POINT 2012: ENDF/B-VII.1 Final Temperature Dependent Cross Section Library

A Brief Library Summary

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January 7, 2012





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Table of Contents

- 1) A Brief Library Summary
- 2) Overview
- 3) Introduction: POINT 2012: ENDF/B-VII.1 Final
- 4) PREPRO 2012 Codes
- 5) Data Processing
- 6) Accuracy of Results
- 7) Contents of the Library
- 8) Requesting POINT 2012 Data
- 9) Installation and Use of POINT 2012
- 10) Acknowledgments
- 11) References
- 12) Appendix A: Contents of ENDF/B-VII.1
- 13) Appendix B: Elemental vs. Isotopic Evaluations
- 14) Appendix C: Completeness of VII.1 and VII.0
- 15) Appendix D: Summary of $\langle v(E) \rangle$ for all isotopes in ENDF/B-VII.1 and VII.0
- 16) Appendix E: The Effects of Temperature and Doppler Broadening

A Brief Library Summary

This is merely an informal memo to briefly summarize the contents of the new ENDF/B-VII.1 Final library, released in December 2011; focus here is only on the **quantity** of data. A later document to planned to more completely document the **quality** of this new library.

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, http://www.nndc.bnl.gov/) and,
- publicly available computer codes (the current PREPRO codes, available on-line at the Nuclear Data Section, IAEA, Vienna, Austria, http://www-nds.iaea.or.at/ndspub/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.

Introduction: POINT 2012: 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-240	97-Bk-247	99-Es-251
30-Zn-64	30-Zn-68	69-Tm-170	81-Tl-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			,		0110 111 1 12	(02 110)	· Craidatic	ms m keb)		
1-H-1-2 20-Ca-446 32-Ge-76 42-Mo-98 50-Sn-113 54-Ke-133 61-Pm-148 68-Er-168 88-Er-168 89-Ac-225 94-Pm-246 94-Pm-248	1 11 1	20 Co 44	32 Co 74	42 Mo 92	40 In 115	54 Vo 131	61 Pm 147			
2-He-3 21-Sc-48 33-As-74 42-Mo-96 50-Sn-114 54-Xe-135 61-Pm-149 68-Er-170 69-Tm-160										
2-He-3 21-Sc-45 33-As-75 42-Mo-96 50-Sn-114 54-Xe-135 61-Pm-151 31-id-6 22-Ti-47 34-Se-76 42-Mo-98 50-Sn-116 54-Xe-135 62-Sm-147 31-id-7 22-Ti-48 34-Se-77 42-Mo-99 50-Sn-116 54-Xe-135 62-Sm-147 51-Id-175 99-Th-227 95-Am-241 4Be-7 22-Ti-48 34-Se-77 42-Mo-109 50-Sn-118 55-Cs-136 62-Sm-147 71-Id-175 99-Th-228 95-Am-242 4Be-9 22-Ti-50 34-Se-79 43-Te-99 50-Sn-119 55-Cs-135 62-Sm-149 72-Hi-147 90-Th-239 95-Am-243 5-B-10 23-V-51 34-Se-82 44-Ru-98 50-Sn-120 55-Cs-136 62-Sm-149 72-Hi-176 90-Th-239 95-Am-244 78-B-11 23-V-51 34-Se-82 44-Ru-98 50-Sn-120 55-Cs-136 62-Sm-150 72-Hi-176 90-Th-239 95-Am-243 78-Di-10-10-10-10-10-10-10-10-10-10-10-10-10-									88-Ra-226	94-Pu-244
2-He-4 3-1-6 22-Ti-46 34-Se-76 34-Se-76 42-Mo-97 50-Sn-115 54-Xe-136 62-Sm-144 62-Sm-147 99-Tm-129 99-Tm-227 95-Am-241 99-Tm-227 95-Am-241 99-Tm-27 95-Am-241 99-Tm-27 95-Am-241 99-Tm-27 95-Am-242										
3-Li-6 22-Ti-47 34-Se-76 42-Mo-98 50-Sn-116 55-Cs-133 62-Sm-147 90-Th-227 95-Am-242 4-Be-7 22-Ti-49 34-Se-78 42-Mo-90 50-Sn-117 55-Cs-133 62-Sm-149 71-Lu-175 90-Th-229 95-Am-242 4-Be-7 22-Ti-50 34-Se-79 43-Tc-99 50-Sn-119 55-Cs-136 62-Sm-149 71-Lu-175 90-Th-229 95-Am-242 95-Am-243 95-Am-242 95-Am-243 95-Am-242 95-Am-243 95-A										
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4-Be-9 22-Ti-50 34-Se-79 43-Tc-99 50-Sn-119 55-Cs-135 62-Sm-149 90-Th-229 95-Am-243 5-B-10 23-V-51 34-Se-82 44-Ru-98 50-Sn-120 55-Cs-136 62-Sm-151 5-B-11 23-V-51 34-Se-82 44-Ru-98 50-Sn-122 55-Cs-136 62-Sm-151 7-N-14 24-Cr-52 35-Br-81 44-Ru-100 50-Sn-124 56-Ba-132 62-Sm-153 8-O-16 24-Cr-53 36-Kr-84 44-Ru-100 50-Sn-125 56-Ba-132 62-Sm-153 8-O-16 24-Cr-53 36-Kr-88 44-Ru-101 50-Sn-125 56-Ba-132 62-Sm-153 8-O-16 24-Cr-53 36-Kr-88 44-Ru-102 51-Sn-125 56-Ba-135 63-Eu-152 8-O-17 25-Mn-55 36-Kr-82 44-Ru-105 51-Sn-125 56-Ba-135 63-Eu-152 11-Na-22 26-Fe-56 36-Kr-84 44-Ru-105 51-Sn-125 56-Ba-137 63-Eu-152 11-Na-22 26-Fe-57 36-Kr-85 44-Ru-105 51-Sn-125 56-Ba-137 63-Eu-152 11-Na-22 26-Fe-58 37-Rh-85 44-Ru-105 51-Sn-125 56-Ba-137 63-Eu-152 11-Na-22 26-Fe-57 36-Kr-85 44-Ru-105 51-Sn-125 56-Ba-136 63-Eu-152 11-Na-22 26-Fe-57 36-Kr-85 44-Ru-105 51-Sn-125 56-Ba-137 63-Eu-152 11-Na-22 26-Fe-58 37-Rh-85 44-Ru-105 51-Sn-125 56-Ba-137 63-Eu-152 11-Na-22 26-Fe-58 37-Rh-85 44-Ru-105 51-Sn-125 56-Ba-137 63-Eu-152 11-Na-22 26-Fe-57 36-Kr-85 44-Ru-105 51-Sn-125 56-Ba-137 63-Eu-152 11-Na-22 26-Fe-58 37-Rh-85 46-Pd-105 52-Te-120 57-La-138 63-Eu-152 11-Na-22 20-C-58 37-Rh-87 46-Pd-105 52-Te-120 57-La-138 63-Eu-152 11-Na-22 20-U-233 37-Rh-87 46-Pd-105 52-Te-120 52										95-Am-242
48.Be.9 22.Ti.50 34.Se.80 44.Ru.96 50.Sn.120 55.Cs135 62.Sm.149 72.Hir.174 90.Th.230 95.Am.244m 58.Br.11 23.V - 51 34.Se.80 44.Ru.98 50.Sn.120 55.Cs.137 62.Sm.151 72.Hir.174 90.Th.230 95.Am.244m								71-Lu-175	90-Th-228	95-Am-242m
5.B. 1.0 5.B. 1.1 5.B										95-Am-243
5-B. 11 6-C-Nat 7-Larlat 90-Th-233 90-Th-234 90-Th-233 90-Th-234 90-Th-233 90-Th-234 90-Th-234 90-Th-233 90-Th-234 90-Cm-244 91-Pa-230 91-										95-Am-244
6-C. Nat										
7-N-14										96-Cm-240
7-N-15									90-Th-233	96-Cm-241
8-O -16									90-Th-234	96-Cm-242
8-O -17										96-Cm-243
9-F. 19										96-Cm-244
11-Na-22										
11-Na-23										
12-Mg-24 26-Fe-58 36-Kr-86 45-Rh-103 51-Sb-126 56-Ba-140 63-Eu-156 74-W - 182 74-W - 182 74-W - 182 74-W - 183 74-W - 184										
12-Mg-25										96-Cm-248
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 -232 97-Bk-246 92-U -234 97-Bk-246 92-U -235 97-Bk-246 92-U -235 97-Bk-246 92-U -236 97-Bk-246 92-U -236 97-Bk-247 92-U -236 97-Bk-247 92-U -236 97-Bk-248 97-Bk-248 97-Bk-247 92-U -236 97-Bk-248 97-Bk-										
13-Al-27 27-Co-59 37-Rb-87 46-Pd-104 52-Te-123 57-La-140 58-Ce-136 54-Gd-154 75-Re-185 92-U-234 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-246 97-Bk-246 97-Bk-246 97-Bk-246 97-Bk-246 97-Bk-246 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-246 97-Bk-246 97-Bk-246 97-Bk-246 97-Bk-246 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-246 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-246 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-246 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-246 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-246 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-248 97-Bk-248 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-248 97-Bk-248 97-Bk-246 97-Bk-248 97-Bk-246 97-Bk-248 97-Bk-24										
14-Si-28										97-Bk-245
14-Si-29										97-Bk-246
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-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 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 80-Hg-196 92-U-238 97-Bk-249 16-S -32 28-Ni-64 38-Sr-90 47-Ag-107 52-Te-129m 58-Ce-141 64-Gd-158 60-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-142 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-143 65-Tb-159 80-Hg-199 92-U-240 98-Cf-248 17-Cl-37 30-Zn-65 40-Zr-90 48-Cd-106 53-I-127 59-Pr-141 66-Dy-156 66-Dy-158 80-Hg-201 93-Np-236 93-Np-236 98-Cf-251										
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18-Ar-38 30-Zn-67 18-Ar-40 30-Zn-68 40-Zr-92 48-Cd-110 53-I -131 60-Nd-142 66-Dy-161 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 82-Pb-204 99-Es-251 20-Ca-40 32-Ge-70 20-Ca-42 32-Ge-72 21-Nb-94 48-Cd-115 54-Xe-129 60-Nd-147 60-Nd-147 60-Nd-148 68-Er-162 82-Pb-208 94-Pu-237 99-Es-254 99-Es-255 99-Es-255								80-Hg-202	93-Np-236	98-Cf-252
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19-K -40 31-Ga-69								81-Tl-205	93-Np-239	99-Es-251
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-42 32-Ge-72 41-Nb-94 48-Cd-1156 54-Xe-129 60-Nd-147 68-Er-162 82-Pb-208 94-Pu-239 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 83-Bi-209 94-Pu-240 99-Es-255									94-Pu-236	99-Es-252
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20 Co 43 32 Co 73 41 Nb 05 40 Ip 113 54 Vo 130 60 Nd 150 68 Ep 164 83-Bi-209 94-Pu-240 99-Es-255								82-Pb-208		99-Es-254m
20-Ca-45 32-Gc-75 41-ND-75 47-ND-75										99-Es-255
	20-Ca-45	32-Ge-13	41-140-32	-1 3-111-113	34-AC-130	00-14u-130	00-E1-104	88-Ra-223	94-Pu-241	100-Fm-255

PREPRO 2012 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 2010 codes were used, and the current version, where the PREPRO 2012 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 2012 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 2012, 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 2012 codes run on virtually any computer, and will soon be 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 2012 version of the ENDF/B Pre-processing codes (PREPRO 2012) 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 2100 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 in given in parenthesis; for details of each code see reference [R3].

Here are the steps, and PREPRO 2012 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 K2100, and 1ev through 10kev, 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 2012) 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 2012 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 2012 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 10⁻⁵ 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 POINT2012 containing fifteen (15) sub-directories,

DOCUMENT - A copy of this report in MSWord and PDF formats. ORIGINAL - The original ENDF/B data before it was processed.

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 - 1800 Kelvin cross sections K1800 K2100 - 2100 Kelvin cross sections - 1 eV cross sections 1eV - 10 eV cross sections 10eV 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 2012 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, 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, Alberto Mengoni at, A.Mengoni@iaea.org

Installation and Use of POINT 2012

I recommend that you,

- 1) Copy the single file from the POINT 2012 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 POINT2012 containing all of the data
- 4) To random access the data execute (double click) POINT2012.htm.

The main POINT2012 directory will contain the fifteen (15) sub-directories, described above. These POINT 2012 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 2012, 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

[R1a] "POINT 2011: A Temperature Dependent ENDF/B-VII.0 data Cross Section Library", Lawrence Livermore National Laboratory, UCRL-TR-479947, rev. 1, May 2011.

[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 V. McLane, et al. National Nuclear Data Center, Brookhaven National Lab. http://www.nndc.bnl.gov/nndcscr/documents/endf/endf102/

[R3] "PREPRO 2010: The 2010 ENDF/B Pre-Processing Codes," by D.E. Cullen, Nuclear Data Section, International Atomic Energy Agency, Vienna, Austria, IAEA-NDS-39, Rev. 14, Oct. 31, 2010; PREPRO 2010 is now publicly available. http://www-nds.iaea.or.at/ndspub/endf/prepro/PREPRO 2012 will be released for public use early in 2012; until then I recommend you use currently available PREPRO 2010 codes.

[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)

1.1.									
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-131	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 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-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-114 50-Sn-115	54-Xe-135	61-Pm-151	69-Tm-168	89-Ac-226	95-Am-240
3-Li-6	22-Ti-40 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-0	22-Ti-47 22-Ti-48	34-Se-77	42-Mo-99	50-Sn-110 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-117 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-119	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-82	44-Ru-98	50-Sn-120 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-122 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-151	73-Ta-180	91-Pa-230	96-Cm-244
9-F -19	26-Fe-54	36-Kr-83	44-Ru-104	51-Sb-121	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-120 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

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 10⁻⁵ 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
12-Mg-Nat	12-Mg- 24 12-Mg- 25 12-Mg- 26 14-Si- 28 14-Si- 29	22-Ti-Nat	22-Ti- 46 22-Ti- 47 22-Ti- 48 22-Ti- 49 22-Ti- 50	42-Mo-Nat	42-Mo- 92 42-Mo- 94 42-Mo- 95 42-Mo- 96 42-Mo- 97
16-S -Nat	14-Si- 29 14-Si- 30 16-S - 32 16-S - 33	23-V -Nat 30-Zn-Nat	23-V - 50 23-V - 51 30-Zn- 64		42-Mo- 98 42-Mo- 99 42-Mo-100
17-Cl-Nat	16-s - 34 16-s - 36 17-cl- 35 17-cl- 37	30-ZII-Nac	30-Zn- 65 30-Zn- 66 30-Zn- 67	49-In-Nat	49-In-113 49-In-115 69-Tm-168 69-Tm-169
19-K -Nat	17-C1- 37 19-K - 39 19-K - 40 19-K - 41	31-Ga-Nat	30-Zn- 68 30-Zn- 70 31-Ga- 69 31-Ga- 71	72-Hf-Nat	69-Tm-170 72-Hf-174 72-Hf-176
20-Ca-Nat	20-Ca- 40 20-Ca- 42 20-Ca- 43	40-Zr-Nat	40-Zr- 90 40-Zr- 91 40-Zr- 92		72-Hf-177 72-Hf-178 72-Hf-179 72-Hf-180
	20-Ca- 44 20-Ca- 46 20-Ca- 48		40-Zr- 93 40-Zr- 94 40-Zr- 95 40-Zr- 96	74-W -Nat	74-W -182 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 VV,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	Comp	leteness	Results
V 11.1	COMB	iciciicss	17 Courto

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	3 4 5 6
=======================================	=======	=======	======
1-H -1 X X	X X	i i	į
1-H -2 X X	X	i i	х х
1-H -3 X X	İ	i i	XXX
2-He-3 X X	X	i i i	i
2-He-4 X X	İ	i i i	i
3-Li-6 X X	x	x x	
4-Be-7 + X		i i i	
4-Be-9 X X	x	i i i	x x
5-B -10 X X	+	x x	
6-C -Nat X X	x	i xxx i	i
28-Ni-59 X X	X		xxx
54-Xe-130 X X	+	+ x x	xxx
88-Ra-223 X X	x	? ? ? X X X	xxx
88-Ra-226 X X	X	? ? ? X X X	x x x
89-Ac-225 X X	x x	? ? ? X X	x x
89-Ac-226 X X	X X	? ? ? 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 1-H -2	X X X X	X X		 	
1-H -3	XX	^			XXX
2-He-3	X X	x	İ	į	j j
2-He-4	XX				
3-Li-6 4-Be-7	X X + X	X		XX	
4-Be-9	ХХ	X	İ	İ	х х
5-B -10	XX	+		X X	
6-C -Nat 8-O -17	X X X X	X X			 + X X
9-F -19	X X	X		X X X	+ X
12-Mg-26	X X	X	İ	xxx	+ X X
16-S -33 16-S -36	X X X X	X X		X X X X X X	+ X X + X X
17-C1-35	+ X	X		X X	XXX
19-K -39	X X	x	İ	xxx	+ X X
19-K -40	XX	X		XXX	+ X X
28-Ni-59 28-Ni-61	X X X X	X X		 + X	+ X X X X
30-Zn-Nat	XX	X		XXX	+ X X
33-As-74	X X	x x	İ	? ?	x x
34-Se-76	X X X X	X		XXX	+ X X
36-Kr-86 37-Rb-87	XX	X X		X X X X X X	+ X X + X X
38-Sr-90	XX	X		XXX	+ X X
39-Y -90	X X	X X		? ?	X X
42-Mo-99	XX	X		XXX	+ X X
44-Ru-100 47-Ag-110m	X X X X	X X		X X X + X X	+ X X X X X
48-Cd-106	хх	X		xxx	+ X X
48-Cd-115m	X X	X X		+ X X	X
50-Sn-112 50-Sn-122	X X X X	X X			+ X X + X X
50-Sn-123	XX	X		XXX	+ X X
52-Te-122	хх	х	İ	xxx	+ X X
52-Te-123	X X	X		XXX	+ X X
52-Te-125 52-Te-127m	X X X X	X X		X X X + X X	+ X X X X X
52-Te-129m	X X	X		+ X X	XXX
53-I -129	X X	X	İ	xxx	+ X X
54-Xe-129	XX	X		XXX	+ X X
54-Xe-130 55-Cs-134	X X X X	+ X		+ X X	X X X + X X
55-Cs-135	X X	X		XXX	+ X X
56-Ba-132	ХХ	X		XXX	+ X X
56-Ba-135 56-Ba-137	X X X X	X X			+ X X + X X
58-Ce-144	XX	X		XXX	+ X X
61-Pm-148	X X	x	İ	XXX	+ X X
63-Eu-151	XX	X		XXX	+ X X
67-Ho-166m 72-Hf-177	X X X X	X X		+ X X + X X	
72-Hf-179	XX	X		+ X X	XXX
77-Ir-193	X X	X X		X X X	+ X
88-Ra-223	XX	X X	3 3 3	XXX	XXX
88-Ra-226 89-Ac-227	X X X X	X	3 3 3	X X X X X X	
90-Th-228	ХХ	X	+ X X	xxx	xxx
90-Th-230	+ X	X	+ X X	XXX	XXX
90-Th-232 90-Th-234	X X X X	X X X	+ X X	X X X X X X	X
91-Pa-231	XX	X X	X X	? ?	X X
91-Pa-233	X X	х х	+ X	? ?	х х
92-U -235	XX	X	XXX	+ X X	X
93-Np-239 94-Pu-238	X X X X	X X	+ X X	X X X + X X	
94-Pu-244	X X	X	+ X X	XXX	XXX
					•

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

Appendix D: Summary of $\langle v(E) \rangle$ 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 < v(E) > (MF/MT=1/452)

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

P = Prompt < v(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) $< \nu(E) >$. In addition there are three evaluations that only include total (T) $< \nu(E) >$: 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 $< \nu(E) >$ (85 evaluations)

		_			·
88-Ra-223	F T	92-U -240	FTDP	96-Cm-244	FTDP
88-Ra-226	F T	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	99-Es-253	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		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 < v(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	F T
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 =
$$\int_{E1}^{E2} [\Sigma c(E)\phi(E)]dE$$
 = 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 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

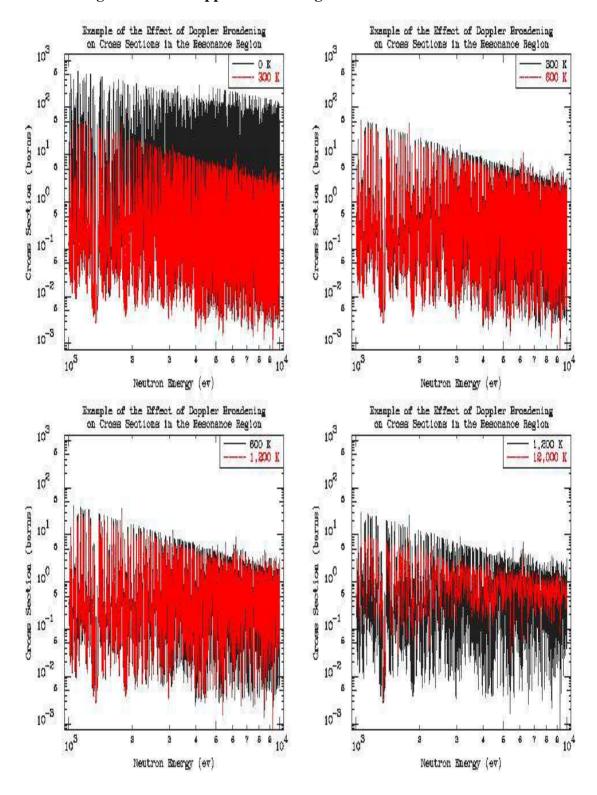


Fig.2: Effect of Doppler Broadening on Resonance Cross Sections

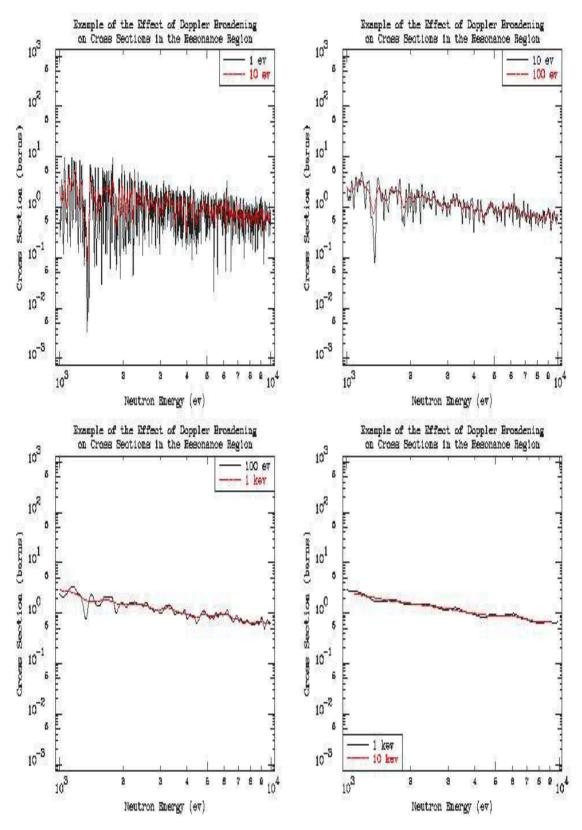
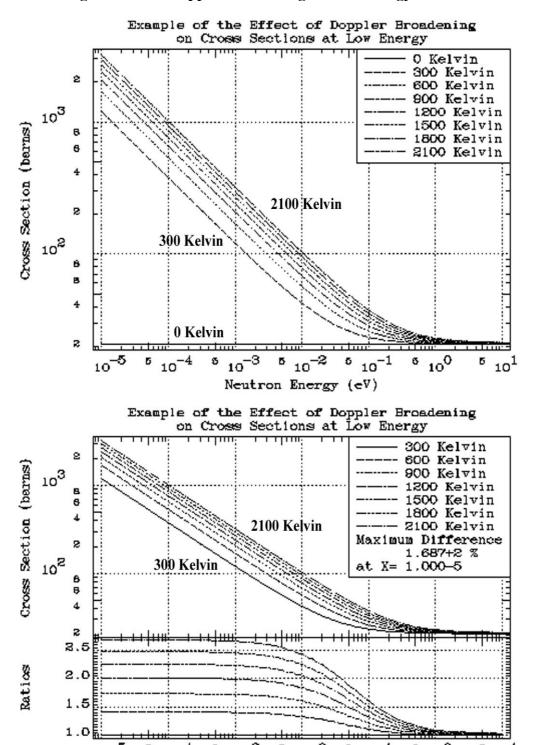


Fig.3: Effect of Doppler Broadening on Low Energy Cross Sections



Neutron Energy (eV)

