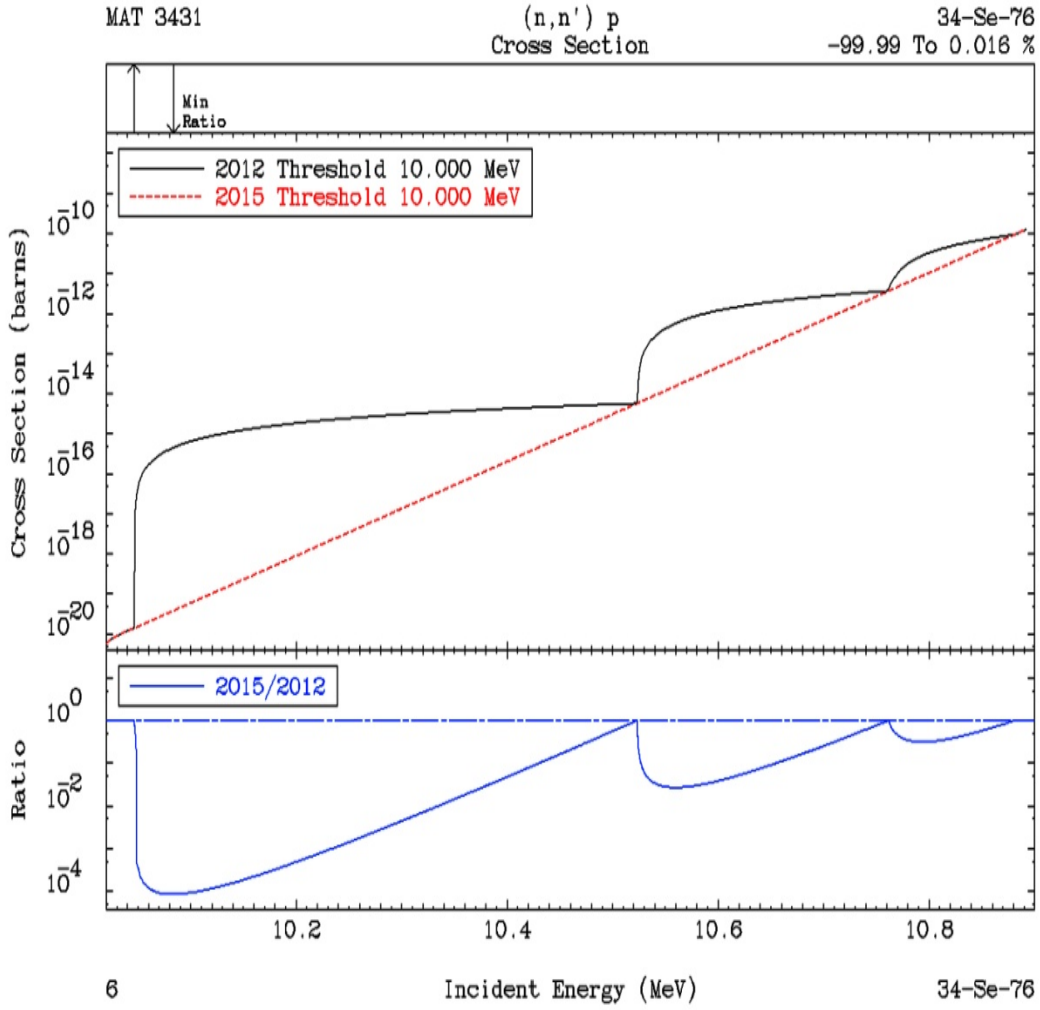
Here the entire shape of the resonance is between 122.599 keV and 122.601 keV, and we can see that all the above tabulated points in both tables start with EXACTLY the same six digit energy 122600. This means that with 9 or 10 digit RECENT output we only have 3 or 4 digits with which to define the entire 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

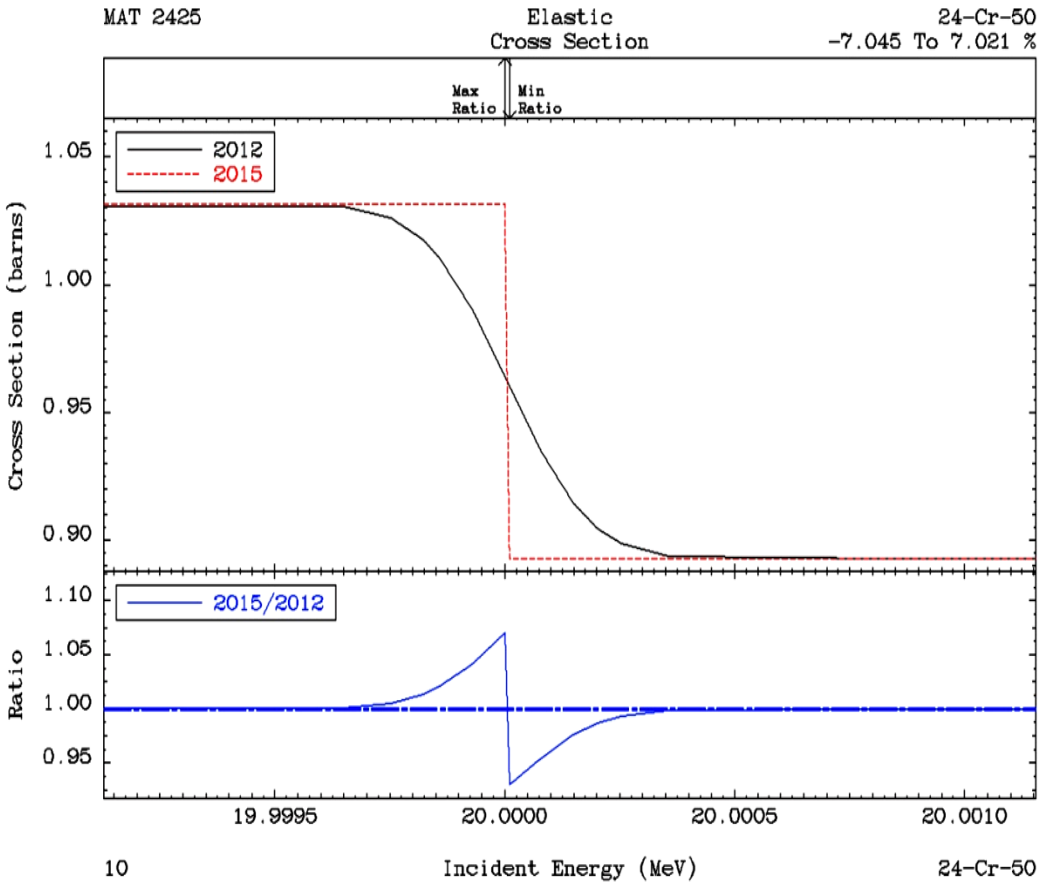
Based on extensive use of the earlier versions of the PREPRO codes over many years, we have been able to define the **BEST Input Parameters** to use with these codes. Note the effect of simply decreasing the minimum cross section from 10^{-10} to 10^{-30} barns to be linearized (tabulated data below 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.



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.



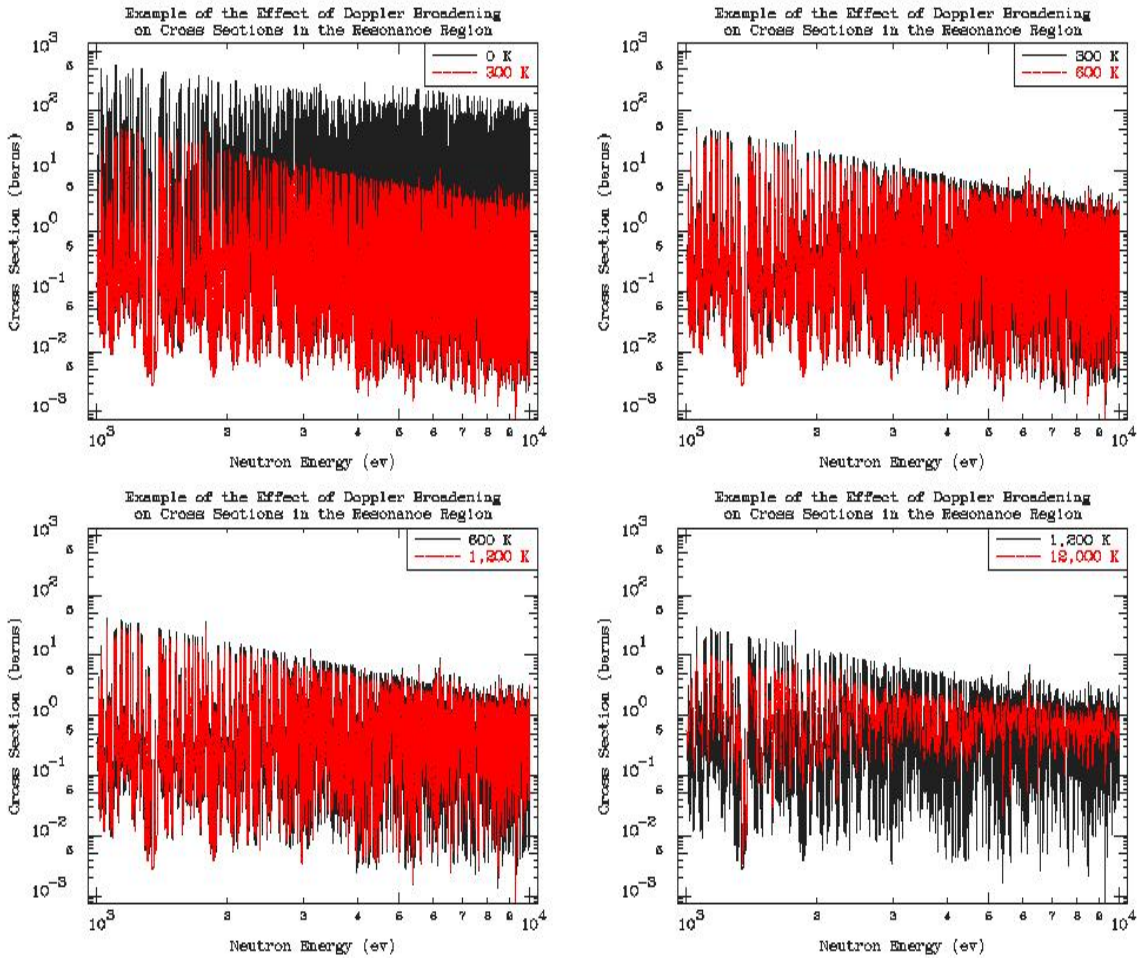
The Effects of Temperature and Doppler Broadening

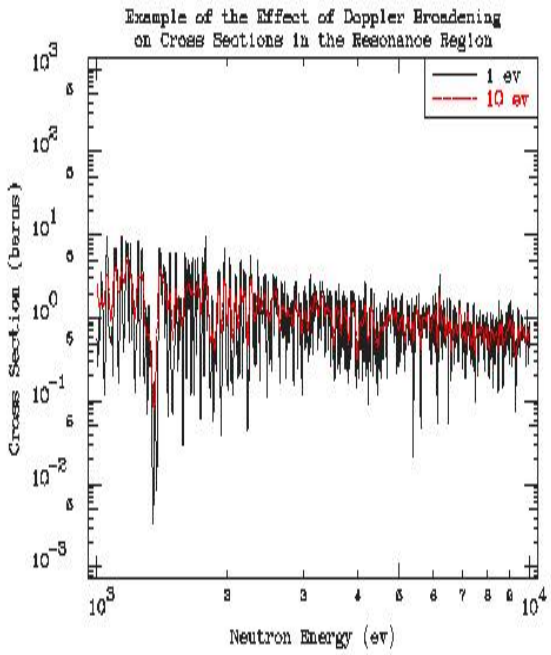
For those readers who are not familiar with the effects of temperature and Doppler broadening on neutron cross sections and transport, for details I suggest that you read Refs [12 – 16]. Here I will give a brief description of these effects. Users of neutron cross sections should be aware that there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

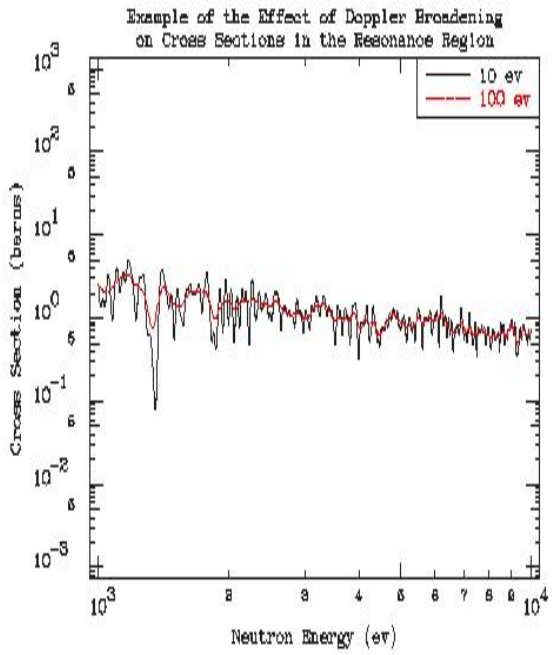
First an important point to understand is that: **neutron cross sections ARE NOT TEMPRATURE DEPENDENT**, in the relative frame-of-reference at the same relative speed the cross sections are temperature INDEPENDENT. Unfortunately, normally we do not perform our calculations in the relative frame-of-reference; 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.

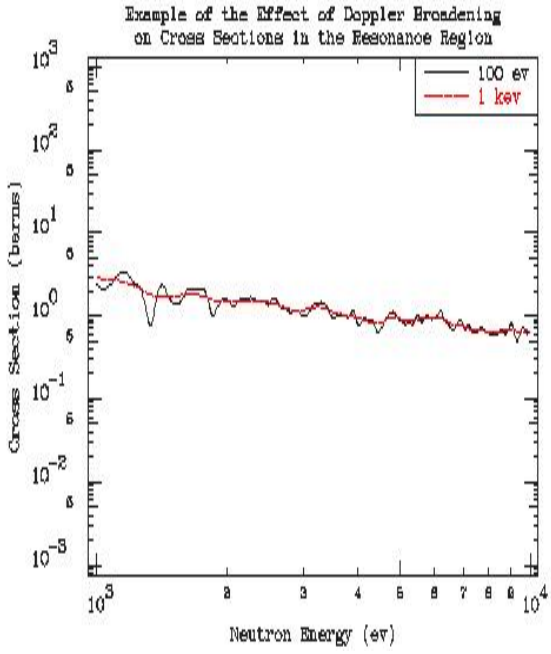
Temperature Effect on Resonance Cross Sections

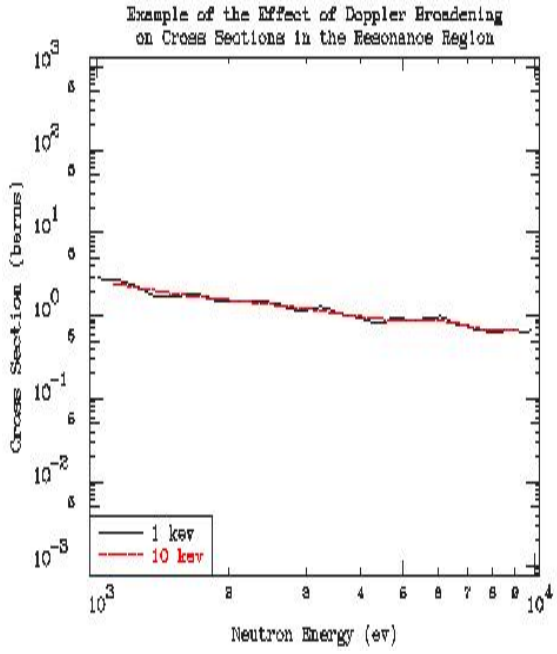
First, I will mention the well-known **effect of temperatures in the neutron resonance region**, where, as the temperature increases, resonances become broader, hence the name **Doppler broadening**. The below figure illustrates the effect of temperature on the ^{238}U capture cross section for neutron-reactor-like 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.




Example of the Effect of Doppler Broadening
on Cross Sections in the Resonance Region
1 ev
10 ev
Cross Section (barns)
Neutron Energy (ev)


Example of the Effect of Doppler Broadening
on Cross Sections in the Resonance Region
10 ev
100 ev
Cross Section (barns)
Neutron Energy (ev)


Example of the Effect of Doppler Broadening
on Cross Sections in the Resonance Region
100 ev
1 kev
Cross Section (barns)
Neutron Energy (ev)


Example of the Effect of Doppler Broadening
on Cross Sections in the Resonance Region
1 kev
10 kev
Cross Section (barns)
Neutron Energy (ev)

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 = $\int_{E1}^{E2}[\Sigma c(E)\phi(E)]dE$ = 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 = $\int_{E1}^{E2}[\Sigma c(E)\phi(E)/\Sigma t(E)]dE$ = including one over total cross section

Consider for example the ^{238}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.**

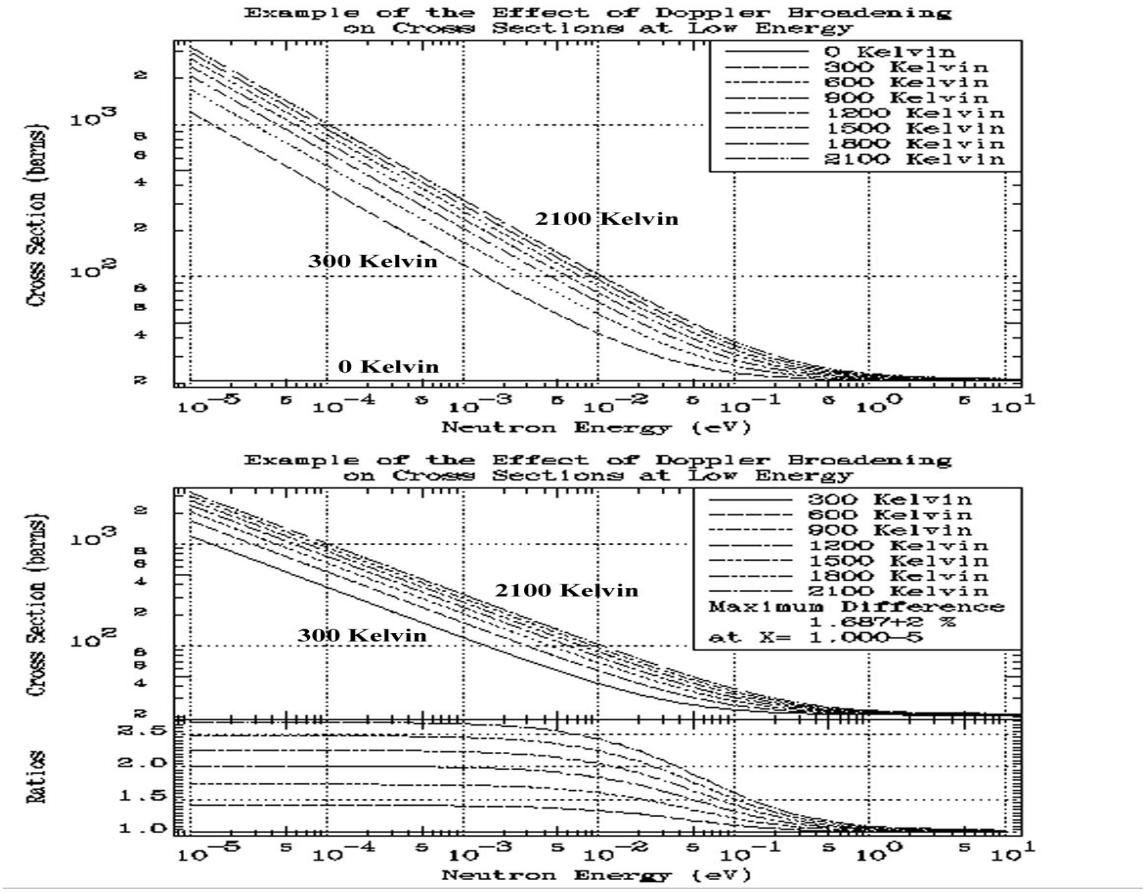
Effect of Temperature on Average Cross Sections

Temp.	Unshielded (barns)	Shielded (barns)
0 K	0.996	0.293
293.6 K	0.966	0.526
600 K	0.996	0.576
1,200 K	0.996	0.630
12,000 K (1 eV)	0.996	0.799
10 eV	0.998	0.905
100 eV	1.000	0.933
1 keV	1.004	0.935
10 keV	1.007	0.939

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.**

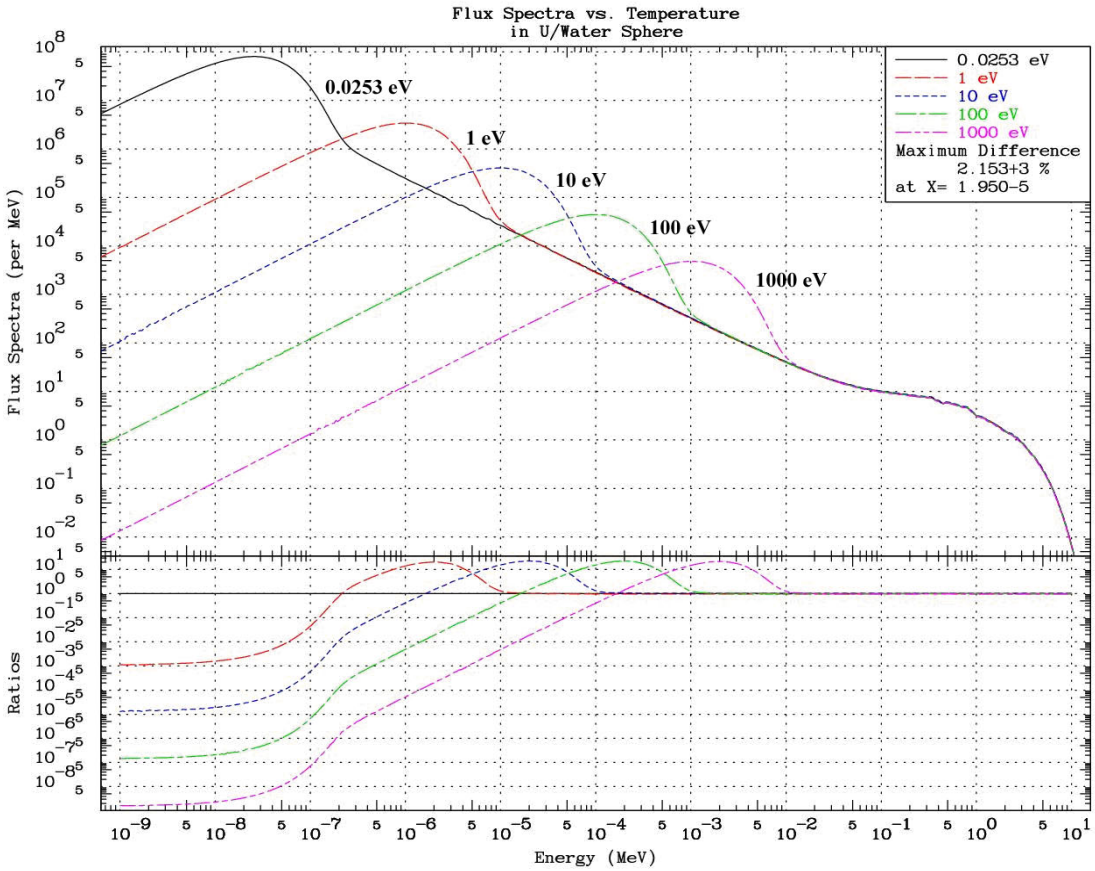


Thermal Scattering

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.



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