POINT 2009:
A Temperature Dependent
ENDF/B-VII.0 Data
Cross Section Library

by
Dermott E. Cullen
Lawrence Livermore National Laboratory, retired

1466 Hudson Way
Livermore, CA 94550

Tel.: 925-443-1911
E. Mail: redcullen1@comcast.net
Website: home.comcast.net/~redcullen1

June 6, 2009

POINT 2009:
A Temperature Dependent
ENDF/B-VII.0
Cross Section Library

by
Dermott E. Cullen
Lawrence Livermore National Laboratory, retired

1466 Hudson Way
Livermore, CA 94550

Tel.: 925-443-1911
E. Mail: redcullen1@comcast.net
Website: home.comcast.net/~redcullen1

June 6, 2009

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. In each case I have used 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/). I have used these in combination to produce the temperature dependent cross sections used in applications and presented in this report.

POINT 2009

ENDF/B-VII.0 was released by CSEWG in November 2006 and is to be frozen for three years until November 2009. As such the Original data included in **POINT 2009** is identical to that included in the earlier release **POINT 2007** [R1]. However, the processed, temperature dependent results may differ because of improvements in the PREPRO ENDF/B Preprocessing Codes, particularly with regard to accuracy, and correct interpretation of the ENDF/B rules as defined by the ENDF/B formats and procedures manual, ENDF-102.

POINT 2007

The version of ENDF/B, preceding ENDF/B-VII.0, namely ENDFV/B-VI, Release 8, contained 328 evaluations [R2]; of the evaluations 13 elemental evaluations are not included in ENDF/B-VII.0 (these have been replaced by isotopic evaluations).

ENDF/B-VII.0 includes 315 evaluations from ENDF/B-VI and 78 evaluations for new isotopes, for a total of 393 evaluations in ENDF/B-VII.0. The contents of ENDF/B-VII.0 are defined in the Appendix A. The appendix includes a variety of what I hope are useful summaries of the VII.0, including,

1) Contents of ENDF/B-VII.0 (78 new + 315 old = 393 total evaluations)
2) Elemental Evaluations Replaced by Isotopic evaluations (16 new, 19 old)
3) New Evaluations for ENDF/B-VII.0 (78 new)
4) Summary of $< \nu(E) >$ for all 65 fissile/fertile isotopes in ENDF/B-VII.0
5) Completeness of ENDF/B-VII.0 Evaluations
6) Same Evaluations in ENDF/B-VI and VII (315)

Deficiencies and Proposed Updates

ENDF/B-VII.0 was released by CSEWG in November 2006 and is to be frozen for three years until November 2009. All recognized ENDF/B-VII.0 deficiencies and proposed updates can be viewed at,

http://www.nndc.bnl.gov/exfor/4web/VII.0-deficiencies.html

These data will be reviewed by CSEWG and these data will serve as the basis for the next version of ENDF/B, namely ENDF/B-VII.1.

Introduction

The latest ENDF/B data library was released in November 2006 and is now freely available through the National Nuclear Data Center (NNDC), Brookhaven National Laboratory. This most recent library is identified as ENDF/B-VII.0; this is the first release of ENDF/B-VII. This release completely supersedes all preceding releases of ENDF/B.

As distributed the ENDF/B-VII.0 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 our applications the ENDF/B-VII.0 library has been processed into 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.

All results are in the computer independent ENDF-6 character format [R2], which allows the data to be easily transported between computers. In its processed form the POINT 2009 library is approximately 11 gigabyte in size and is distributed on three DVDs (see, below for the details of the contents of each DVD).

PREPRO 2009 Codes

In addition to the changes in the ENDF/B-VII.0 evaluations, it should be noted that between the last version of this report, where the PREPRO 2007 codes were used, and the current version, where the PREPRO 2009 codes were used, there have been major improvements in the ENDF/B Pre-processing codes (PREPRO). The major 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 2009 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 2009, 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 2009 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/

Requesting POINT 2009 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, Enrico Sartori at Sartori@nea.fr

3) Otherwise: contact the Nuclear Data Section, International Atomic Energy Agency, Vienna, Austria, Alberto Mengoni at,
A.Mengoni@iaea.org

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 2009 version of the ENDF/B Pre-processing codes (PREPRO 2009) 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 2009 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 2009) 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 2009 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.0 general purpose library. A table in the appendix summarizes the contents of the ENDF/B-VII.0 general purpose library. This library contains evaluations for 393 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 2009 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 11 gigabyte of storage and is distributed on three DVDs; see below for details of the DVDs.

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 DVDs is divided into fifteen (15) directories, across three DVDS,

Part 1 (first DVD)

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

Part 2 (second DVD)
K1200 - 1200 Kelvin cross sections
K1500 - 1500 Kelvin cross sections
K1800 - 1800 Kelvin cross sections
K2100 - 2100 Kelvin cross sections

Part 3 (third DVD)
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 394 files, one file for each of the 393 evaluation, plus one HTML file to allow interactive data retrieval. Each file 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.

Installation and Use of POINT 2009

I recommend that you create a directory named POINT 2009 and copy the entire contents of **ALL three** DVDs into this directory; this will allow you simple access to the data at all temperatures. These POINT 2009 directories include HTML routines to allow interactive retrieval of the data. The result will be a directory of about 11 gigabytes. To put that in perspective, today it costs less than $1 U.S. to purchase, install, and maintain on-line one gigabyte of disk storage. Therefore the cost of maintaining this 11 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 **Kevin McLaughlin** and **Andre Trkov**, of the Nuclear Data Section, International Atomic Energy Agency, for supplying the ENDF/B Pre-processing codes, PREPRO 2009, used in this project. I thank **Nancy Larsen, Bob MacFarlane**, **Maurice Greene**, and **Mike Dunn**, for their intercomparison 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 **Dave Heinrichs** for proofreading the draft of this report and making many helpful corrections and improvements, which I incorporated in the final report.

References

[R1] "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] now available, "PREPRO 2007: The 2007 ENDF/B Pre-Processing Codes," by D.E. Cullen, Nuclear Data Section, International Atomic Energy Agency, Vienna, Austria, IAEA-NDS-39, Rev. 12, Nov. 22, 2004; PREPRO 2009 will soon to publicly available. http://www-nds.iaea.or.at/ndspub/endf/prepro/

[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.0 (**78 new** + 315 old = 393 total evaluations)

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

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** (included in ENDF/B-VI, but not included in ENDF/B-VII); the below table summarizes the elemental evaluations deleted and the isotopic evaluations designed to replace them. The only remaining elemental evaluations in ENDF/B-VII are:

6-C–Nat 6-C-12 98.93%/ 6-C-13 1.07% missing
23-V –Nat 23-V-50 99.75%/ 23-V-51 0.25% missing
30-Zn-Nat 5 isotopes, all missing

All of these isotopes in VII.0 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. However, 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.

Elemental Evaluations Replaced by Isotopic evaluations (16 new, 19 old)

Element	Isotope	Element	Isotope	Element	Isotope
12-Mg-Nat	12-Mg- 24	22-Ti-Nat	22-Ti- 46	42-Mo-Nat	42-Mo- 92
	12-Mg- 25		22-Ti- 47		42-Mo- 94
	12-Mg- 26		22-Ti- 48		42-Mo- 95
14-Si-Nat	14-Si- 28		**22-Ti- 49**		42-Mo- 96
	14-Si- 29		22-Ti- 50		42-Mo- 97
	14-Si- 30	31-Ga-Nat	**31-Ga- 69**		42-Mo- 98
16-S -Nat	16-S - 32		**31-Ga- 71**		42-Mo- 99
	16-S - 33	40-Zr-Nat	40-Zr- 90		42-Mo-100
	16-S - 34		40-Zr- 91	49-In-Nat	49-In-113
	16-S - 36		40-Zr- 92		49-In-115
17-Cl-Nat	17-Cl- 35		40-Zr- 93	72-Hf-Nat	72-Hf-174
	17-Cl- 37		40-Zr- 94		72-Hf-176
19-K -Nat	**19-K - 39**		40-Zr- 95		72-Hf-177
	19-K - 40		40-Zr- 96		72-Hf-178
	19-K - 41				72-Hf-179
20-Ca-Nat	**20-Ca- 40**				72-Hf-180
	20-Ca- 42			74-W -Nat	74-W -182
	20-Ca- 43				74-W -183
	20-Ca- 44				74-W -184
	20-Ca- 46				74-W -186
	20-Ca- 48				

New Evaluations for ENDF/B-VII.0 (78 new)

After six versions of ENDF/B over almost 40 years, most of the important isotopes have already been evaluated and included in earlier versions of ENDF/B. The new ENDF/B-VII evaluations were difficult to do, since usually there is little experimental data for rarer isotopes. Most of the new evaluations are complete in the sense that they include major cross sections from 10^{-5} eV to 20 MeV. The except is 4-Be-7 which only extends up to 8.1 MeV, and only includes elastic and charged particle reactions; this is a theoretical evaluation that should not have been included in ENDF/B-VII.0. Many of the other evaluations are pretty bad; better than nothing, but crude, so **CAVEAT EMPTOR!**

The below table includes a list of all 78 new evaluations. If there are no comments, I judge the evaluation to be o.k.

78 New Evaluations

Material	Comments	Material	Comments
4-Be- 7	Useless partial	67-Ho-166M	Crude
11-Na- 22	Crude	68-Er-162	
12-Mg- 25		68-Er-164	
12-Mg- 26		68-Er-168	
16-S - 33		68-Er-170	
16-S - 34		80-Hg-196	Crude
16-S - 36	Crude	80-Hg-198	Crude, check capture
18-Ar- 36	Crude	80-Hg-199	
18-Ar- 38	Crude	80-Hg-200	
19-K - 39		80-Hg-201	
19-K - 40	Very crude	80-Hg-202	Crude, check capture
20-Ca- 40	o.k. to 20 MeV	80-Hg-204	Very crude
20-Ca- 42	"	82-Pb-204	
20-Ca- 43	"	88-Ra-223	Very crude
20-Ca- 44	"	88-Ra-224	Very crude
20-Ca- 46	Very crude	88-Ra-225	Very crude
20-Ca- 48	o.k. to 20 MeV	88-Ra-226	
22-Ti- 49		89-Ac-225	Very crude
27-Co- 58	Very crude	89-Ac-226	Very crude
27-Co- 58M	Very crude	89-Ac-227	Very crude
30-Zn-Nat	Check (n,alpha)	90-Th-227	Very crude
31-Ga- 69		90-Th-228	Rubbish
31-Ga- 71		90-Th-229	(n,n') down to 100 eV
32-Ge- 70		90-Th-233	Very crude
33-As- 74		90-Th-234	Rubbish
34-Se- 79	Crude	92-U -239	Weird resonances
47-Ag-110M	(n,n') down to 3 eV?	92-U -240	
50-Sn-113	Resonance gap	92-U -241	Weird resonances
54-Xe-123	Very crude	93-Np-235	Very crude
56-Ba-130		94-Pu-246	Very crude
56-Ba-132	Crude	95-Am-244	Very crude
56-Ba-133		95-Am-244M	Very crude
57-La-138		96-Cm-249	
58-Ce-136		96-Cm-250	Crude
58-Ce-138		97-Bk-250	Weird resonances
58-Ce-139		98-Cf-254	Very crude
64-Gd-153		99-Es-254	Very crude
66-Dy-156		99-Es-255	Very crude
66-Dy-158		100-Fm-255	Very crude

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

For applications 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). Below is a summary of all fissile/fertile materials in ENDF/B-VII.0, indicating the neutrons per fission data included for each isotope. In all cases the Total (T) is included, however in some cases no other data is included, so that we cannot define either Prompt (P) or Delayed (D). I will have to add the missing data before I can use these isotopes in my applications.

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

Isotope	<nu>	Comments	Isotope	<nu>	Comments
ZA088223	T	No Delayed	ZA094241	T D P	
ZA088226	T	No Delayed	ZA094242	T D P	
ZA089227	T	No Delayed	ZA094243	T	No Delayed
ZA090227	T D P		ZA094244	T	No Delayed
ZA090228	T D P		ZA094246	T D P	
ZA090229	T D P		ZA095241	T D P	
ZA090230	T	No Delayed	ZA095242	T D P	
ZA090232	T D P		ZA095242.M	T D P	
ZA090233	T D P		ZA095243	T D P	
ZA090234	T D P		ZA095244	T D P	
ZA091231	T D P		ZA095244.M	T D P	
ZA091232	T D P		ZA096241	T	No Delayed
ZA091233	T D P		ZA096242	T D P	
ZA092232	T D P		ZA096243	T D P	
ZA092233	T D P		ZA096244	T D P	
ZA092234	T D P		ZA096245	T D P	
ZA092235	T D P		ZA096246	T D P	
ZA092236	T D P		ZA096247	T D P	
ZA092237	T D P		ZA096248	T	No Delayed
ZA092238	T D P		ZA096249	T D P	
ZA092239	T D P		ZA096250	T D P	
ZA092240	T D P		ZA097249	T D P	
ZA092241	T D P		ZA097250	T D P	
ZA093235	T D P		ZA098249	T D P	
ZA093236	T D P		ZA098250	T	No Delayed
ZA093237	T D P		ZA098251	T D P	
ZA093238	T D P		ZA098252	T	No Delayed
ZA093239	T	No Delayed	ZA098253	T	No Delayed
ZA094236	T D P		ZA098254	T D P	
ZA094237	T	No Delayed	ZA099254	T D P	
ZA094238	T D P		ZA099255	T D P	
ZA094239	T D P		ZA100255	T D P	
ZA094240	T D P				

Completeness of ENDF/B-VII.0 Evaluations

For ENDF/B-VI.8, I judged that only about half of the 328 evaluations were complete and physically acceptable enough to be used in neutron transport calculations. In contrast in ENDF/B-VII.0, only a few evaluations are incomplete (10^{-5} eV to 20 MeV) or physically unacceptable (negative cross sections). Below is a summary (no comment = o.k.)

Material				Comments
ZA001001	mt= 50	no inelastic		
ZA001002	mt= 50	no inelastic		
ZA001003	mt= 102	no capture		
ZA001003	mt= 50	no inelastic		
ZA002003	mt= 50	no inelastic		
ZA002004	mt= 102	no capture		
ZA002004	mt= 50	no inelastic		
ZA004007	**mt= 2**	**cross section ends**	**8.1000D+06 eV**	**Incomplete only elastic**
ZA004007	**mt= 1**	**no total**		**up to 8.1 MeV**
ZA004007	**mt= 102**	**no capture**		
ZA004007	**mt= 50**	**no inelastic**		
ZA004009	mt= 50	no inelastic		
ZA005010	mt= 102	cross section ends	5.0000D+05 eV	
ZA017035	mt= 2	cross section start	1.4519D-05 eV	Negative elastic
ZA018040	mt= 2	cross section <=0	9.7825D+05 eV	Negative elastic
ZA020040	mt= 2	cross section <=0	5.0000D+05 eV	Negative elastic
ZA021045	mt= 102	cross section ends	5.0000D+06 eV	
ZA026056	mt= 2	cross section <=0	1.1971D+06 eV	Negative elastic
ZA027058	mt= 102	cross section <=0	8.4925D+00 eV	Negative capture
ZA027058.M	mt= 51	level energy > 0	2.4900D+04 eV	
ZA028059	**mt= 50**	**no inelastic**		**Incomplete**
ZA028061	mt= 2	cross section <=0	7.4355D+05 eV	Negative elastic
ZA041093	mt= 2	cross section <=0	2.3344D+03 eV	Negative elastic
ZA047110.M	mt= 51	level energy > 0	1.1760D+05 eV	
ZA047110.M	mt= 52	level energy > 0	1.0660D+05 eV	
ZA048108	mt= 102	cross section ends	1.0000D+07 eV	
ZA048110	mt= 102	cross section ends	1.0000D+07 eV	
ZA048112	mt= 102	cross section ends	1.0000D+07 eV	
ZA048115.M	mt= 51	level energy > 0	1.8100D+05 eV	
ZA048116	mt= 102	cross section ends	1.0000D+07 eV	
ZA052127.M	mt= 51	level energy > 0	8.8260D+04 eV	
ZA052127.M	mt= 52	level energy > 0	2.7140D+04 eV	
ZA052129.M	mt= 51	level energy > 0	1.0550D+05 eV	
ZA054130	mt= 102	cross section ends	1.0000D+07 eV	
ZA061148.M	mt= 51	level energy > 0	1.3790D+05 eV	
ZA061148.M	mt= 52	level energy > 0	6.2200D+04 eV	
ZA064152	mt= 2	cross section <=0	3.3186D+01 eV	Negative elastic
ZA066160	mt= 2	cross section <=0	3.3293D+02 eV	Negative elastic
ZA067166.M	mt= 51	level energy > 0	5.9850D+03 eV	
ZA082207	mt= 2	cross section <=0	4.7500D+05 eV	Negative elastic
ZA090228	mt= 18	cross section <=0	3.0000D+03 eV	
ZA090230	mt= 2	cross section <=0	1.2856D+00 eV	Negative elastic
ZA092240	mt= 2	cross section <=0	2.2262D+00 eV	Negative elastic
ZA094238	mt= 2	cross section <=0	5.9743D+01 eV	Negative elastic
ZA094242	mt= 2	cross section <=0	2.2348D+00 eV	Negative elastic
ZA094244	mt= 2	cross section <=0	2.0770D+01 eV	Negative elastic
ZA095242.M	mt= 51	level energy > 0	4.8600D+04 eV	
ZA095242.M	mt= 52	level energy > 0	4.5000D+03 eV	
ZA095244.M	mt= 51	level energy > 0	8.8000D+04 eV	
ZA096241	mt= 102	cross section ends	4.0000D+06 eV	
ZA096242	mt= 2	cross section <=0	1.3448D+01 eV	Negative elastic
ZA096242	mt= 18	cross section <=0	2.7600D+02 eV	
ZA096248	mt= 2	cross section <=0	6.8142D+00 eV	Negative elastic
ZA098250	mt= 2	cross section <=0	1.4329D+01 eV	Negative elastic
ZA098252	mt= 2	cross section <=0	1.6674D+01 eV	Negative elastic
ZA098253	**mt= 18**	**cross section ends**	**1.1000D+04 eV**	**Incomplete only to 11 keV**
ZA098253	**mt= 102**	**cross section ends**	**1.1000D+04 eV**	
ZA098253	**mt= 50**	**no inelastic**		
ZA099253	**mt= 102**	**cross section ends**	**1.1000D+04 eV**	**Incomplete only to 11 keV**

ZA099253 mt= 50 no inelastic

Same Evaluations in ENDF/B-VI and VII (315)

Above I stated that ENDF/B-VII.0 includes 315 evaluations from ENDF/B-VI. By this I mean that there are evaluations for the same 315 elements or isotopes in both VI and VII. The contents of these evaluations may be identical to ENDF/B-VI, or completely different. Below I provide a brief, one line summary comparing the contents of ENDF/B-VII.0 to VI.8. These summaries are based only on my comparing major cross sections (total, elastic, capture and fission) for the 315 same evaluations. For more details of any given evaluation the reader can use the COMPLOT code [R3] to “see” comparisons.

The intent here is to hopefully save users time and effort by telling them which evaluations have or have not changed. For example, many metals and fissile isotopes have not changed. There are also materials where the cross sections are what I call “similar”, but which I mean similar resonance structure, but actual cross section values may be quite different.

1) Many single level Breit-Wigner (SLBW) resonances have been changed to multi-level (MLBW). In many case this eliminates negative elastic cross sections, and results in what I identify in the following table as “similar”. WARNING – because of the use of non-physical average J values, switching from SLBW to MLBW does not always eliminate negative cross sections. WARNING – “similar” here means similar resonance structure; the actual energy dependent cross sections may be very different.
2) Many incomplete ENDF/B-VI evaluations have now been extended up to 20 MeV and are now complete in VII.0. Also the high energy range of many other evaluations were re-done using nuclear model code calculations; this has changed some high energy cross sections by 10 to 20%.
3) Many evaluations now include resonance parameters from the latest 2006 version of the atlas of nuclear resonances, BNL-325 [R4]; this has allowed many resonance regions to be extended to higher energies. However, in many cases no additional evaluation was performed to eliminate resonance gaps in the experimentally measured resonance parameters, and many isotopes do not included an unresolved resonance energy range.
4) I try to identify evaluations where the major cross sections differ substantially; roughly speaking my criteria was differences of at least ~ 1% .
5) I also compared <nu>, where smaller differences can be important. For the major fuel, U-233, U-235, and Pu-235, there have been minor ~ 0.5% changes in <nu> which may be reflected in calculated integral parameters, such as K-eff. Some minor fissile/fertile have changes in <nu> of 5 to 10%

315 Same Materials (1-H - 1 to 44-Ru- 99)

1-H - 1	Elastic 0.3% lower < 10 keV	32-Ge- 73	New - completely different
1-H - 2	Same	32-Ge- 74	New - completely different
1-H - 3	Elastic 30% higher < 1 MeV	32-Ge- 76	New - completely different
2-He- 3	Same	33-As- 75	New - resonances > 2 keV
2-He- 4	Same	34-Se- 74	Different
3-Li- 6	Elastic 7% higher < 0.1 eV	34-Se- 76	Different
3-Li- 7	Same	34-Se- 77	Different
4-Be- 9	Elastic 10% different > 10 eV	34-Se- 78	Different
5-B – 10	Elastic 8% higher ~ 100 keV	34-Se- 80	Different
5-B – 11	Same	34-Se- 82	Different
6-C –Nat	Same	35-Br- 79	Different
7-N – 14	Same	35-Br- 81	Different
7-N – 15	Same	36-Kr- 78	Different
8-O – 16	Elastic 7% higher 4 to 9 MeV	36-Kr- 80	Different
8-O – 17	Same	36-Kr- 82	Different
9-F – 19	Different resonances < 1 MeV	36-Kr- 83	Different
11-Na- 23	Same	36-Kr- 84	Different
12-Mg- 24	Same	36-Kr- 85	Different
13-Al- 27	Different resonances < 1 MeV	36-Kr- 86	Different
14-Si- 28	Same	37-Rb- 85	Different - fewer resonances
14-Si- 29	Same	37-Rb- 86	Different
14-Si- 30	Same	37-Rb- 87	Different - fewer resonances
15-P – 31	Same	38-Sr- 84	Different
16-S – 32	Different resonances	38-Sr- 86	Different
17-Cl- 35	Different – resonances > 200 keV	38-Sr- 87	Different
17-Cl- 37	Different – resonances > 200 keV	38-Sr- 88	Different
18-Ar- 40	Completely different	38-Sr- 89	Different - both rubbish
19-K – 41	Same	38-Sr- 90	Different - both rubbish
21-Sc- 45	Same	39-Y – 89	Different
22-Ti- 46	Same	39-Y – 90	Different – old rubbish
22-Ti- 47	Same	39-Y – 91	Different - both rubbish
22-Ti- 48	Same	40-Zr- 90	Different – fewer resonances
22-Ti- 50	Same	40-Zr- 91	Different - similar resonances
23-V –Nat	Same	40-Zr- 92	Different – fewer resonances
24-Cr- 50	Same	40-Zr- 93	Different – old rubbish
24-Cr- 52	Same	40-Zr- 94	Similar
24-Cr- 53	Same	40-Zr- 95	Different - both rubbish
24-Cr- 54	Same	40-Zr- 96	Similar
25-Mn- 55	Same	41-Nb- 93	Same
26-Fe- 54	Same	41-Nb- 94	Different - both rubbish
26-Fe- 56	Same	41-Nb- 95	Different - both rubbish
26-Fe- 57	Same	42-Mo- 92	Very different > 20 keV
26-Fe- 58	Same	42-Mo- 94	Very different > 6 keV
27-Co- 59	Same	42-Mo- 95	Same < 2 keV – 40% higher energy
28-Ni- 58	Same	42-Mo- 96	Very different > 4 keV
28-Ni- 59	Very narrow resonance differences	42-Mo- 97	Different
28-Ni- 60	Same	42-Mo- 98	Different – old rubbish
28-Ni- 61	Same	42-Mo- 99	Different - both rubbish
28-Ni- 62	Same	42-Mo-100	Very different > 4 keV
28-Ni- 64	Same	43-Tc- 99	Very different > 1 keV
29-Cu- 63	Same	44-Ru- 96	Different - both rubbish
29-Cu- 65	Same	44-Ru- 98	Different - both rubbish
32-Ge- 72	New - completely different	44-Ru- 99	Different > 100 eV

315 Same Materials (44-Ru- 100 to 61-Pm-148)

44-Ru-100	Old Rubbish – new poor
44-Ru-101	50% higher < 10 eV
44-Ru-102	Similar
44-Ru-103	Old Rubbish – new poor
44-Ru-104	Different > 1 keV
44-Ru-105	Similar - both rubbish
44-Ru-106	Similar - both rubbish
45-Rh-103	Same < 4 keV – 40% higher energy
45-Rh-105	Different - both rubbish
46-Pd-102	Old rubbish – new poor
46-Pd-104	Different – old rubbish
46-Pd-105	Same < 2 keV – 20% higher energy
46-Pd-106	Different – old rubbish
46-Pd-107	Very similar
46-Pd-108	Different – old poor
46-Pd-110	Different - old rubbish
47-Ag-107	Different > 3 keV
47-Ag-109	Similar < 5 keV - 7% > 100 keV
47-Ag-111	New - old rubbish
48-Cd-106	No resonances 600 eV - 3 keV
48-Cd-108	No resonances 350 eV – 2.6 keV
48-Cd-110	Similar
48-Cd-111	Different < 1 eV 60% lower
48-Cd-112	Similar < 2 keV
48-Cd-113	Similar < 2 keV
48-Cd-114	Same
48-Cd-115M	New - old rubbish
48-Cd-116	Similar
49-In-113	New resonances > 50 eV
49-In-115	Very different > 1 keV
50-Sn-112	Similar
50-Sn-114	Different - more resonances
50-Sn-115	Different – both poor
50-Sn-116	New resonances > 2 keV
50-Sn-117	Different
50-Sn-118	Similar
50-Sn-119	Different
50-Sn-120	New resonances > 15 keV
50-Sn-122	New resonances > 900 eV
50-Sn-123	Different - both rubbish
50-Sn-124	New resonances > 700 eV
50-Sn-125	New - old rubbish
50-Sn-126	Different - both rubbish
51-Sb-121	More resonances > 2.5 keV
51-Sb-123	More resonances > 2.5 keV
51-Sb-124	Different - both rubbish
51-Sb-125	Different - both rubbish
51-Sb-126	Different - old rubbish
52-Te-120	Different - both rubbish
52-Te-122	More resonances > 4 keV
52-Te-123	More resonances > 500 eV
52-Te-124	More resonances > 6 keV
52-Te-125	More resonances > 1 keV
52-Te-126	More resonances > 6 keV
52-Te-127M	Different - both rubbish
52-Te-128	More resonances > 3.5 keV
52-Te-129M	Different - both rubbish
52-Te-130	Different
52-Te-132	Different - old rubbish
53-I -127	More resonances > 1 keV
53-I -129	More resonances > 150 eV
53-I -130	Different - old rubbish
53-I -131	Different - both rubbish
53-I -135	Different - both rubbish
54-Xe-124	Similar
54-Xe-126	Different resonances
54-Xe-128	Similar
54-Xe-129	Similar
54-Xe-130	Similar
54-Xe-131	Same
54-Xe-132	Different
54-Xe-133	Different - both rubbish
54-Xe-134	Different
54-Xe-135	Same - both rubbish > 10 eV
54-Xe-136	New - old rubbish
55-Cs-133	Same - 14% > 100 keV
55-Cs-134	Similar
55-Cs-135	Similar
55-Cs-136	Different - new rubbish
55-Cs-137	Similar - both rubbish
56-Ba-134	Similar < 10 keV
56-Ba-135	Similar < 1 keV
56-Ba-136	Different
56-Ba-137	Different
56-Ba-138	Similar
56-Ba-140	Different – old rubbish
57-La-139	Different
57-La-140	Different - old rubbish
58-Ce-140	Different - old rubbish
58-Ce-141	Different - old rubbish
58-Ce-142	Different - old rubbish
58-Ce-143	Different - old rubbish
58-Ce-144	Different - both rubbish
59-Pr-141	Similar
59-Pr-142	Different - old rubbish
59-Pr-143	Different - old rubbish
60-Nd-142	Different
60-Nd-143	Similar - 4% > 100 keV
60-Nd-144	Different
60-Nd-145	Similar - 5% > 100 keV
60-Nd-146	Different
60-Nd-147	Different > 30 eV
60-Nd-148	Different
60-Nd-150	Different
61-Pm-147	No resonances > 100 eV
61-Pm-148	Different - both rubbish

315 Same Materials (61-Pm-148M to 99-Es-293)

61-Pm-148M	Similar - not great
61-Pm-149	Different - both rubbish
61-Pm-151	Different - old rubbish
62-Sm-144	Similar
62-Sm-147	Similar > 10 eV
62-Sm-148	Different - old rubbish
62-Sm-149	Very similar
62-Sm-150	Very similar
62-Sm-151	Same - 15% > 10 keV
62-Sm-152	Similar
62-Sm-153	Different - old rubbish
62-Sm-154	Different
63-Eu-151	Very similar
63-Eu-152	Same - 30% > 100 eV
63-Eu-153	Same - 16% > 100 eV
63-Eu-154	Different
63-Eu-155	Very similar
63-Eu-156	Different - both rubbish
63-Eu-157	Different - old rubbish
64-Gd-152	Different < 10 eV
64-Gd-154	Similar
64-Gd-155	Same - 20% > 200 eV
64-Gd-156	Different
64-Gd-157	Similar, same < 400 eV
64-Gd-158	Different
64-Gd-160	Different
65-Tb-159	Different > 100 eV
65-Tb-160	Different - old rubbish
66-Dy-160	Very similar
66-Dy-161	Similar
66-Dy-162	Similar < 5 keV
66-Dy-163	Similar
66-Dy-164	Similar < 7 keV
67-Ho-165	Different
68-Er-166	Similar < 2 keV
68-Er-167	Similar < 500 eV
71-Lu-175	Same
71-Lu-176	Same
72-Hf-174	Same
72-Hf-176	Same
72-Hf-177	Same
72-Hf-178	Same
72-Hf-179	Same
72-Hf-180	Same
73-Ta-181	Same
73-Ta-182	Same
74-W -182	Same
74-W -183	Same
74-W -184	Same
74-W -186	Same
75-Re-185	Same
75-Re-187	Same
77-Ir-191	Very similar
77-Ir-193	Similar
79-Au-197	Similar
82-Pb-206	Very similar
82-Pb-207	Very similar, 3% ~ 10 MeV
82-Pb-208	Very similar
83-Bi-209	Same
90-Th-230	Same
90-Th-232	Different resonances
91-Pa-231	Similar < 15 eV
91-Pa-232	Similar
91-Pa-233	Similar < 40 eV
92-U -232	Same < 200 eV
92-U -233	Similar to 60 eV
92-U -234	Similar
92-U -235	Same - 1% ~ 20 MeV
92-U -236	Same - 6% ~ 500 keV
92-U -237	Similar – weird resonances
92-U -238	Similar < 10 keV
93-Np-236	Same
93-Np-237	Similar < 150 eV
93-Np-238	Different - both rubbish
93-Np-239	Same - both rubbish
94-Pu-236	Same
94-Pu-237	Same
94-Pu-238	Same
94-Pu-239	Same
94-Pu-240	Same
94-Pu-241	Same
94-Pu-242	Same
94-Pu-243	Same
94-Pu-244	Same
95-Am-241	Same
95-Am-242	Different - old bad
95-Am-242M	Similar - 30% > 3.5 eV
95-Am-243	Same
96-Cm-241	Same
96-Cm-242	Same
96-Cm-243	Same
96-Cm-244	Similar < 500 eV
96-Cm-245	Same
96-Cm-246	Same
96-Cm-247	Different
96-Cm-248	Same – negative elastic
97-Bk-249	Same
98-Cf-249	Same
98-Cf-250	Same
98-Cf-251	Same
98-Cf-252	Same
98-Cf-253	Same – partial to 11 keV
99-Es-253	Same – partial to 11 keV

Appendix B: 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 $U^{\mathbf{238}}$ 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

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

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

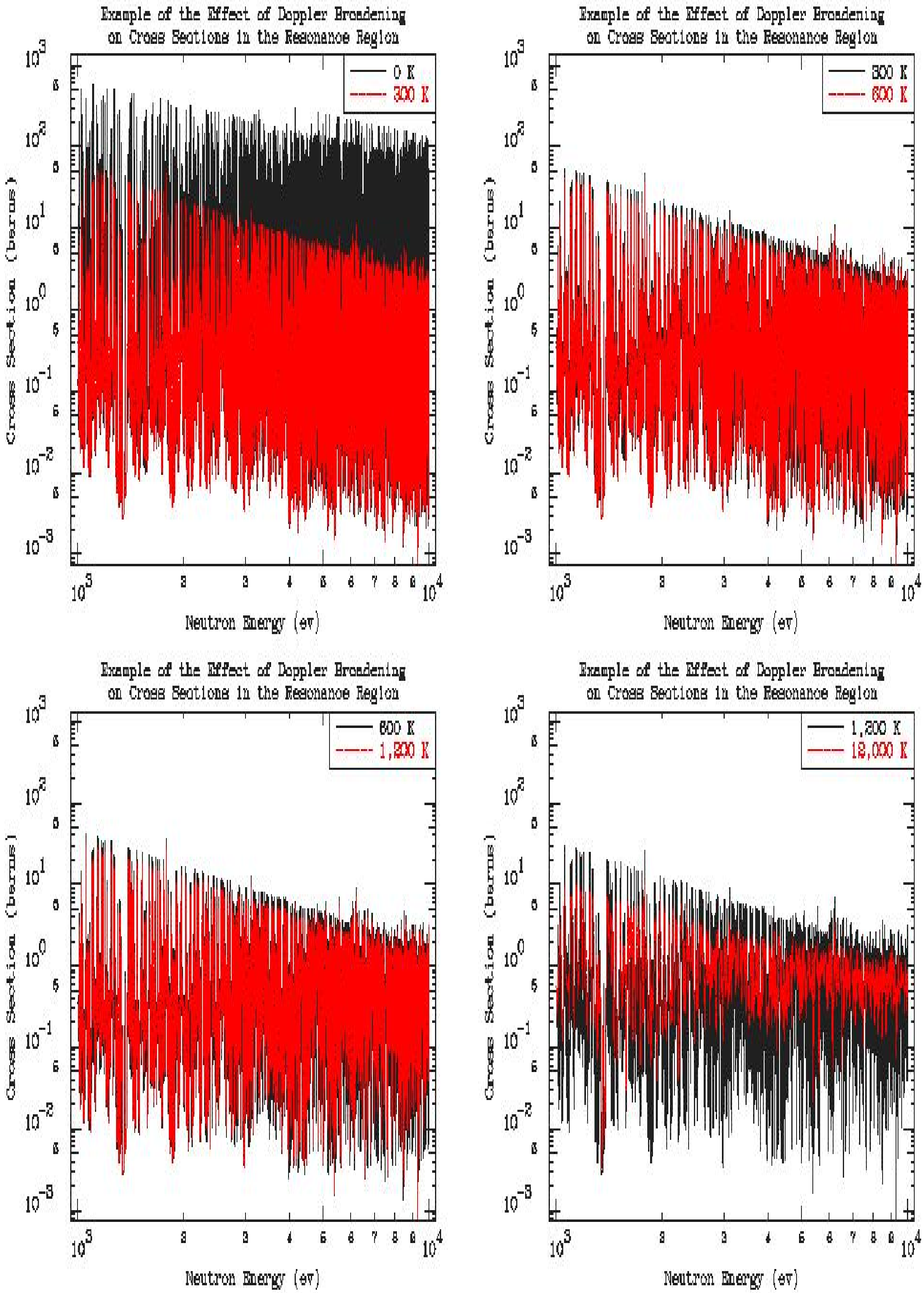

Fig.2: Effect of Doppler Broadening on Resonance Cross Sections

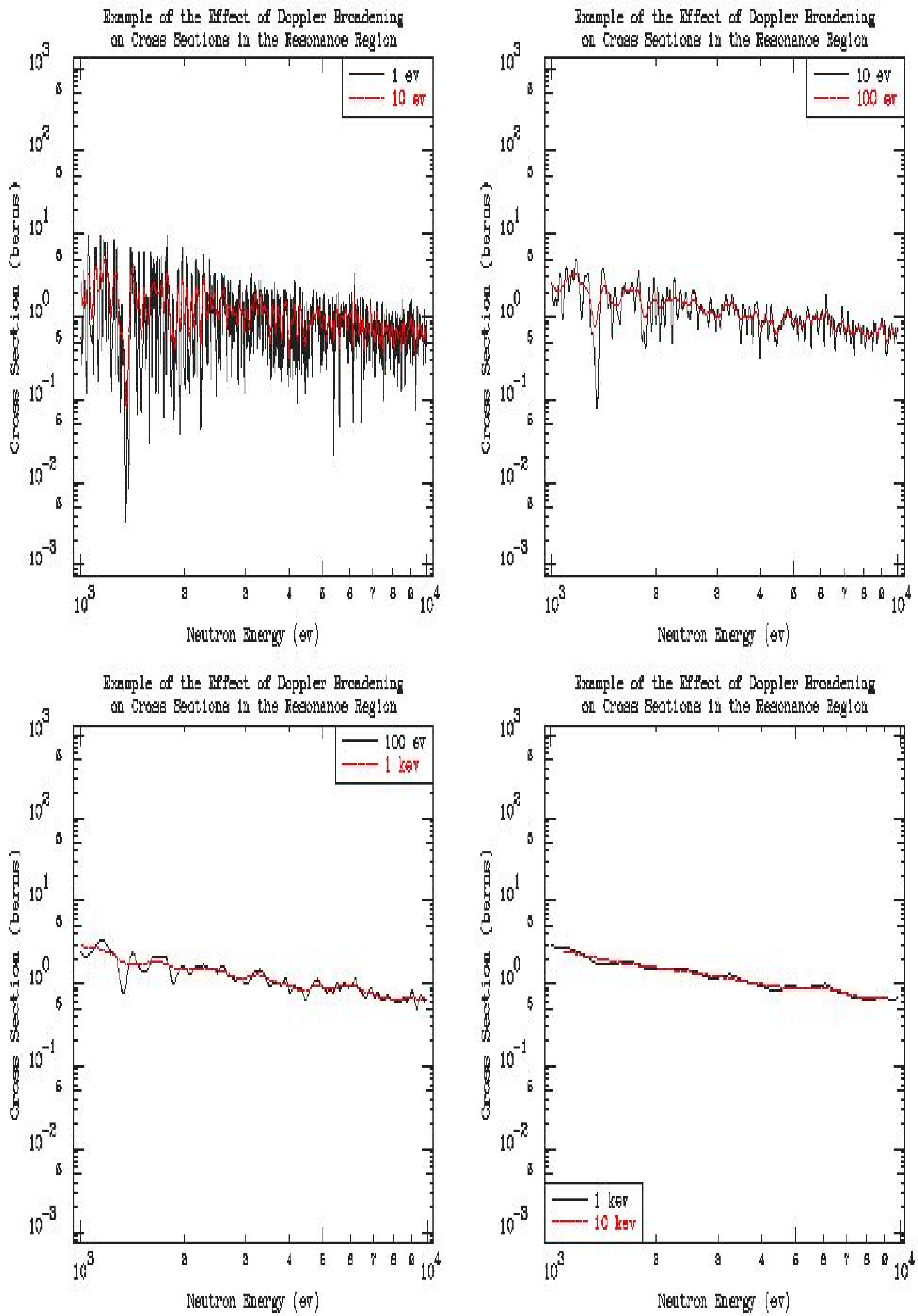

Fig.3: Effect of Doppler Broadening on Low Energy Cross Sections

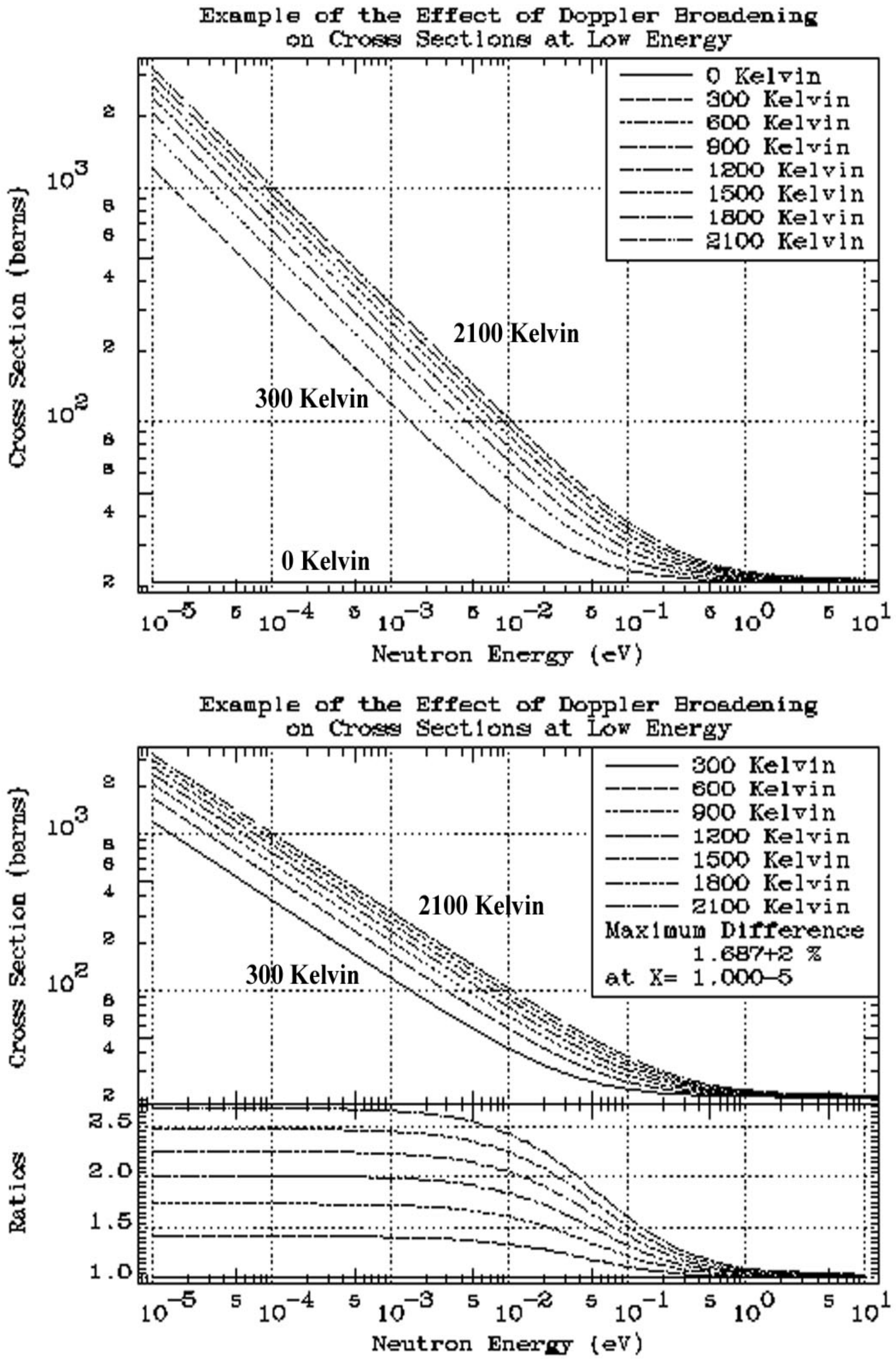

Fig.4: Effect of Doppler Broadening on Neutron Spectrum