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# POINT 2015: ENDF/B-VII.1 Final Temperature Dependent Cross Section Library

by
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**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, <a href="http://www.nndc.bnl.gov/">http://www.nndc.bnl.gov/</a>) and, 2) publicly available computer codes (the current PREPRO codes, available on-line at the Nuclear Data Section, IAEA, Vienna, Austria, <a href="http://www-nds.iaea.or.at/ndspub/endf/prepro/">http://www-nds.iaea.or.at/ndspub/endf/prepro/</a>) 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, March 2015

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#### Overview

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 [R1]. In each case I have used my personal computer at home and publicly available data and codes:

- publicly available nuclear data (the current ENDF/B data, available on-line at the National Nuclear Data Center, Brookhaven National Laboratory, <a href="http://www.nndc.bnl.gov/">http://www.nndc.bnl.gov/</a>) and,
- publicly available computer codes (the current PREPRO codes, available on-line at the Nuclear Data Section, IAEA, Vienna, Austria, <a href="http://www-nds.iaea.or.at/ndspub/endf/prepro/">http://www-nds.iaea.or.at/ndspub/endf/prepro/</a>) 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.

#### **POINT 2015 versus POINT 2012**

Both POINT 2012 and POINT 2015 are based on exactly the same ENDF/B-VII.1 evaluations. The difference between them is 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 (PREPRO 2015) that were used to create POINT 2015. Compared to earlier versions of the PREPRO codes the 2015 version has the following features,

**FORTRAN, C** C++ Compatible ENDF results: I have added the ENDF2C code to PREPRO, to insure that ALL PREPRO output in the ENDF format are completely FORTRAN, C and C++ compatible. As of today (January 2015) 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 insure 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 of 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 will be able to avoid this problem. PREPRO2015 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).

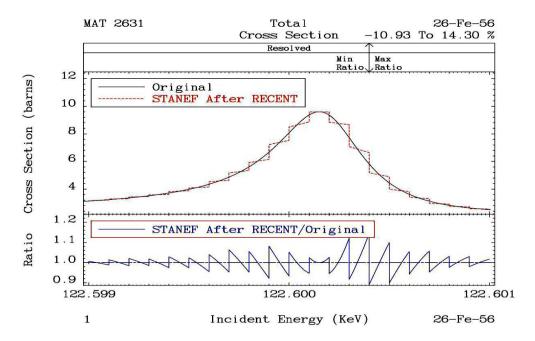
#### **Before ENDF2C**

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1.002000+3 1.996800+0
                                                                 0 128 3
                                                                             125
0.000000+0 0.000000+0
                                                              149 128 3
                                                                             126
      149
                                                                   128 3
1.000000-5 3.420300+0 1.000000-4 3.403000+0 2.530000-2 3.395510+0 128 3
1.000000+2 3.395010+0 1.000000+3 3.394900+0 2.000000+3 3.394800+0 128 3
3.000000+3 3.394400+0 4.000000+3 3.389400+0 5.000000+3 3.385000+0 128
                                                                             130
1.000000+4 3.367000+0 2.000000+4 3.342000+0 3.000000+4 3.321000+0 128
4.000000+4 3.302000+0 5.000002+4 3.285000+0 6.000002+4 3.270000+0 128 3
                                    After ENDF2C
1002.00000 1.99680000
                               O
                                          O
                                                     0
                                                                 0 128 3
                                                                               1
0.0
           0.0
                                                              149 128 3
       149
1.00000E-5 3.42030000 1.00000E-4 3.40300000 .025300000 3.39551000 128 3
100.000000 3.39501000 1000.00000 3.39490000 2000.00000 3.39480000 128 3
3000.00000 3.39440000 4000.00000 3.38940000 5000.00000 3.38500000 128 3
                                                                               6
10000.0000 3.36700000 20000.0000 3.34200000 30000.0000 3.32100000 128 3
                                                                               7
40000.0000 3.30200000 50000.0200 3.28500000 60000.0200 3.27000000 128 3
```

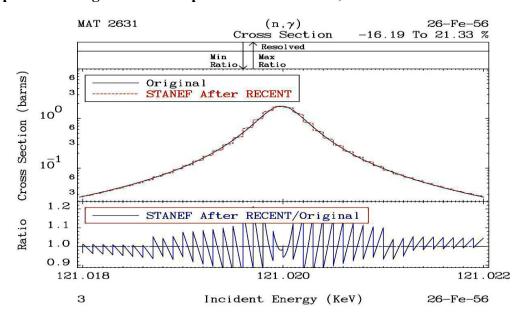
Note that in the above example we can see that the numerical values are EXACTY the same in both cases. However, the ENDF2C output include 9 digits of precision, and is completely FORTRAN, C and C++ compatible. In comparison the ENDF 7-digit, so called "E-less" data, such as 1.234567+3 (as opposed to 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.** For example consider: 9 digits: 12324.56789, versus 7 digits: 1.234567+3. Here in we can see that 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 2015 output data using 9 or 10 digits of accuracy compared to STANEF using 7 digits. To see the real danger of using 7-digit output with today's modern evaluations let's see what happens when we run the 9-digit RECENT output through STANEF 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. Rather than the smooth profile produced by the RECENT 9-digit output, the 7-digit STANEF output produces **Ziggurats** = stepped pyramids. To understand the problem we need merely compare the 9-digit RECENT output near the peak of the resonance,

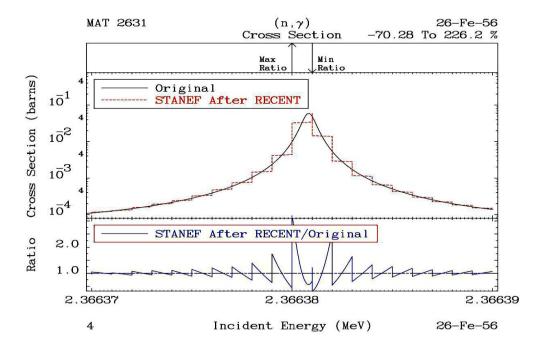
```
122600.007 8.18440080 122600.018 8.34734256 122600.021 8.391426722631 3 1 6030
122600.028 8.49343634 122600.055 8.86885730 122600.077 9.139853322631 3
122600.099 9.36221564 122600.120 9.51387393 122600.131 9.565109362631 3
122600.142 9.59483076 122600.153 9.60178112 <mark>122600.164 9.585085692631 3 1 6033 122600.176 9.53939892 122600.178 9.52899291 122600.180 9.517793222631 3 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 6034 1 60</mark>
122600.182 9.50580250 122600.184 9.49302393 122600.196 9.400050502631 3
122600.207 9.29106975 122600.218 9.16076388 122600.229 9.010880802631 3 122600.240 8.84348060 122600.251 8.66085453 122600.261 8.483667022631 3
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
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
122600.592 3.67214930 122600.614 3.53482178 122600.625 3.471802962631 3
122600.636 3.41225491 122600.658 3.30276311 122600.679 3.209061382631 3 122600.701 3.12093801 122600.722 3.04533219 122600.744 2.974035832631 3
                                                                                                                                                                                                 1 6044
122600.766 2.90992540 122600.788 2.85219006 122600.809 2.802371112631 3
122600.831 2.75512041 122600.853 2.71238188 122600.875 2.673669622631 3
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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 STANEF 7-digit output over the same energy range,

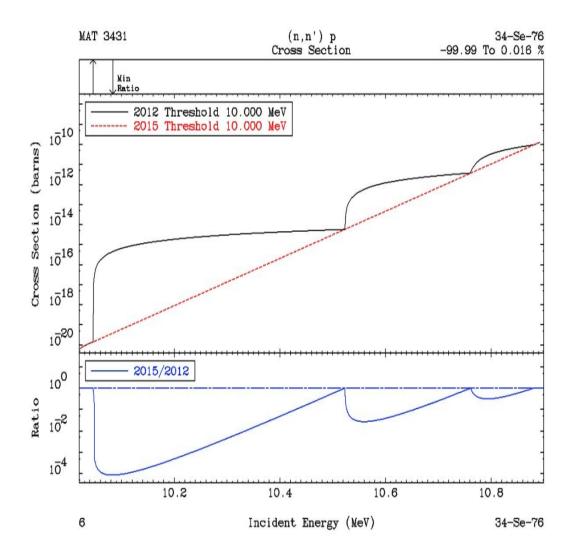
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1.226000+5 8.493436+0 1.226001+5 8.868857+0 1.226001+5 9.139853+02631 3
 1.226001+5 9.362216+0 1.226001+5 9.513874+0 1.226001+5 9.565109+02631 3
1.226001+59.594831+01.226002+59.601781+01.226002+59.585086+02631314521
1.226002+5 9.539399+0 1.226002+5 9.528993+0 1.226002+5 9.517793+02631
1.226002+5 9.33399+0 1.226002+5 9.326993+0 1.226002+5 9.31779362631 3
1.226002+5 9.505802+0 1.226002+5 9.493024+0 1.226002+5 9.400051+02631 3
1.226002+5 9.291070+0 1.226002+5 9.160764+0 1.226002+5 9.010881+02631 3
1.226002+5 8.843481+0 1.226003+5 8.660855+0 1.226003+5 8.483667+02631 3
1.226003+5 8.065878+0 1.226003+5 7.625405+0 1.226003+5 7.341331+02631 3
1.226003+5\ 7.078967+0\ 1.226004+5\ 6.645197+0\ 1.226004+5\ 6.250367+02631\ 3
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1.226004+5 5.862783+0 1.226004+5 5.505146+0 1.226004+5 5.178660+02631 3
1.226005+5 4.895771+0 1.226005+5 4.628253+0 1.226005+5 4.398676+02631 3
 1.226005+5 4.183017+0 1.226005+5 3.990472+0 1.226006+5 3.818722+02631 3
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1.226006+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.302763+0 \ \ 1.226007+5 \ \ 3.209061+02631 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 1.226007+5 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 3.412255+0 \ \ 
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1.226008+5 2.909925+0 1.226008+5 2.852190+0 1.226008+5 2.802371+02631 3
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1.226008+5 \ 2.755120+0 \ 1.226009+5 \ 2.712382+0 \ 1.226009+5 \ 2.673670+02631 \ 3
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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
```

Here the entire shape of the resonance is between 122.599 keV and 122.601 keV, and we can see that all of the above tabulated points in both tables start with EXACTLY the same six digit energy 122600. This means that with 9-digit RECENT output we only have three digits with which to define the entire shape of the resonance, which is adequate, but with 7-digit STANEF 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 STANEF ENERGIS 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 to 7-digit energies.

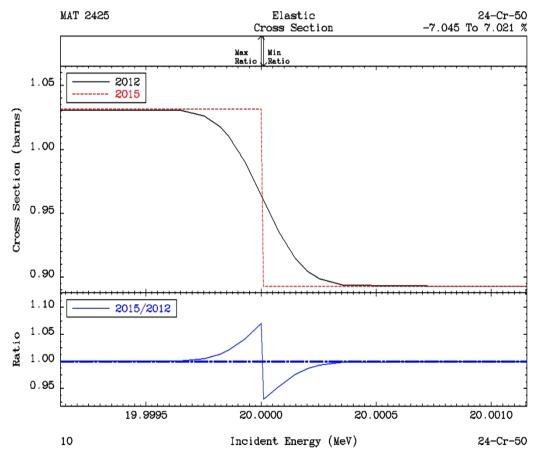
The bottom line here is to understand that due to the details included in modern evaluations it is physically impossible for 7-digit output to accurately represent the energy dependent cross sections to anywhere near our target allowable uncertainty (0.1%). In this case we find differences in the total 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 isn't even the worse 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!!!!!



Improved BEST Input Parameters, based on extensive use of the earlier versions of the PREPRO codes. Of particular note is decreasing the minimum cross section from 10<sup>-10</sup> to 10<sup>-30</sup> 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<sup>-20</sup> barn s using log-log interpolation (INT=5). PREPRO2012 ignored the interpolation code below 10<sup>-10</sup> and copied the original tabulated values and indicated lin-lin interpolation (INT=2). In contrast PREPRO2015 linearized the cross sections over the entire tabulated range. Here the cross section can be quite small, but extend 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 it is now accurately included.



**Doppler Broadening High Energy Cutoff:** Today many modern evaluations extend to very high energies well above the traditional ENDF 20 MeV end 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.



# **Introduction: POINT 2015: ENDF/B-VII.1 Final**

The latest **ENDF/B-VII.1 Final** data library was recently released and is now freely available through the National Nuclear Data Center (NNDC), Brookhaven National Laboratory. **This release completely supersedes all preceding releases of ENDF/B**.

Individual files and/or the complete tarball can also be downloaded from: http://www.nndc.bnl.gov/

Compared to VII.0 which included 393 evaluations, VII.1 included 423 evaluations; this includes 32 new evaluations; 2 natural evaluations were dropped (23-V – Nat, and 30-Zn-Nat). The 32 new evaluations are; note the isotopes of 23-V and 30-Zn; these have replaced the natural evaluations in VII.0.

#### 32 New Evaluation in VII.1 (not in VII.0)

23-V-50	30-Zn-66	69-Tm-168	74-W-180	91-Pa-229	93-Np-234	97-Bk-246	98-Cf-248
23-V-51	30-Zn-67	69-Tm-169	81-Tl-203	91-Pa-230	95-Am-440	97-Bk-247	99-Es-251
30-Zn-64	30-Zn-68	69-Tm-170	81-T1-205	92-U-230	96-Cm-240	97-Bk-248	99-Es-252
30-Zn-65	30-Zn-70	73-Ta-180	90-Th-231	92-U-231	97-Bk-245	98-Cf-246	99-Es-254m

### 423 Evaluations in VII.1 (32 new evaluations in RED)

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-44 20-Ca-46	32-Ge-74 32-Ge-76	42-Mo-94	50-Sn-112	54-Xe-131	61-Pm-148	68-Er-167	88-Ra-225	94-Pu-243
1-H -3	20-Ca-40 20-Ca-48	32-Ge-70 33-As-74	42-Mo-95	50-Sn-112 50-Sn-113	54-Xe-132	61-Pm-148m	68-Er-168	88-Ra-226	94-Pu-244
2-He-3	20-Ca-46 21-Sc-45	33-As-74	42-Mo-96	50-Sn-113	54-Xe-134	61-Pm-149	68-Er-170	89-Ac-225	94-Pu-246
2-He-3 2-He-4	21-30-45 22-Ti-46	34-Se-74	42-Mo-97	50-Sn-114 50-Sn-115	54-Xe-135	61-Pm-151	69-Tm-168	89-Ac-226	95-Am-240
2-11e-4 3-Li-6	22-Ti-40 22-Ti-47	34-Se-74	42-M0-97 42-Mo-98	50-Sn-116	54-Xe-135 54-Xe-136	62-Sm-144	69-Tm-169	89-Ac-227	95-Am-241
3-Li-0 3-Li-7	22-11-47 22-Ti-48	34-Se-70 34-Se-77	42-Mo-99	50-Sn-110 50-Sn-117	54-Ae-130 55-Cs-133	62-Sm-147	69-Tm-170	90-Th-227	95-Am-242
3-L1-7 4-Be-7	22-11-48 22-Ti-49	34-Se-77 34-Se-78		50-Sn-117 50-Sn-118	55-Cs-133 55-Cs-134	62-Sm-147 62-Sm-148	71-Lu-175	90-Th-228	95-Am-242m
4-Be-7 4-Be-9	22-Ti-49 22-Ti-50	34-Se-78 34-Se-79	42-Mo-100 43-Tc-99	50-Sn-119	55-Cs-134 55-Cs-135	62-Sm-149	71-Lu-176	90-Th-229	95-Am-243
5-B -10	22-11-50 23-V -50	34-Se-79 34-Se-80	43-10-99 44-Ru-96	50-Sn-119 50-Sn-120	55-Cs-136	62-Sm-150	72-Hf-174	90-Th-230	95-Am-244
5-B -10 5-B -11	23-V -50 23-V -51	34-Se-80 34-Se-82	44-Ru-98	50-Sn-120 50-Sn-122	55-Cs-130 55-Cs-137	62-Sm-151	72-Hf-176	90-Th-231	95-Am-244m
							72-Hf-177	90-Th-232	96-Cm-240
6-C -Nat	24-Cr-50	35-Br-79	44-Ru-99	50-Sn-123	56-Ba-130	62-Sm-152	72-Hf-178	90-Th-233	96-Cm-241
7-N -14	24-Cr-52	35-Br-81	44-Ru-100	50-Sn-124	56-Ba-132	62-Sm-153	72-Hf-179	90-Th-234	96-Cm-242
7-N -15	24-Cr-53	36-Kr-78	44-Ru-101	50-Sn-125	56-Ba-133	62-Sm-154	72-Hf-180	91-Pa-229	96-Cm-243
8-0 -16	24-Cr-54	36-Kr-80	44-Ru-102	50-Sn-126	56-Ba-134	63-Eu-151	73-Ta-180	91-Pa-230	96-Cm-244
8-O -17	25-Mn-55	36-Kr-82	44-Ru-103	51-Sb-121	56-Ba-135	63-Eu-152	73-Ta-181	91-Pa-231	96-Cm-245
9-F -19	26-Fe-54	36-Kr-83	44-Ru-104	51-Sb-123	56-Ba-136	63-Eu-153	73-Ta-182	91-Pa-232	96-Cm-246
11-Na-22	26-Fe-56	36-Kr-84	44-Ru-105	51-Sb-124	56-Ba-137	63-Eu-154	74-W -180	91-Pa-233	96-Cm-247
11-Na-23	26-Fe-57	36-Kr-85	44-Ru-106	51-Sb-125	56-Ba-138	63-Eu-155	74-W -182	92-U -230	96-Cm-248
12-Mg-24	26-Fe-58	36-Kr-86	45-Rh-103	51-Sb-126	56-Ba-140	63-Eu-156	74-W -183	92-U -231	96-Cm-249
12-Mg-25	27-Co-58	37-Rb-85	45-Rh-105	52-Te-120	57-La-138	63-Eu-157	74-W -184	92-U -232	96-Cm-250
12-Mg-26	27-Co-58m	37-Rb-86	46-Pd-102	52-Te-122	57-La-139	64-Gd-152	74-W -186	92-U -233	97-Bk-245
13-Al-27	27-Co-59	37-Rb-87	46-Pd-104	52-Te-123	57-La-140	64-Gd-153	75-Re-185	92-U -234	97-Bk-246
14-Si-28	28-Ni-58	38-Sr-84	46-Pd-105	52-Te-124	58-Ce-136	64-Gd-154	75-Re-187	92-U -235	97-Bk-247
14-Si-29	28-Ni-59	38-Sr-86	46-Pd-106	52-Te-125	58-Ce-138	64-Gd-155	77-Ir-191	92-U -236	97-Bk-248
14-Si-30	28-Ni-60	38-Sr-87	46-Pd-107	52-Te-126	58-Ce-139	64-Gd-156	77-Ir-193	92-U -237	97-Bk-249
15-P -31	28-Ni-61	38-Sr-88	46-Pd-108	52-Te-127m	58-Ce-140	64-Gd-157	79-Au-197	92-U -238	97-Bk-250
16-S -32	28-Ni-62	38-Sr-89	46-Pd-110	52-Te-128	58-Ce-141	64-Gd-158	80-Hg-196	92-U -239	98-Cf-246
16-S -33	28-Ni-64	38-Sr-90	47-Ag-107	52-Te-129m	58-Ce-142	64-Gd-160	80-Hg-198	92-U -240	98-Cf-248
16-S -34	29-Cu-63	39-Y -89	47-Ag-109	52-Te-130	58-Ce-143	65-Tb-159	80-Hg-199	92-U -241	98-Cf-249
16-S -36	29-Cu-65	39-Y -90	47-Ag-110m	52-Te-132	58-Ce-144	65-Tb-160	80-Hg-200	93-Np-234	98-Cf-250
17-Cl-35	30-Zn-64	39-Y -91	47-Ag-111	53-I -127	59-Pr-141	66-Dy-156	80-Hg-201	93-Np-235	98-Cf-251
17-Cl-37	30-Zn-65	40-Zr-90	48-Cd-106	53-I -129	59-Pr-142	66-Dy-158	80-Hg-202	93-Np-236	98-Cf-252
18-Ar-36	30-Zn-66	40-Zr-91	48-Cd-108	53-I -130	59-Pr-143	66-Dy-160	80-Hg-204	93-Np-237	98-Cf-253
18-Ar-38	30-Zn-67	40-Zr-92	48-Cd-110	53-I -131	60-Nd-142	66-Dy-161	81-Tl-203	93-Np-238	98-Cf-254
18-Ar-40	30-Zn-68	40-Zr-93	48-Cd-111	53-I -135	60-Nd-143	66-Dy-162	81-Tl-205	93-Np-239	99-Es-251
19-K -39	30-Zn-70	40-Zr-94	48-Cd-112	54-Xe-123	60-Nd-144	66-Dy-163	82-Pb-204	94-Pu-236	99-Es-252
19-K -40	31-Ga-69	40-Zr-95	48-Cd-113	54-Xe-124	60-Nd-145	66-Dy-164	82-Pb-206	94-Pu-237	99-Es-253
19-K -41	31-Ga-71	40-Zr-96	48-Cd-114	54-Xe-126	60-Nd-146	67-Ho-165	82-Pb-207	94-Pu-238	99-Es-254
20-Ca-40	32-Ge-70	41-Nb-93	48-Cd-115m	54-Xe-128	60-Nd-147	67-Ho-166m	82-Pb-208	94-Pu-239	99-Es-254m
20-Ca-42	32-Ge-72	41-Nb-94	48-Cd-116	54-Xe-129	60-Nd-148	68-Er-162	83-Bi-209	94-Pu-240	99-Es-255
20-Ca-43	32-Ge-73	41-Nb-95	49-In-113	54-Xe-130	60-Nd-150	68-Er-164	88-Ra-223	94-Pu-241	100-Fm-255

#### PREPRO 2015 Codes

In addition to the changes in the ENDF/B-VII.1 evaluations, it should be noted that between the last version of this report, where the PREPRO 2012 codes were used, and the current version, where the PREPRO 2015 codes were used, there have been improvements in the ENDF/B Preprocessing 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 used by the current evaluations. The result is more accurate cross section data throughout the POINT 2015 library.

**WARNING** – due to recent changes in ENDF-6 Formats and Procedures only the latest version of the ENDF/B Pre-processing codes, namely PREPRO 2015, can be used to accurately process all current ENDF/B-VII evaluations. If you fail to heed this warning and you use any earlier versions of these codes the results will be inaccurate.

The PREPRO 2015 codes run on virtually any computer, and are available FREE on-line from the Nuclear Data Section, IAEA, Vienna, Austria, website at,

http://www-nds.iaea.or.at/ndspub/endf/prepro/

#### **Data Processing**

As distributed the original evaluated data includes cross sections represented in the form of a combination of resonance parameters and/or tabulated energy dependent cross sections, nominally at 0 Kelvin temperature. For use in applications, this data has been processed using the 2015 version of the ENDF/B Pre-processing codes (PREPRO 2015) 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 eight 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. 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, are described below; the name of each code is given in parenthesis; for details of each code see reference [R3].

Here are the steps, and PREPRO 2015 codes, used to process the data, in the order in which the codes were used.

- 1) Linearly interpolable, tabulated cross sections (**LINEAR**)
- 2) Including the resonance contribution (**RECENT**)
- 3) Doppler broaden all cross sections to temperature (**SIGMA1**)
- 4) Check data, define redundant cross sections by summation (FIXUP)
- 5) Update evaluation dictionary in MF/MT=1/451 (**DICTIN**)

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

The result is linearly interpolable in energy, tabulated, temperature dependent cross sections, in the 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 final results, i.e., it is the same in all of the directories, ORIGINAL, as well as K0 through K1800, and 1ev through 10key, on the DVDs.

#### **Accuracy of Results**

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 2015) 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 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. 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. For use in POINT 2015 all cross sections were reconstructed to within an accuracy of 0.01% in the thermal range, and 0.1 % at all other energies and temperatures; this is beyond the accuracy to which this data in known, so that I assume that the data processing does not add any significant additional error to the inherent error of the data.

# **Contents of the Library**

This library **contains** all of the evaluations in the ENDF/B-VI.1 general purpose library. The below table summarizes the contents of the ENDF/B-VII.1 general purpose library. This library contains evaluations for 423 materials (isotopes or naturally occurring elemental mixtures of isotopes).

This library **does not contain** data from special purpose ENDF/B-VII 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

In the POINT 2015 library each evaluation is stored as a separate file. The following table defines each material and the corresponding filename. The entire library is in the computer independent ENDF-6 character format, which allows the data to be easily transported between computers. The entire library requires approximately 15 gigabyte of storage and is distributed on one DVD compressed; see below for details of the DVD.

This library contains data for some metastable materials, which are indicated by an "M" at the end of their descriptions.

The majority of these evaluations are complete, in the sense that they include all cross sections over the energy range 10<sup>-5</sup> eV to at least 20 MeV. See the appendix for a list of all evaluations, plus a separate list of incomplete evaluations; there are now only a few.

The DVD is compressed; when uncompressed you will find a single directory named POINT2015 containing fifteen (15) sub-directories,

DOCUMENT - A copy of this report in MSWord and PDF formats.

ENDF2C - The original ENDF/B data After being processed by ENDF2C.

K0 - 0 Kelvin cross sections K293.6 - 293.6 Kelvin cross sections K600 - 600 Kelvin cross sections
K900 - 900 Kelvin cross sections
K1200 - 1200 Kelvin cross sections
K1500 - 1500 Kelvin cross sections
K1800 - 1800 Kelvin cross sections
1eV - 1 eV cross sections
10eV - 10 eV cross sections

100eV - 100 eV cross sections 1keV - 1 keV cross sections 10keV - 10 keV cross sections

With the exception of DOCUMENT, each of these directories contains 424 files, one file for each of the 423 evaluation, plus one HTML file to allow interactive data retrieval. Each evaluation is a complete ENDF/B "tape" [R2], including a starting "tape" identification line, and ending with a "tape" end line [R2]. In this form, each file can be used by a wide variety of available computer codes that treat data in the ENDF/B format, e.g., all of the PREPRO codes.

# **Requesting POINT 2015 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 at, <a href="mailto:services@bnlnd2.dne.bnl.gov">services@bnlnd2.dne.bnl.gov</a>
- 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 at nds.contact-point@iaea.org.

#### **Installation and Use of POINT 2015**

I recommend that you,

- 1) Copy the single file from the POINT 2015 DVD 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 POINT2015 containing all of the data
- 4) To random access the data execute (double click) POINT2015.htm.

The main POINT2015 directory will contain the fifteen (15) sub-directories, described above. These POINT 2015 directories include HTML routines to allow interactive retrieval of the data. The result will be a directory of about 15 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 16 gigabyte library on-line is trivial.

#### Acknowledgments

I thank **Said Mughabghab** for his detailed explanation of the use of his newly published resonance parameters [R4] in ENDF/B-VII.0 evaluations. I thank **Ramon E. Arcilla, Jr.**, of the National Nuclear Data Center (NNDC), Brookhaven National Laboratory, for supplying the original ENDF/B-VII.0, used in this project. I thank **Liam Costello**, of the Nuclear Data Section, International Atomic Energy Agency, for supplying the ENDF/B Pre-processing codes, PREPRO 2015, used in this project. I thank **Janice Arwood** (RSICC, Oak Rdige) for carefully checking and recommending improvements. I thank **Nancy Larsen, Bob MacFarlane, Maurice Greene**, and **Mike Dunn**, for their comparison of their cross section processing codes (SAMMY, NJOY and AMPX) against the PREPRO codes. These comparisons have led to significant improvements in the accuracy and reliability of the results produced by all four codes (SAMMY, NJOY, AMPX, PREPRO). I thank **Andre Trkov, Skip Kahler, Robert MacFarlane, Mike Herman** and **Dave Heinrichs** for proofreading the draft of this report and making many helpful corrections and improvements, which I incorporated in the final report.

#### References

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[R1b] "POINT 2009: A Temperature Dependent ENDF/B-VII.0 data Cross Section Library, June 6, 2009.

[R1c] "POINT 2007: A Temperature Dependent ENDF/B-VII.0 data Cross Section Library", Lawrence Livermore National Laboratory, UCRL-TR-228089, February 2007.

[R2] Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6, BNL-NCS-44945, Rev. 11/95, edited by A. Trkov, M. Herman and D. A. Brown, National Nuclear Data Center, Brookhaven National Lab. <a href="http://www.nndc.bnl.gov/csewg/docs/endf-manual.pdf">http://www.nndc.bnl.gov/csewg/docs/endf-manual.pdf</a>

[R3] "PREPRO 2015: 2015 ENDF/B Pre-Processing Codes (ENDF/B-VII Tested)," by D.E. Cullen, Owned, Maintained and Distributed by the Nuclear Data Section, International Atomic Energy Agency, Vienna, Austria, IAEA-NDS-39, Rev. 16, Jan. 31, 2015; publicly available on <a href="https://www-nds.iaea.org/public/endf/prepro/PREPRO 2015">https://www-nds.iaea.org/public/endf/prepro/PREPRO 2015</a>

[R4] "Atlas of Nuclear Resonances", by S.F. Mughabghab, National Nuclear Data Center, Brookhaven National Laboratory, published by Elsevier, March 2006.

[R5] "Exact Doppler Broadening of Tabulated Cross Sections," by D.E. Cullen and C.R. Weisbin, Nuclear Science and Engineering 60, p. 199 (1975)

[R6] "THERMAL: A Routine Designed to Calculate Neutron Thermal Scattering," by D.E. Cullen, Lawrence Livermore National Laboratory, UCRL-ID-120560-Rev-1, Sept. 1995. http://home.comcast.net/~redcullen1

[R7] "Verification of High Temperature Free Atom Thermal Scattering in MERCURY Compared to TART", by D.E. Cullen, Scott McKinley and Christian Hagmann, Lawrence Livermore National Laboratory, UCRL-TR-226340, August 1, 2006.

[R8] "TART2005: A Coupled Neutron-Photon 3-D, Time Dependent, Combinatorial Geometry Monte Carlo Transport Code," by D.E. Cullen, Lawrence Livermore National Laboratory, UCRL-SM-218009, Nov. 22, 2005.

**Appendix A:** Contents of ENDF/B-VII.1 (32 new + 391 old = 423 total evaluations)

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-74	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-112	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-113	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
2-11e-4 3-Li-6	22-Ti-40 22-Ti-47	34-Se-74 34-Se-76	42-Mo-98	50-Sn-116	54-Xe-135 54-Xe-136	62-Sm-144	69-Tm-169	89-Ac-227	95-Am-241
3-Li-0 3-Li-7	22-11-47 22-Ti-48	34-Se-70 34-Se-77	42-M0-99	50-Sn-117	54-Ae-130 55-Cs-133	62-Sm-147	69-Tm-170	90-Th-227	95-Am-242
3-L1-7 4-Be-7	22-11-48 22-Ti-49	34-Se-77 34-Se-78	42-Mo-100	50-Sn-117 50-Sn-118	55-Cs-133 55-Cs-134	62-Sm-148	71-Lu-175	90-Th-228	95-Am-242n
4-Be-7 4-Be-9	22-11-49 22-Ti-50	34-Se-78 34-Se-79	42-M0-100 43-Tc-99	50-Sn-119	55-Cs-134 55-Cs-135	62-Sm-149	71-Lu-176	90-Th-229	95-Am-243
	22-11-50 23-V -50				55-Cs-136	62-Sm-150	72-Hf-174	90-Th-230	95-Am-244
5-B -10	23-V -50 23-V -51	34-Se-80	44-Ru-96	50-Sn-120 50-Sn-122	55-Cs-130 55-Cs-137		72-Hf-176	90-Th-231	95-Am-244n
5-B -11		34-Se-82	44-Ru-98			62-Sm-151	72-Hf-177	90-Th-232	96-Cm-240
6-C -Nat	24-Cr-50	35-Br-79	44-Ru-99	50-Sn-123	56-Ba-130	62-Sm-152	72-Hf-178	90-Th-233	96-Cm-241
7-N -14	24-Cr-52	35-Br-81	44-Ru-100	50-Sn-124	56-Ba-132	62-Sm-153	72-Hf-179	90-Th-234	96-Cm-242
7-N -15	24-Cr-53	36-Kr-78	44-Ru-101	50-Sn-125	56-Ba-133	62-Sm-154	72-Hf-180	91-Pa-229	96-Cm-243
8-0 -16	24-Cr-54	36-Kr-80	44-Ru-102	50-Sn-126	56-Ba-134	63-Eu-151	73-Ta-180	91-Pa-230	96-Cm-244
8-0 -17	25-Mn-55	36-Kr-82	44-Ru-103	51-Sb-121	56-Ba-135	63-Eu-152	73-Ta-181	91-Pa-231	96-Cm-245
9-F -19	26-Fe-54	36-Kr-83	44-Ru-104	51-Sb-123	56-Ba-136	63-Eu-153	73-Ta-182	91-Pa-232	96-Cm-246
11-Na-22	26-Fe-56	36-Kr-84	44-Ru-105	51-Sb-124	56-Ba-137	63-Eu-154	74-W -180	91-Pa-233	96-Cm-247
11-Na-23	26-Fe-57	36-Kr-85	44-Ru-106	51-Sb-125	56-Ba-138	63-Eu-155	74-W -182	92-U -230	96-Cm-248
12-Mg-24	26-Fe-58	36-Kr-86	45-Rh-103	51-Sb-126	56-Ba-140	63-Eu-156	74-W -183	92-U -231	96-Cm-249
12-Mg-25	27-Co-58	37-Rb-85	45-Rh-105	52-Te-120	57-La-138	63-Eu-157	74-W -184	92-U -232	96-Cm-250
12-Mg-26	27-Co-58m	37-Rb-86	46-Pd-102	52-Te-122	57-La-139	64-Gd-152	74-W -186	92-U -233	97-Bk-245
13-Al-27	27-Co-59	37-Rb-87	46-Pd-104	52-Te-123	57-La-140	64-Gd-153	75-Re-185	92-U -234	97-Bk-246
14-Si-28	28-Ni-58	38-Sr-84	46-Pd-105	52-Te-124	58-Ce-136	64-Gd-154	75-Re-187	92-U -235	97-Bk-247
14-Si-29	28-Ni-59	38-Sr-86	46-Pd-106	52-Te-125	58-Ce-138	64-Gd-155	77-Ir-191	92-U -236	97-Bk-248
14-Si-30	28-Ni-60	38-Sr-87	46-Pd-107	52-Te-126	58-Ce-139	64-Gd-156	77-Ir-193	92-U -237	97-Bk-249
15-P -31	28-Ni-61	38-Sr-88	46-Pd-108	52-Te-127m	58-Ce-140	64-Gd-157	79-Au-197	92-U -238	97-Bk-250
16-S -32	28-Ni-62	38-Sr-89	46-Pd-110	52-Te-128	58-Ce-141	64-Gd-158	80-Hg-196	92-U -239	98-Cf-246
16-S -33	28-Ni-64	38-Sr-90	47-Ag-107	52-Te-129m	58-Ce-142	64-Gd-160	80-Hg-198	92-U -240	98-Cf-248
16-S -34	29-Cu-63	39-Y -89	47-Ag-109	52-Te-130	58-Ce-143	65-Tb-159	80-Hg-199	92-U -240 92-U -241	98-Cf-249
16-S -36	29-Cu-65	39-Y -90	47-Ag-110m	52-Te-132	58-Ce-144	65-Tb-160	80-Hg-200	93-Np-234	98-Cf-250
17-Cl-35	30-Zn-64	39-Y -91	47-Ag-111	53-I -127	59-Pr-141	66-Dy-156	80-Hg-201	93-Np-235	98-Cf-251
17-Cl-37	30-Zn-65	40-Zr-90	48-Cd-106	53-I -129	59-Pr-142	66-Dy-158	80-Hg-202	93-Np-236	98-Cf-252
18-Ar-36	30-Zn-66	40-Zr-91	48-Cd-108	53-I -130	59-Pr-143	66-Dy-160	80-Hg-204	93-Np-237	98-Cf-253
18-Ar-38	30-Zn-67	40-Zr-92	48-Cd-110	53-I -131	60-Nd-142	66-Dy-161	81-Tl-203	93-Np-238	98-Cf-254
18-Ar-40	30-Zn-68	40-Zr-93	48-Cd-111	53-I -135	60-Nd-143	66-Dy-162			
19-K -39	30-Zn-70	40-Zr-94	48-Cd-112	54-Xe-123	60-Nd-144	66-Dy-163	81-T1-205 82-Pb-204	93-Np-239	99-Es-251 99-Es-252
19-K -40	31-Ga-69	40-Zr-95	48-Cd-113	54-Xe-124	60-Nd-145	66-Dy-164		94-Pu-236	
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

# **Appendix B: Elemental vs. Isotopic Evaluations**

Successive versions of ENDF/B have replaced elemental evaluations by isotopic evaluations. Between ENDF/B-VI and VII 13 elemental evaluations were deleted, i.e., included in ENDF/B-VI, but not included in ENDF/B-VII, with VII.0 only including elemental evaluations for three elements: 6-C, 23-V, and 30-Zn. Between VII.0 and VII.1 2 elemental evaluations were deleted (23-V, and 30-Zn), and replaced by isotopic evaluations, leaving only 6-C: 6-C-12 98.93%/ 6-C-13 1.07% missing – so that 6C-Nat is almost entirely the single isotope 6-C-12.

In addition evaluations for the isotopes of 68-Tm and 81-Tl have been added.

All of these isotopes in VII.1 are complete, in the sense that they include major cross sections (elastic, capture, inelastic) over the energy range 10<sup>-5</sup> eV up to at least 20 MeV.

WARNING: Be aware that evaluating isotopes is difficult and the quality of minor isotopes may be poor. To my knowledge as yet the summing these isotopes to define equivalent elemental evaluations has not been verified against experimental measurements.

# New Isotopic evaluations in VII.1 (28 new, 19 old)

Element	Isotope	Element	Isotope	Element	Isotope
Element  12-Mg-Nat  14-Si-Nat  16-S -Nat  17-Cl-Nat  19-K -Nat  20-Ca-Nat	12-Mg- 24  12-Mg- 25  12-Mg- 26  14-Si- 28  14-Si- 30  16-S - 32  16-S - 33  16-S - 34  16-S - 36  17-Cl- 35  17-Cl- 37  19-K - 39  19-K - 40  19-K - 41  20-Ca- 40  20-Ca- 42  20-Ca- 44  20-Ca- 46	Element 22-Ti-Nat 23-V -Nat 30-Zn-Nat 31-Ga-Nat 40-Zr-Nat	22-Ti- 46 22-Ti- 47 22-Ti- 48 22-Ti- 49 22-Ti- 50 23-V - 50 23-V - 51 30-Zn- 65 30-Zn- 66 30-Zn- 67 30-Zn- 68 30-Zn- 68 30-Zn- 70 31-Ga- 69 31-Ga- 71 40-Zr- 90 40-Zr- 91 40-Zr- 92 40-Zr- 93 40-Zr- 94	Element 42-Mo-Nat 49-In-Nat 72-Hf-Nat	42-Mo- 92 42-Mo- 94 42-Mo- 95 42-Mo- 96 42-Mo- 97 42-Mo- 98 42-Mo- 99 42-Mo-100 49-In-113 49-In-115 <b>69-Tm-168</b> <b>69-Tm-169</b> <b>69-Tm-170</b> 72-Hf-174 72-Hf-176 72-Hf-177 72-Hf-178 72-Hf-178 72-Hf-179 72-Hf-180
	20-Ca- 48		40-Zr- 95 40-Zr- 96		74-W -183 74-W -184 74-W -186 81-T1-203 81-T1-205

# **Appendix C: Completeness of VII.1 and VII.0**

Here I present the results of simple tests to check the completeness of VII,1 and VII.0. Compared to the results for VII.0, the VII.1 show great improvement.

The results presented here should not be interpreted as indicating **ERRORS**, but rather as **WARNINGS**, that we should check the indicated data; in many cases I judge the data to be o.k. 4-Be-7 is a partial evaluations that failed almost all tests, and should never have been included in a ENDF/B general purpose library. Here I checked,

- 1) MT=2, 102, 18, 4, 16 (elastic, capture, fission, inelastic, n,2n).
- 2) MF=3, 4, 5, 6 (cross sections, angular, energy, double differential)

For these test I assume,

- 1) Every evaluation includes MT=2, 102, 4 and 16; this is obviously not true for some light isotopes, but for completeness they are included here, i.e., this is merely to inform users. Of the heavier isotopes only 28-Ni-59 appears to be a problem with no inelastic data.
- 2) All cross sections are positive (>0) above their threshold up to at least 20 MeV. This is not true for some reactions which do not extend up to at least 20 MeV, particularly high energy capture, which is o.k. There are also a number of cases where the elastic is negative due to the resonance contribution.
- 3) No isotopes with Z<90 include MT=18 (fission). For VII.0 this test found the obvious ERROR in 43-Tc-99, which has positive fission widths = NONSENSE!!! This was corrected for VII.1. It also flagged isotopes of 88Ra and 89-Ac, which are questionable.
- 4) I included many more completeness tests, but these were the only ones that failed.

# **VII.1 Completeness Results**

Evaluation	MT=2	MT=102	MT=18	MT=4	MT=16
=======	3 4 5 6	=======	=======   3 4 5 6	: =======   3 4 5 6	3 4 5 6
=======		=======	=======	=======	======
1-H -1	X X	X X		i	i i
1-H -2	X X	X		İ	X X
1-H -3	X X			1	X X X
2-He-3	X X	X		1	1
2-He-4	X X			1	1
3-Li-6	X X	X		X X	1
4-Be-7	+ X			1	1
4-Be-9	X X	X		1	X X
5-B -10	X X	+		X X	1
6-C -Nat	X X	X		X X X	1
28-Ni-59	X X	X			X X X
54-Xe-130	X X	+		+ X X	X X X
88-Ra-223	X X	X	3 3 3	X X X	X X X
88-Ra-226	X X	X	3 3 3	X X X	X X X
89-Ac-225	X X	X X	3 3 3	X X	X X
89-Ac-226	X X	X X	3 3 3	X X	X X
89-Ac-227	X X	X X	? ? ?	X X	X X

The above rather short list for VII.1 can be compared to the below much longer list for VII.0 to see the improvements in completeness.

# VII.0 Completeness Results

Evaluation					MT=16
	3 4 5 6	3 4 5 6	3 4 5 6	3 4 5 6	
1-H -1	X X	X X			i i
1-н -2 1-н -3	X X X X	X		l I	X
2-He-3		   X	i i	i İ	
2-He-4	X X	İ	İ	İ	i i
3-Li-6	XX	X	1	X X	!
4-Be-7 4-Be-9	+ X X X	   X		l I	
5-B -10	XX	+	İ	I X X	
6-C -Nat	X X	X	İ	X X X	i i
8-0 -17	XX	X	1		+ X X
9-F -19 12-Mg-26	X X X X	X   X		X X X   X X X	+
16-S -33	XX	X		X X X	+ X X
16-S -36	X X	X	İ	X X X	+ X X
17-C1-35	+ X	X		•	X X
19-K -39 19-K -40	X X X X	X   X	1	X X X   X X X	+ X X     + X X
28-Ni-59	XX	X	i	21 21 21	+ X X
28-Ni-61	X X	X	İ	+ X	X X
30-Zn-Nat	X X	X	1	X X X	+ X X
33-As-74 34-Se-76	X X X X	X X   X   X	1	? ?   X X X	X X
36-Kr-86	X X	X	i	X X X	+ X X
37-Rb-87	X X	X	I	X X X	+ X X
38-Sr-90	XX	X		X X X	+ X X
39-Y -90 42-Mo-99	X X X X	X X   X     X	1	? ?   X X X	X X     + X X
44-Ru-100	XX	X		X X X	+ X X
47-Ag-110m	X X	X		+ X X	X X X
48-Cd-106	XX	X		X X X	+ X X
48-Cd-115m 50-Sn-112	X X X X	X X   X		+ X X   X X X	X
50-Sn-122	XX	X	İ	XXX	+ X X
50-Sn-123	X X	X	!	X X X	+ X X
52-Te-122	X X X X	X   X		X X X   X X X	+ X X     + X X
52-Te-123 52-Te-125	XX	X		X X X   X X X	+ X X     + X X
52-Te-127m	XX	X	İ	•	XXX
52-Te-129m	XX	X	1	+ X X	X X X
53-I -129 54-Xe-129	X X X X	X   X		X X X   X X X	+ X X     + X X
54-Xe-130	XX	^		+ X X	X X X
55-Cs-134	X X	X	İ	X X X	+ X X
55-Cs-135	XX	X	1	X X X	+ X X
56-Ba-132 56-Ba-135		X   X	l I	X X X   X X X	+ X X     + X X
56-Ba-137	XX	X			+ X X
58-Ce-144	X X	X	1	X X X	+ X X
61-Pm-148	XX	X		X X X	+ X X
63-Eu-151 67-Ho-166m	X X X X	X   X X		X X X   + X X	+ X X     X X
72-Hf-177	X X	X	i	•	XXX
72-Hf-179	X X	X	!	+ X X	X X X
77-Ir-193 88-Ra-223	X X X X	X X   X     X	? ? ?	X X X   X     X X X   X   X   X   X	+ X     X X X
88-Ra-226	XX	X	? ? ?	X X X	X X X
89-Ac-227	X X	l X	? ? ?	X X X	X X X
90-Th-228	XX	X	+ X X	X X X	X X X
90-Th-230 90-Th-232	+ X X X	X   X X		X X X   X X X	X X X     X X X
90-Th-234	XX	X		X X X	X X X
91-Pa-231	X X	X X	X X	? ?	X X
91-Pa-233	XX			? ?	X X
92-U -235 93-Np-239	X X X X	X   X		+ X X   X X X	X X X
94-Pu-238	XX	X			X X X
94-Pu-244	X X	X		X X X	X X X

94-Pu-246	Χ	Χ	- 1	Х	1	+	Χ	Χ	- 1	Χ	Χ	Х		Χ	Χ	Х		
95-Am-242m	Χ	Χ	- 1	Х	1	Χ	Χ	Χ		+	Χ		Χ	Χ			Χ	
95-Am-244m	Χ	Χ	- 1	Х	1	Χ	Χ	Χ		+	Χ	Χ		Χ	Χ	Χ		
96-Cm-241	Χ	Χ	- 1	+	1	Χ	Χ	Χ		+	Χ	Χ		Χ	Χ	Χ		
96-Cm-242	Χ	Χ	- 1	Х	1	+	Χ	Χ		+	Χ	Χ		Χ	Χ	Χ		
96-Cm-248	+	Χ	- 1	Х	1	Χ	Χ	Χ		+	Χ	Χ		Χ	Χ	Χ		
98-Cf-250	Χ	Χ		Х	1	+	Χ	Χ		Χ	Χ	Χ		+	Χ	Χ		
98-Cf-251	Χ	Χ		Х	1	Χ	Χ	Χ		Χ	Χ	Χ		+	Χ	Χ		
98-Cf-252	Χ	Χ	- 1	X	1	Χ	Χ	Χ		Χ	Χ	Χ		+	Χ	Χ		
98-Cf-253	Χ	Χ	- 1	+	1	+	Χ	Χ										
99-Es-253	Χ	Χ	- 1	+	1													

# Appendix D: Summary of $\langle \nu(E) \rangle$ for all isotopes in ENDF/B-VII.1 and VII.0

For applications involving fission (F) I require both prompt and delayed neutrons per fission. In the ENDF/B format the evaluator can optionally include: Total (T), Delayed (D) and/or Prompt (P); given any two of these three we can uniquely define the third. Below is a summary of all fissile/fertile materials in ENDF/B-VII.1, indicating the neutrons per fission data included for each isotope. This table indicates each evaluation that includes,

```
F = Fission cross section (MF/MT=3/18)

T = Total < \nu(E) > (MF/MT=1/452)

D = Delayed < \nu(E) > (MF/MT=1/455)

P = Prompt < \nu(E) > (MF/MT=1/456)
```

This table indicates VII.1 is in much better shape than VII.0, where more evaluations only included total (T) < v(E) >. In addition there are three evaluations that only include total (T) < v(E) >: 88-Ra-233, 88-Ra-226, and 94-Pu-243. It is also questionable whether or not 88-Ra and 89-Ac should be identified as fissile/fertile.

# Summary of all fissile/fertile isotopes in ENDF/B-VII.1 < v(E) > (85 evaluations)

88-Ra-223	F T	92-U -240	FTDP	96-Cm-244	FTDP
88-Ra-226	FT	92-U -241	FTDP	96-Cm-245	FTDP
89-Ac-225	FTDP	93-Np-234	FTDP	96-Cm-246	FTDP
89-Ac-226	FTDP	93-Np-235	FTDP	96-Cm-247	FTDP
89-Ac-227	FTDP	93-Np-236	FTDP	96-Cm-248	FTDP
90-Th-227	FTDP	93-Np-237	FTDP	96-Cm-249	FTDP
90-Th-228	FTDP	93-Np-238	FTDP	96-Cm-250	FTDP
90-Th-229	FTDP	93-Np-239	FTDP	97-Bk-245	FTDP
90-Th-230	FTDP	94-Pu-236	FTDP	97-Bk-246	FTDP
90-Th-231	FTDP	94-Pu-237	FTDP	97-Bk-247	FTDP
90-Th-232	FTDP	94-Pu-238	FTDP	97-Bk-248	FTDP
90-Th-233	FTDP	94-Pu-239	FTDP	97-Bk-249	FTDP
90-Th-234	FTDP	94-Pu-240	FTDP	97-Bk-250	FTDP
91-Pa-229	FTDP	94-Pu-241	FTDP	98-Cf-246	FTDP
91-Pa-230	FTDP	94-Pu-242	FTDP	98-Cf-248	FTDP
91-Pa-231	FTDP	94-Pu-243	F T	98-Cf-249	FTDP
91-Pa-232	FTDP	94-Pu-244	FTDP	98-Cf-250	FTDP
91-Pa-233	FTDP	94-Pu-246	FTDP	98-Cf-251	FTDP
92-U -230	FTDP	95-Am-240	FTDP	98-Cf-252	FTDP
92-U -231	FTDP	95-Am-241	FTDP	98-Cf-253	FTDP
92-U -232	FTDP	95-Am-242	FTDP	98-Cf-254	FTDP
92-U -233	FTDP	95-Am-242m	FTDP	99-Es-251	FTDP
92-U -234	FTDP	95-Am-243	FTDP	99-Es-252	FTDP
92-U -235	FTDP	95-Am-244	FTDP		FTDP
92-U -236	FTDP	95-Am-244m	FTDP	99-Es-254	FTDP
92-U -237	FTDP	96-Cm-240	FTDP	99-Es-254m	FTDP
92-U -238	FTDP	96-Cm-241	FTDP	99-Es-255	FTDP
92-U -239	FTDP	96-Cm-242	FTDP	100-Fm-255	FTDP
		96-Cm-243	FTDP		

# Summary of all fissile/fertile isotopes in ENDF/B-VII.0 $< \nu(E) >$ (65 evaluations)

Comparing the above table for VII.1 and the below table for VII.0 we can see that the  $\langle \nu(E) \rangle$  data is much improved, but VII.1 still has the same three deficiencies that we found in VII.0, namely evaluations that only include total (T)  $\langle \nu(E) \rangle$ : 88-Ra-233, 88-Ra-226, and 94-Pu-243.

88-Ra-223	F T	92-U -241	FTDP	96-Cm-241	F T
88-Ra-226	F T	93-Np-235	FTDP	96-Cm-242	FTDP
89-Ac-227	F T	93-Np-236	FTDP	96-Cm-243	FTDP
90-Th-227	FTDP	93-Np-237	FTDP	96-Cm-244	FTDP
90-Th-228	FTDP	93-Np-238	FTDP	96-Cm-245	FTDP
90-Th-229	FTDP	93-Np-239	F T	96-Cm-246	FTDP
90-Th-230	F T	94-Pu-236	FTDP	96-Cm-247	FTDP
90-Th-232	FTDP	94-Pu-237	F T	96-Cm-248	F T
90-Th-233	FTDP	94-Pu-238	FTDP	96-Cm-249	FTDP
90-Th-234	FTDP	94-Pu-239	FTDP	96-Cm-250	FTDP
91-Pa-231	FTDP	94-Pu-240	FTDP	97-Bk-249	FTDP
91-Pa-232	FTDP	94-Pu-241	FTDP	97-Bk-250	FTDP
91-Pa-233	FTDP	94-Pu-242	FTDP	98-Cf-249	FTDP
92-U -232	FTDP	94-Pu-243	F T	98-Cf-250	F T
92-U -233	FTDP	94-Pu-244	F T	98-Cf-251	FTDP
92-U -234	FTDP	94-Pu-246	FTDP	98-Cf-252	FT
92-U -235	FTDP	95-Am-241	FTDP	98-Cf-253	F T
92-U -236	FTDP	95-Am-242	FTDP	98-Cf-254	FTDP
92-U -237	FTDP	95-Am-242m	FTDP	99-Es-254	FTDP
92-U -238	FTDP	95-Am-243	FTDP	99-Es-255	FTDP
92-U -239	FTDP	95-Am-244	FTDP	100-Fm-255	FTDP
92-U -240	FTDP	95-Am-244m	FTDP		

### **Appendix E: 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 references [R5] and [R6], listed below. 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,

1) There is the well known effect in the neutron resonance region, where as the temperature increases resonances become broader, hence the name Doppler broadening. Figure 1 below illustrates the effect of temperature on the  $U^{238}$  capture cross section for neutron reactor like temperatures, and figure 2 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 figure 1 and 2 each sub-figure shows exactly the same 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). This temperature effect will have a very important effect on resonance self-shielding in any neutron transport calculation. You should note from these figures that due to the large resonance spacing in  $U^{238}$  the resonance structure can still be seen up to very high temperatures.

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 = 
$$\int_{E_1}^{E_2} [\Sigma c(E)\phi(E)/\Sigma t(E)] dE$$
 = including one over total cross section

Consider for example the U238 capture cross section between 1 and 10 keV as shown in fig. 1 and 2. If we calculate the unshielded and shielded average capture cross section for the energy interval over the range of temperatures shown in figs. 1 and 2, we obtain the results shown below in table 1.

What we see from these results is that the unshielded average capture cross section is virtually independent of temperature, being about 1 barn over the entire temperature range. In contrast the shielded average cross section varying 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.

Table 1: Effect of Temperature on Average Cross Sections

Ter	mp.	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

- 2) 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 [R5]. Figure 3 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 400 higher in energy. From the lower half of figure 2 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 very important for thermal and low energy neutron systems.
- 3) Yet another important effect of temperature is that at lower energies neutrons do not slow down 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 or a free gas model is used to model the interaction of neutrons with target atoms that are moving about with thermal motion. Figure 4 illustrates the effect of temperature on the neutron spectrum over a wide range of temperatures [R7]. 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. See reference [R6], below for a routine designed to be used in conjunction with the SIGMA1 method of Doppler broadening [R5], to handle neutron thermal scattering. This routine [R6] is completely compatible for use with the cross sections included here, since these cross sections were Doppler broadened using the SIGMA1 method [R5]. The combination of SIGMA1 [R5] Doppler broadened cross sections and THERMAL [R6] to handle thermal scattering, is currently used in the TART Monte Carlo transport code [R8].

Fig.1: Effect of Doppler Broadening on Resonance Cross Sections

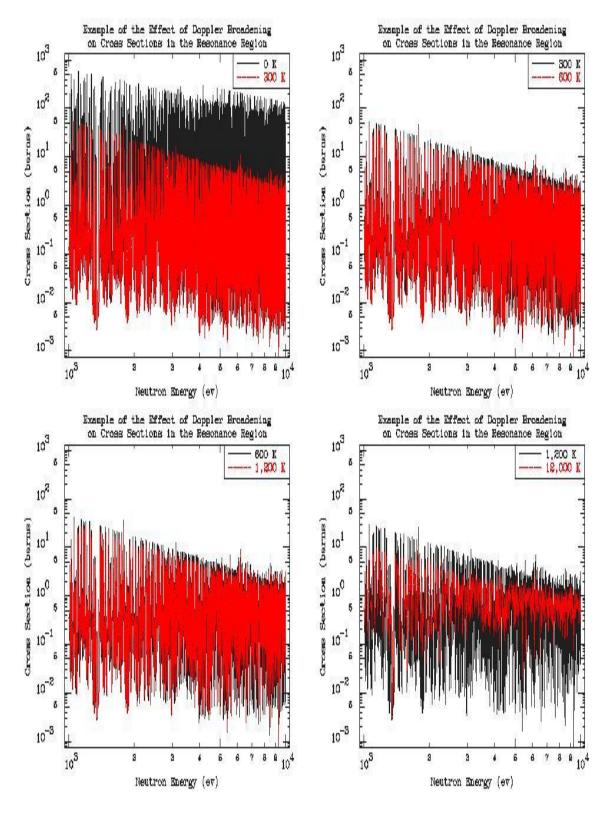


Fig.2: Effect of Doppler Broadening on Resonance Cross Sections

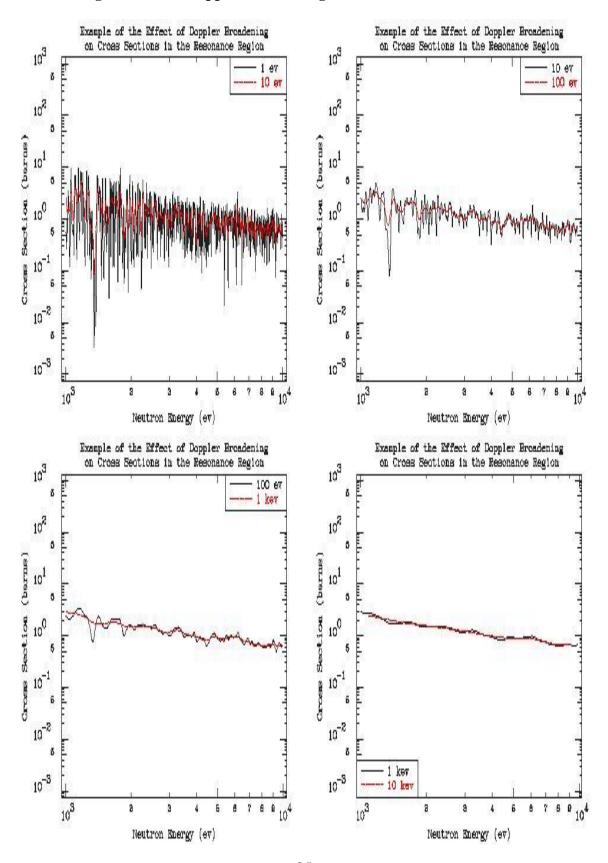
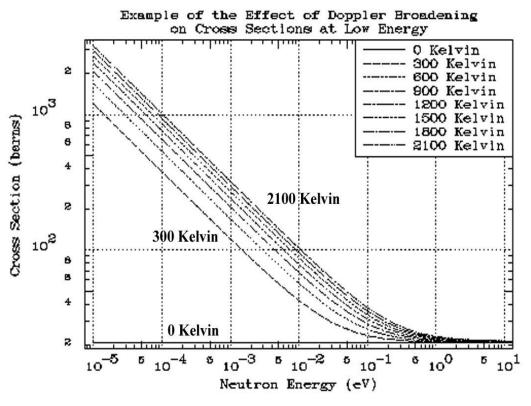


Fig.3: Effect of Doppler Broadening on Low Energy Cross Sections



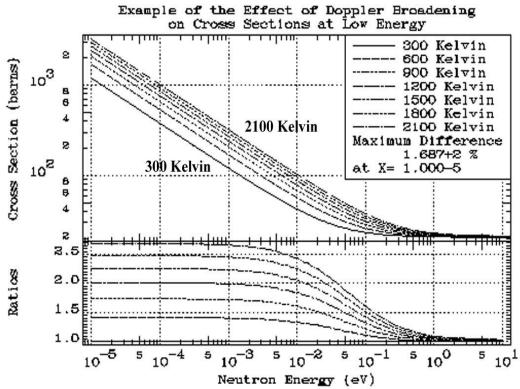


Fig.4: Effect of Doppler Broadening on Neutron Spectrum

