

REPORT

Processing of the JEFF-3.2T3 Cross Section Library with the NJOY Code System into Various Formats for Testing Purposes

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1. Introduction: Report contents

The source of the evaluated nuclear data is JEFF-3.2T3. This library comprises 472 materials. The nuclides to be processed are all those of the General Purpose Library JEFF-3.2T3, including important light nuclei, the structural materials, the fission products, control rod materials and burnable poisons, all major and minor actinides.

The processing code system to be used is NJOY99.393 [**NJOY-99, NJOY99_up393**]. The NJOY modules used in this processing are: *moder*, *reconr*, *broadr*, *heart*, *gaspr*, *purr*, *acer*, *group*, *matxsr*, *error*, *covr*, *viewr*. The processed data also contains production and gas production data whenever such data are contained in JEFF-3.2T3. Kinematic KERMA factors and total damage energy production data are processed. The processed PENDF library at 300K has been verified: visually (no discontinuities, correct processing in all range) and compared with ENDF/B-VII.1, JEFF-3.1.2 and TENDL-2012.

In summary, the most important conclusions of this work are:

A) In Section 2, the processing steps of JEFF-3.2T3 in ACE format is explained.

- a. **Sections 2.1 and 2.2 illustrates some corrections in the official up393 patch and in JEFF-3.2T3 Library**
- b. **In Sections 2.3-2.8 examples of NJOY inputs and some procedures are shown**
 - PENDF, GENDF, MATXSR, ACE formats are processed and explained in Section 2.3-2.6.
 - In section 2.7 the processing of the STL, including additional materials such as Mg and Ca(CaH₂).
 - In Section 2.8, processing covariance data are reported, including errors.
 - In Section 2.9, checking ACE outputs has permitted to identify problems in PTABLE option for some nuclides. To be mentioned the problems in Pu238, S36 and K39.

B) In Sections 3 and 4, a QA procedure, including a validation criticality Suite of 123 cases taken from ICSBEP, is summarized

- checking messages and warnings
- comparison and visualization of important reactions and nuclides comparing with PREPRO system and JANIS4.0. Comparing JEFF-3.2T3 with ENDF/B-VII.1, JEFF-3.1.2 and TENDL-2012
- Criticality Validation Suite from ICSBEP and compared results with ENDF/B-VII.1, JEFF-3.1.2 and JEFF-3.2T2 using the same processing scheme.

- C) Finally, Section 5 describes the** work to process JEFF-3.2T3 with INTER code to be compared with other data libraries (JEFF-3.1.2, ENDF/B-VII.1 TENDL-2012,...).

In addition, a comparison for the MT444 (damage energy cross-section) shows large differences between nuclear data libraries. It can be concluded that JEFF-3.2T3 should improved MF5/MF6 and MT5 above 20 MeV to take into account accurate damage energy cross-sections.

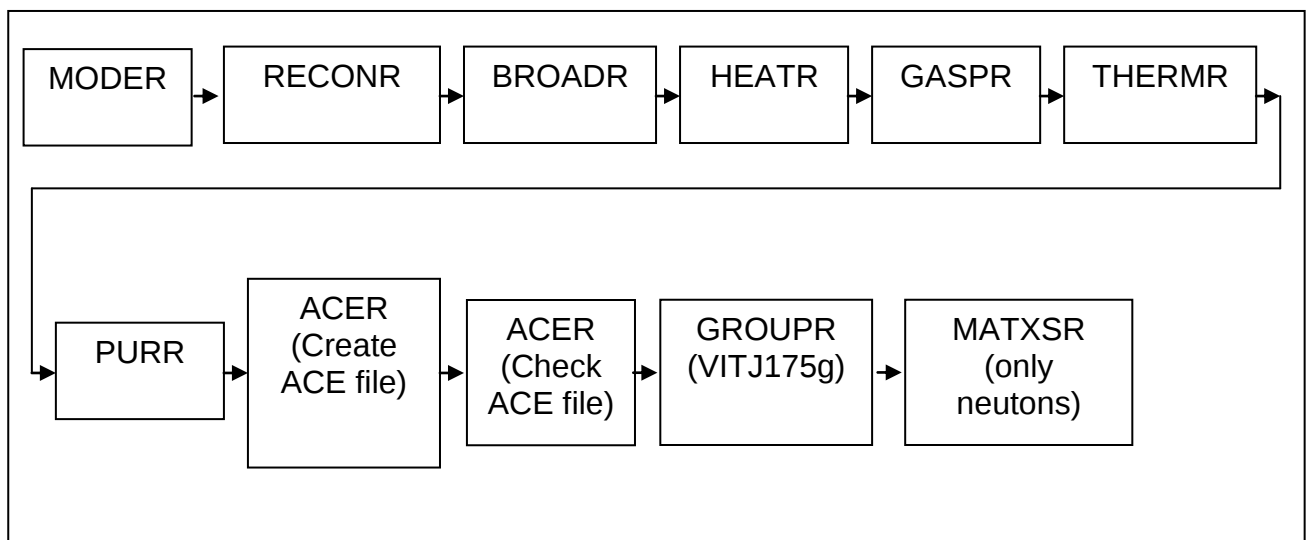
- D)** As results of this work, a list of “**9 ANNEXES**” has been included in the final documentation.

2. Processing evaluated nuclear data in different formats.

NJOY is a modular computer code used for converting evaluated nuclear data in the ENDF format into different type of libraries useful for applications calculations.

The processing sequence for generating formatted library suitable for use by different codes is shown below.

Figure 1. NJOY processing sequence for a formatted neutron library



The list of NJOY modules can be described by:

- **MODER:** Convert between ENDF/B standard coded mode and the NJOY blocked binary mode
- **RECONR:** Reconstruct pointwise cross sections from ENDF resonance parameters and interpolation schemes
- **BROADR:** Doppler-broadens and thins pointwise cross sections
- **HEATR:** Generate pointwise heat production cross section (KERMA factors) and radiation damage production cross sections
- **GASPR:** Add gas production to PENDF
- **THERMR:** Generate neutron scattering cross sections and point-to-point scattering kernels in the thermal range for free or bound atoms
- **PURR:** Prepare unresolved region probability tables for the MCNP continuous energy Monte Carlo code

- **ACER:** Prepare libraries in ACE format for the Los Alamos continuous energy Monte Carlo code MCNP
- **GROUPE:** Generate self-shielded multigroup cross sections and group-to-group scattering and photon production matrices
- **MATXS:** Convert multigroup data into the comprehensive MATXS cross section interface format.

For each material the processing sequence can be divided into three calculations:

- To produce point-wise data in PENDF format
- Module ACER generates the ACE formatted file that can be directly used in MCNP calculations. Here, error checking and consistency checks are also performed.
- Modules GROUPE and MATXS are used to process the library into a multigroup neutron energy structure. A multigroup energy structure option, ign=1 (USER option, 238-group structure based on SCALE6) with a weight function option, iwt=2 (constant), has been chosen.

2.1 Corrections in JEFF-3.2T3

In this work two corrections are suggested:

- The gzipped Library “JEFF32T3N.tar.gz” has problems in the unzipped files: JEFF32T3N2434.ASC and JEFF32T3N0925.ASC
Individual files for these materials taken from NEA Data Bank are used in this work
- Problems found in Nb93 to process MF40 are due to a typo error in the file: JEFF32T3N4125.ASC
A recommended update can be found in ANNEX 6.1

2.2 Corrections in NJOY99.393

In this work some corrections/suggestions have been identified in NJOY code.

The initial version used to process this library is NJOY99.393 taken from **Official Updates (LANL)** in: <http://t2.lanl.gov/codes/njoy99/>.

- a) Processing JEFF-3.2 using GROUPR module after ACER module failed for some isotopes (H3, He3, Y90, ...). A modification, uposc2, in ACER subroutine is proposed to correct this problem.

```
*ident uposc2
*/ acer -- nov2011
*/ - processing JEFF-3.1.2 with VDF6.6A in WindowsXP
*i up45.9
    if (ngmt.eq.0) call closz(-iold)
    if (ngmt.eq.0) call closz(-inew)
```

- b) Processing Nb93 with MF10 fails in GROUPR

```
group / Prepare multigroup data for neutrons
21 23 0 24
4125 17 0 2 6 1 1 1/
'(JEFF3.2T3) NJOY99.364 NEA DEC2011 '/
300.
1.E+10
3 /
40410931 4 /
0/
0/
```

The error message is:

```
***error in getsig***desired lfs not found
```

An new updated, uposc5, solve this problem:

```
*ident uposc5
*/ groupr -- nov2011
*/ - processing JEFF-3.1.2 with VDF6.6A in WindowsXP
*i up347.64
    if (mfd.gt.100000000) lfs=mod(mfd,10)
```

However, a new error occurs in ERRORR module

```
---message from covcal---WARNING! izap=0 for mf40, mt 4 is nonstandard
covcal may skip this mt, or covr plot title will be ambiguous

---message from rdgout---mf 3 mt 4 not found.
calculation is continued by sigma=0.0.
```

This new message is related with up324:

```
*ident up324
*/ errorr - 17february2010; adapted from upnea062 by Andre Trkov.
*/ - Add MF40 processing capability
*/ NOTE: When running with mfcov=40 the User must input a groupr
*/ generated genf file created with mfd=10. This coding
*/ has been tested for a single LFS state in MF10 and a
*/ single covariance set for that state in MF40.
```

```

*/  NOTE: The Fall, 2009 CSEWG meeting accepted a format change
*/      to include IZAP in the L1 location of the CONT record
*/      initiating an MF40 subsection. This coding assumes that
*/      endf formatted input files have been corrected, and will
*/      warn the user when reading an izap value of zero. Files
*/      with izap=0 and non-zero LFS values will likely not be
*/      processed.
*/  - Write -14 in the errorj output tape header record as a flag
*/      for subsequent modules that this tape contains mf40 data;
*/  - Change of convention in GENDF files generated by ERRORR;
*/      originally the C1 and C2 records were zero but for consistency
*/      with GENDF files produced by groupr, C1 is now set to ZA and
*/      C2 is either set to zero or when processing MF40 is set to
*/      10*ZA+LFS. We also include temperature in the C1 location of
*/      the second mf1, mt451 record as done by GROUPE.
*/  - Make sure matrix elements are zero in groups where the cross
*/      section is zero.

```

Then, it has been found a typo mistake in the file: "JEFF32T3N4125.ASC"

Original File

```

...
...
4.109300+4 9.210510+1 0 0 1 0412540 4 1
0.000000+0-3.082000+4 0 1 0 1412540 4 2
1.000000+1 1.000000+0 0 4 0 1412540 4 3
0.000000+0 0.000000+0 1 5 528 32412540 4 4
1.000000-5 4.000000+4 5.000000+4 6.000000+4 8.000000+4 1.000000+5412540 4 5
1.500000+5 2.000000+5 3.000000+5 4.000000+5 5.000000+5 6.000000+5412540 4 6
...
...

```

Updated File:

```

...
...
4.109300+4 9.210510+1 0 0 1 0412540 4 0
0.000000+0-3.082000+4 41093 1 0 1412540 4 2
1.000000+1 1.000000+0 0 4 0 1412540 4 3
0.000000+0 0.000000+0 1 5 528 32412540 4 4
1.000000-5 4.000000+4 5.000000+4 6.000000+4 8.000000+4 1.000000+5412540 4 5
1.500000+5 2.000000+5 3.000000+5 4.000000+5 5.000000+5 6.000000+5412540 4 6
...
...

```

The proposed update can be found in ANNEX 6.1.

- c) BROADR module returns zero value for processed cross-sections with a value lower than 1.0e-15 b. It should be taken into account a revision of this limit.

data sigmin/1.d15/

broadr.1256

2.3 *NJOY inputs to process JEFF-3.2 in PENDF, ACE, GENDF and MATXS*

Each NJOY module performs a well-defined processing task. These modules are linked by input and output files (tapes).

A reference input file for each material (fissile and non-fissile) at a specific temperature has been generated.

Examples of NJOY inputs are given in Figures 2 and 3.

Figure 2. NJOY input used to process Am242 (MAT 9546) at 293.6K

```
moder / Extract/convert neutron evaluated data
1 21
'95-Am-242 from JEFF32'/
20 9546
0/
reconr / Reconstruct XS for neutrons
21 22
'JEFF32 PENDF for 95-Am-242'/
9546 2/
0.001 0.0 0.003/ err tempr errmax
'JEFF32: 95-Am-242'/
'Processed by NJOY99.393, NEA_July_2013'/
0/
broadr / Doppler broaden XS
21 22 23
9546 1 0 0 0./
0.001 2.0e+6 0.003/ errthn thnmax errmax
293.6
0/
heatr / Add heating kerma and damage energy
21 23 24/
9546 7 0 0 0 2/
302 303 304 318 402 443 444/
gaspr / Add gas production
21 24 25
thermr / Add thermal scattering data
0 25 61
0 9546 12 1 1 0 1 221 1/
293.6
0.001 4.0
purr / Process Unresolved Resonance Range if any
21 61 26
9546 1 5 20 64/ matd ntemp nsigz nbin nladr
293.6
1.E+10 1.E+04 1.E+03 1.E+02 1.E+01
0/
acer / Prepare ACE files
21 26 0 27 28
1 0 1 .03 /
'95-Am-242 from JEFF32, NJOY99.393, NEA_July2013'/
9546 293.6
1 1/
/
acer / Check ACE files
0 27 0 29 30
```

```

7 1 1 -1/
/
groupr / Prepare multigroup data for neutrons
21 26 0 31
9546 1 0 2 6 1 5 1/
'95-Am-242 from JEFF32(JEFF32) NJOY 99.393 NEA JULY2011 '/'
293.6
1.E+10 1.E+04 1.E+03 1.E+02 1.E+01
      238 / Card 6A
1.0000E-05 1.0000E-04 5.0000E-04 7.5000E-04 1.0000E-03 1.2000E-03
1.5000E-03 2.0000E-03 2.5000E-03 3.0000E-03 4.0000E-03 5.0000E-03
7.5000E-03 1.0000E-02 2.5300E-02 3.0000E-02 4.0000E-02 5.0000E-02
6.0000E-02 7.0000E-02 8.0000E-02 9.0000E-02 1.0000E-01 1.2500E-01
1.5000E-01 1.7500E-01 2.0000E-01 2.2500E-01 2.5000E-01 2.7500E-01
3.0000E-01 3.2500E-01 3.5000E-01 3.7500E-01 4.0000E-01 4.5000E-01
5.0000E-01 5.5000E-01 6.0000E-01 6.2500E-01 6.5000E-01 7.0000E-01
7.5000E-01 8.0000E-01 8.5000E-01 9.0000E-01 9.2500E-01 9.5000E-01
9.7500E-01 1.0000E+00 1.0100E+00 1.0200E+00 1.0300E+00 1.0400E+00
1.0500E+00 1.0600E+00 1.0700E+00 1.0800E+00 1.0900E+00 1.1000E+00
1.1100E+00 1.1200E+00 1.1300E+00 1.1400E+00 1.1500E+00 1.1750E+00
1.2000E+00 1.2250E+00 1.2500E+00 1.3000E+00 1.3500E+00 1.4000E+00
1.4500E+00 1.5000E+00 1.5900E+00 1.6800E+00 1.7700E+00 1.8600E+00
1.9400E+00 2.0000E+00 2.1200E+00 2.2100E+00 2.3000E+00 2.3800E+00
2.4700E+00 2.5700E+00 2.6700E+00 2.7700E+00 2.8700E+00 2.9700E+00
3.0000E+00 3.0500E+00 3.1500E+00 3.5000E+00 3.7300E+00 4.0000E+00
4.7500E+00 5.0000E+00 5.4000E+00 6.0000E+00 6.2500E+00 6.5000E+00
6.7500E+00 7.0000E+00 7.1500E+00 8.1000E+00 9.1000E+00 1.0000E+01
1.1500E+01 1.1900E+01 1.2900E+01 1.3750E+01 1.4400E+01 1.5100E+01
1.6000E+01 1.7000E+01 1.8500E+01 1.9000E+01 2.0000E+01 2.1000E+01
2.2500E+01 2.5000E+01 2.7500E+01 3.0000E+01 3.1250E+01 3.1750E+01
3.3250E+01 3.3750E+01 3.4600E+01 3.5500E+01 3.7000E+01 3.8000E+01
3.9100E+01 3.9600E+01 4.1000E+01 4.2400E+01 4.4000E+01 4.5200E+01
4.7000E+01 4.8300E+01 4.9200E+01 5.0600E+01 5.2000E+01 5.3400E+01
5.9000E+01 6.1000E+01 6.5000E+01 6.7500E+01 7.2000E+01 7.6000E+01
8.0000E+01 8.2000E+01 9.0000E+01 1.0000E+02 1.0800E+02 1.1500E+02
1.1900E+02 1.2200E+02 1.8600E+02 1.9250E+02 2.0750E+02 2.1000E+02
2.4000E+02 2.8500E+02 3.0500E+02 5.5000E+02 6.7000E+02 6.8300E+02
9.5000E+02 1.1500E+03 1.5000E+03 1.5500E+03 1.8000E+03 2.2000E+03
2.2900E+03 2.5800E+03 3.0000E+03 3.7400E+03 3.9000E+03 6.0000E+03
8.0300E+03 9.5000E+03 1.3000E+04 1.7000E+04 2.5000E+04 3.0000E+04
4.5000E+04 5.0000E+04 5.2000E+04 6.0000E+04 7.3000E+04 7.5000E+04
8.2000E+04 8.5000E+04 1.0000E+05 1.2830E+05 1.5000E+05 2.0000E+05
2.7000E+05 3.3000E+05 4.0000E+05 4.2000E+05 4.4000E+05 4.7000E+05
4.9950E+05 5.5000E+05 5.7300E+05 6.0000E+05 6.7000E+05 6.7900E+05
7.5000E+05 8.2000E+05 8.6110E+05 8.7500E+05 9.0000E+05 9.2000E+05
1.0100E+06 1.1000E+06 1.2000E+06 1.2500E+06 1.3170E+06 1.3560E+06
1.4000E+06 1.5000E+06 1.8500E+06 2.3540E+06 2.4790E+06 3.0000E+06
4.3040E+06 4.8000E+06 6.4340E+06 8.1870E+06 1.0000E+07 1.2840E+07
1.3840E+07 1.4550E+07 1.5680E+07 1.7330E+07 2.0000E+07
3/
3 221 'Free Gas'/
3 251 'mubar'/
3 252 'xi'/
3 253 'gamma'/
3 259 '1/v'/
3 452/
3 455/
6/
6 221 'Free Gas'/
0/
0/

```

```
matxsr / Produce MATXS file
31 0 41/
1 'JEFF32:Am242 '/
1 2 2 1
'JEFF32 95-Am-242 from JEFF32'/
'Processed by NJOY-99.364 at NEA DEC2011 '/
'n' /
238
'nscat' 'ntherm' /
1 1/
1 1/
Am242 9546/
stop
```

Figure 3. NJOY input used to process H1 (MAT125) at 293.6K.

```
moder / Extract/convert neutron evaluated data
1 21
'1-H-1 from JEFF32'/
20 125
0/
reconr / Reconstruct XS for neutrons
21 22
'JEFF32 PENDF for 1-H-1'/
125 2/
0.001 0.0 0.003/ err tempr errmax
'JEFF32: 1-H-1'/
'Processed by NJOY99.393, NEA_July_2013'/
0/
broadr / Doppler broaden XS
21 22 23
125 1 0 0 0./
0.001 2.0e+6 0.003/ errthn thnmax errmax
293.6
0/
heatr / Add heating kerma and damage energy
21 23 24/
125 7 0 0 0 2/
302 303 304 318 402 443 444/
gaspr / Add gas production
21 24 25
thermr / Add thermal scattering data
0 25 61
0 125 12 1 1 0 1 221 1/
293.6
0.001 4.0
purr / Process Unresolved Resonance Range if any
21 61 26
125 1 1 20 64/ matd ntemp nsigz nbin nladr
293.6
1.E+10
0/
acer / Prepare ACE files
21 26 0 27 28
1 0 1 .03 /
'1-H-1 from JEFF32, NJOY99.393, NEA_July2013'/
125 293.6
1 1/
/
```

```

acer / Check ACE files
0 27 0 29 30
7 1 1 -1/
/
groupr / Prepare multigroup data for neutrons
21 26 0 31
125 1 0 2 6 1 1 1/
'1-H-1 from JEFF32(JEFF32) NJOY 99.393 NEA JULY2011 '/'
293.6
1.E+10
238 / Card 6A
1.0000E-05 1.0000E-04 5.0000E-04 7.5000E-04 1.0000E-03 1.2000E-03
1.5000E-03 2.0000E-03 2.5000E-03 3.0000E-03 4.0000E-03 5.0000E-03
7.5000E-03 1.0000E-02 2.5300E-02 3.0000E-02 4.0000E-02 5.0000E-02
6.0000E-02 7.0000E-02 8.0000E-02 9.0000E-02 1.0000E-01 1.2500E-01
1.5000E-01 1.7500E-01 2.0000E-01 2.2500E-01 2.5000E-01 2.7500E-01
3.0000E-01 3.2500E-01 3.5000E-01 3.7500E-01 4.0000E-01 4.5000E-01
5.0000E-01 5.5000E-01 6.0000E-01 6.2500E-01 6.5000E-01 7.0000E-01
7.5000E-01 8.0000E-01 8.5000E-01 9.0000E-01 9.2500E-01 9.5000E-01
9.7500E-01 1.0000E+00 1.0100E+00 1.0200E+00 1.0300E+00 1.0400E+00
1.0500E+00 1.0600E+00 1.0700E+00 1.0800E+00 1.0900E+00 1.1000E+00
1.1100E+00 1.1200E+00 1.1300E+00 1.1400E+00 1.1500E+00 1.1750E+00
1.2000E+00 1.2250E+00 1.2500E+00 1.3000E+00 1.3500E+00 1.4000E+00
1.4500E+00 1.5000E+00 1.5900E+00 1.6800E+00 1.7700E+00 1.8600E+00
1.9400E+00 2.0000E+00 2.1200E+00 2.2100E+00 2.3000E+00 2.3800E+00
2.4700E+00 2.5700E+00 2.6700E+00 2.7700E+00 2.8700E+00 2.9700E+00
3.0000E+00 3.0500E+00 3.1500E+00 3.5000E+00 3.7300E+00 4.0000E+00
4.7500E+00 5.0000E+00 5.4000E+00 6.0000E+00 6.2500E+00 6.5000E+00
6.7500E+00 7.0000E+00 7.1500E+00 8.1000E+00 9.1000E+00 1.0000E+01
1.1500E+01 1.1900E+01 1.2900E+01 1.3750E+01 1.4400E+01 1.5100E+01
1.6000E+01 1.7000E+01 1.8500E+01 1.9000E+01 2.0000E+01 2.1000E+01
2.2500E+01 2.5000E+01 2.7500E+01 3.0000E+01 3.1250E+01 3.1750E+01
3.3250E+01 3.3750E+01 3.4600E+01 3.5500E+01 3.7000E+01 3.8000E+01
3.9100E+01 3.9600E+01 4.1000E+01 4.2400E+01 4.4000E+01 4.5200E+01
4.7000E+01 4.8300E+01 4.9200E+01 5.0600E+01 5.2000E+01 5.3400E+01
5.9000E+01 6.1000E+01 6.5000E+01 6.7500E+01 7.2000E+01 7.6000E+01
8.0000E+01 8.2000E+01 9.0000E+01 1.0000E+02 1.0800E+02 1.1500E+02
1.1900E+02 1.2200E+02 1.8600E+02 1.9250E+02 2.0750E+02 2.1000E+02
2.4000E+02 2.8500E+02 3.0500E+02 5.5000E+02 6.7000E+02 6.8300E+02
9.5000E+02 1.1500E+03 1.5000E+03 1.5500E+03 1.8000E+03 2.2000E+03
2.2900E+03 2.5800E+03 3.0000E+03 3.7400E+03 3.9000E+03 6.0000E+03
8.0300E+03 9.5000E+03 1.3000E+04 1.7000E+04 2.5000E+04 3.0000E+04
4.5000E+04 5.0000E+04 5.2000E+04 6.0000E+04 7.3000E+04 7.5000E+04
8.2000E+04 8.5000E+04 1.0000E+05 1.2830E+05 1.5000E+05 2.0000E+05
2.7000E+05 3.3000E+05 4.0000E+05 4.2000E+05 4.4000E+05 4.7000E+05
4.9950E+05 5.5000E+05 5.7300E+05 6.0000E+05 6.7000E+05 6.7900E+05
7.5000E+05 8.2000E+05 8.6110E+05 8.7500E+05 9.0000E+05 9.2000E+05
1.0100E+06 1.1000E+06 1.2000E+06 1.2500E+06 1.3170E+06 1.3560E+06
1.4000E+06 1.5000E+06 1.8500E+06 2.3540E+06 2.4790E+06 3.0000E+06
4.3040E+06 4.8000E+06 6.4340E+06 8.1870E+06 1.0000E+07 1.2840E+07
1.3840E+07 1.4550E+07 1.5680E+07 1.7330E+07 2.0000E+07
3/
3 221 'Free Gas'/
3 251 'mubar'/
3 252 'xi'/
3 253 'gamma'/
3 259 '1/v'/
6/
6 221 'Free Gas'/
0/
0/

```

```
matxsr / Produce MATXS file
31 0 41/
1 'JEFF32:H1      '/
1 2 2 1
'JEFF32 1-H-1 from JEFF32'/
'Processed by NJOY-99.364 at NEA DEC2011 '/
'n' /
238
'nscat' 'ntherm' /
1 1/
1 1/
H1      125/
Stop
```

2.4 NJOY step-by-step

In this section, a summary of the most important processing options used by NJOY in a typical input file (U-235 at 293.6K) is presented below.

MODER

Convert ENDF “tapes” back and forth between formatted (that is, ASCII, EBCDIC, etc.) and blocked binary modes.

```
moder / Extract/convert neutron evaluated data
1 21
'92-U-235 from JEFF32'/
20 9228
0/
```

- Input unit : 20 (tape20, JEFF-3.1 cross section library)
- Material : 9228 (U-235)

MODER reads the JEFF-3.2T3 file (tape20) which contains the material (for U-235 the material number is 9228), extract it and put the ENDF file in binary mode in tape21.

RECONR

Reconstruct pointwise (energy-dependent) cross sections from ENDF resonance parameters and interpolation schemes.

```
reconr / Reconstruct XS for neutrons
21 22
'JEFF32 PENDF for 92-U-235'/
9228 2/
0.001 0.0 0.003/ err tempr errmax
'JEFF32: 92-U-235'/
'Processed by NJOY99.393, NEA_July_2013'/
0/
```

- Reconstruction tolerance : 1%
- Resonance-integral-check tolerance : 1%

- Reconstruction temperature : 0.0 K

RECONR read tape21, extract material 9228 and reconstruct cross section at 0K with a reconstruction tolerance of 1%. The resulting pointwise cross section is written in tape22.

BROADR

Doppler-broadens and thins pointwise cross sections.

```
broadr / Doppler broaden XS
21 22 23
9228 1 0 0 0./
0.001 2.0e+6 0.003/ errthn thnmax errmax
293.6
0/
```

- Thinning tolerance : 1%
- Integral criterion tolerance : 1%
- Thnmax value : 2MeV (The upper limit for broadening and thinning is: the lowest of the input values THNAMX, or the lowest reaction threshold, or the start of the resolved range.)
- Temperature : 293.6 K

BROADR reads tape21-tape22 and Doppler-broadens at 293.6K for material 9228. The tolerance used is 1%. The results are written in tape23.

HEATR

Generate pointwise heat production cross sections (KERMA factors) and radiation-damage-production cross sections.

```
heatr / Add heating kerma and damage energy
21 23 24/
9228 7 0 0 0 2/
302 303 304 318 402 443 444/
```

- MT=302: Elastic
- MT=303: Non-elastic
- MT=304: Inelastic
- MT=318: Fission
- MT=402: Capture
- MT=443: Total kinematic kerma
- MT=444: Total damage energy production

HEATR computes energy-balance heating and damage energy for material 9228 at 293.6K. Input files are tape21-tape23. The output file is tape24.

GASPR

Add gas production (mt203-207) to PENDF.

```
gaspr / Add gas production
21 24 25
```

GASPR add gas production reactions to PENDF tape24. Output file is tape25

THERMR

Produce cross sections and energy-to-energy matrices for free or bound scatterers in the thermal energy range.

```
thermr / Add thermal scattering data
0 25 61
0 9228 12 1 1 0 1 221 1/
293.6
0.001 4.0
```

- Number of angles bins : 12
- Tolerance : 0.1%
- Max. Energy : 4 eV
- Scattering option : 221 (free gas)
- Temperature : 293.6 K

THERMR generates neutron scattering cross sections and point-to-point scattering kernels in the thermal range. The input file is only tape25, the output file is tape61. The generation of neutron scattering cross sections is doing for material 9228 with 12 equi-probable angles at 293.6K. Free gas option is chosen and no elastic cross sections in the thermal range. A tolerance of 0.1% and the maximum energy for thermal treatment is 4 eV.

PURR

Prepare unresolved-region probability tables for the MCNP continuous-energy Monte Carlo code.

```
purr / Process Unresolved Resonance Range if any
21 61 26
9228 1 5 20 64/ matd ntemp nsigz nbin nladr
293.6
1.E+10 1.E+04 1.E+03 1.E+02 1.E+01
0/
```

- Number of probability bins : 15
- Number of resonance ladders: 32
- Temperature : 293.6 K
- Bondarenko σ_0 values : 1.E+10 1.E+04 1.E+03 1.E+02 1.E+01

PURR calculates probability tables for treating unresolved-resonance self-shielding for Monte Carlo codes. Inputs tgape21-tape61, output in tape 26. Calculation performed for material 9228 at 293.6K with five σ_0 values (1.0E+10, infinite dilute cross section). A total number of 15 probability bins and 32 resonance ladders were selected.

ACER (cross section libraries)

Prepare libraries in ACE format for the Los Alamos continuous-energy Monte Carlo code MCNP.

```
acer / Prepare ACE files
21 26 0 27 28
1 0 1 .03 /
'92-U-235 from JEFF32, NJOY99.393, NEA_July2013'/
9228 293.6
1 1/
/
acer / Check ACE files
0 27 0 29 30
7 1 1 -1/
/
```

- Type of ACE file : 1 (ascii)
- ZAID suffix : .03
- No thinning
- Temperature : 293.6 K

ACER prepares a data library for MCNP (in ASCII). Input files: tape21-26, output files: tape27 (ACE file) and tape28 (XSDIR file). The material processed is 9228 at 293.6K. The id suffix for this material is ".03".

Second ACER module checks previous ACE file and prepare new tape29(ACE file) and tape30(XSDIR file).

GROUPR (multigroup cross section libraries)

GROUPR computes a 238 multigroup library for material 9228 at 293.6K. Input files are tape21-tape26. The output file is tape31.

```
grouppr / Prepare multigroup data for neutrons
21 26 0 31
9228 1 0 2 6 1 5 1/
'92-U-235 from JEFF32(JEFF32) NJOY 99.393 NEA JULY2011 '/
293.6
1.E+10 1.E+04 1.E+03 1.E+02 1.E+01
238 / Card 6A
1.0000E-05 1.0000E-04 5.0000E-04 7.5000E-04 1.0000E-03 1.2000E-03
1.5000E-03 2.0000E-03 2.5000E-03 3.0000E-03 4.0000E-03 5.0000E-03
7.5000E-03 1.0000E-02 2.5300E-02 3.0000E-02 4.0000E-02 5.0000E-02
6.0000E-02 7.0000E-02 8.0000E-02 9.0000E-02 1.0000E-01 1.2500E-01
1.5000E-01 1.7500E-01 2.0000E-01 2.2500E-01 2.5000E-01 2.7500E-01
3.0000E-01 3.2500E-01 3.5000E-01 3.7500E-01 4.0000E-01 4.5000E-01
```

```

5.0000E-01 5.5000E-01 6.0000E-01 6.2500E-01 6.5000E-01 7.0000E-01
7.5000E-01 8.0000E-01 8.5000E-01 9.0000E-01 9.2500E-01 9.5000E-01
9.7500E-01 1.0000E+00 1.0100E+00 1.0200E+00 1.0300E+00 1.0400E+00
1.0500E+00 1.0600E+00 1.0700E+00 1.0800E+00 1.0900E+00 1.1000E+00
1.1100E+00 1.1200E+00 1.1300E+00 1.1400E+00 1.1500E+00 1.1750E+00
1.2000E+00 1.2250E+00 1.2500E+00 1.3000E+00 1.3500E+00 1.4000E+00
1.4500E+00 1.5000E+00 1.5900E+00 1.6800E+00 1.7700E+00 1.8600E+00
1.9400E+00 2.0000E+00 2.1200E+00 2.2100E+00 2.3000E+00 2.3800E+00
2.4700E+00 2.5700E+00 2.6700E+00 2.7700E+00 2.8700E+00 2.9700E+00
3.0000E+00 3.0500E+00 3.1500E+00 3.5000E+00 3.7300E+00 4.0000E+00
4.7500E+00 5.0000E+00 5.4000E+00 6.0000E+00 6.2500E+00 6.5000E+00
6.7500E+00 7.0000E+00 7.1500E+00 8.1000E+00 9.1000E+00 1.0000E+01
1.1500E+01 1.1900E+01 1.2900E+01 1.3750E+01 1.4400E+01 1.5100E+01
1.6000E+01 1.7000E+01 1.8500E+01 1.9000E+01 2.0000E+01 2.1000E+01
2.2500E+01 2.5000E+01 2.7500E+01 3.0000E+01 3.1250E+01 3.1750E+01
3.3250E+01 3.3750E+01 3.4600E+01 3.5500E+01 3.7000E+01 3.8000E+01
3.9100E+01 3.9600E+01 4.1000E+01 4.2400E+01 4.4000E+01 4.5200E+01
4.7000E+01 4.8300E+01 4.9200E+01 5.0600E+01 5.2000E+01 5.3400E+01
5.9000E+01 6.1000E+01 6.5000E+01 6.7500E+01 7.2000E+01 7.6000E+01
8.0000E+01 8.2000E+01 9.0000E+01 1.0000E+02 1.0800E+02 1.1500E+02
1.1900E+02 1.2200E+02 1.8600E+02 1.9250E+02 2.0750E+02 2.1000E+02
2.4000E+02 2.8500E+02 3.0500E+02 5.5000E+02 6.7000E+02 6.8300E+02
9.5000E+02 1.1500E+03 1.5000E+03 1.5500E+03 1.8000E+03 2.2000E+03
2.2900E+03 2.5800E+03 3.0000E+03 3.7400E+03 3.9000E+03 6.0000E+03
8.0300E+03 9.5000E+03 1.3000E+04 1.7000E+04 2.5000E+04 3.0000E+04
4.5000E+04 5.0000E+04 5.2000E+04 6.0000E+04 7.3000E+04 7.5000E+04
8.2000E+04 8.5000E+04 1.0000E+05 1.2830E+05 1.5000E+05 2.0000E+05
2.7000E+05 3.3000E+05 4.0000E+05 4.2000E+05 4.4000E+05 4.7000E+05
4.9950E+05 5.5000E+05 5.7300E+05 6.0000E+05 6.7000E+05 6.7900E+05
7.5000E+05 8.2000E+05 8.6110E+05 8.7500E+05 9.0000E+05 9.2000E+05
1.0100E+06 1.1000E+06 1.2000E+06 1.2500E+06 1.3170E+06 1.3560E+06
1.4000E+06 1.5000E+06 1.8500E+06 2.3540E+06 2.4790E+06 3.0000E+06
4.3040E+06 4.8000E+06 6.4340E+06 8.1870E+06 1.0000E+07 1.2840E+07
1.3840E+07 1.4550E+07 1.5680E+07 1.7330E+07 2.0000E+07
3/
3 221 'Free Gas'/
3 251 'mubar'/
3 252 'xi'/
3 253 'gamma'/
3 259 '1/v'/
3 452/
3 455/
5 455/
6/
6 221 'Free Gas'/
0/
0/

```

- Neutron groups : 238, SCALE6 – energy structure
- Gamma groups : 0
- Neutron weight function : constant
- Legendre order : P6
- Temperature : 293.6K
- Bondarenko σ_0 values : 1.E+10 1.E+04 1.E+03 1.E+02 1.E+01
- Reactions : all MT in file 3, MT=302, ...MT=444,
Mt=251, MT=252, MT=253 and MT=259, for
actinides MT=452 and MT=455

MATXSR (multigroup cross section libraries)

MATXSR generates a 238-SCALE6 library for material 9228 at 293.6K. Input files are tape31. The output file is tape36.

```
matxsr / Produce MATXS file
31 0 41/
1 'JEFF32:U235  '/
1 2 2 1
'JEFF32 92-U-235 from JEFF32'/
'Processed by NJOY-99.364 at NEA DEC2011 '/
'n' /
238
'nscat' 'ntherm' /
1 1/
1 1/
U235 9228/
```

- Type of particles : neutrons (n)
- Data types : 2 (nscat, ntherm)
- Number of neutrons groups : 238, SCALE6

2.5 Processing JEFF-3.2T3 in ACE format

The library contains pointwise cross section data files for use in the Monte Carlo code MCNP.

For each material two files were given:

- Cross section data file in the ACE type 1 (ASCII) format: *file.ace*
- Information required by *xmdir* file of MCNP code system: *file.dir*

These files were rewritten by the UpdXSDIR code **[UpdXSDIR]** to give the correct ACE filename and to update the route to 0.

Both files were prepared by the ACER module of NJOY99-393. Also, probability tables (ptable) have been generated for those materials with unresolved resonance data (see Table 1).

Table 1. Information on the JEFF-3.2T3 ACE library at 293.6K. A list of 97 new materials/isotopes are included in JEFF-3.2T3.

No.	Nuclide	ZAID	PT Tables			ACE filename	XSDIR filename	Comment
			JEFF3.1.1	JEFF3.1.2	JEFF-32T3			
1	1-H-1	1001.03c	-	-	-	H1.ACE	H1.DIR	
2	1-H-2	1002.03c	-	-	-	H2.ACE	H2.DIR	
3	1-H-3	1003.03c	-	-	-	H3.ACE	H3.DIR	
4	2-He-3	2003.03c	-	-	-	He3.ACE	He3.DIR	
5	2-He-4	2004.03c	-	-	-	He4.ACE	He4.DIR	
6	3-Li-6	3006.03c	-	-	-	Li6.ACE	Li6.DIR	
7	3-Li-7	3007.03c	-	-	-	Li7.ACE	Li7.DIR	
8	4-Be-9	4009.03c	-	-	-	Be9.ACE	Be9.DIR	
9	5-B-10	5010.03c	-	-	-	B10.ACE	B10.DIR	
10	5-B-11	5011.03c	-	-	-	B11.ACE	B11.DIR	
11	6-C-0	6000.03c	-	-	-	C0.ACE	C0.DIR	
12	6-C-13	6013.03c	-	-	-	C13.ACE	C13.dir	No in JEFF-3.1.1/2
13	7-N-14	7014.03c	-	-	-	N14.ACE	N14.DIR	
14	7-N-15	7015.03c	-	-	-	N15.ACE	N15.DIR	
15	8-O-16	8016.03c	-	-	-	O16.ACE	O16.DIR	
16	8-O-17	8017.03c	-	-	-	O17.ACE	O17.DIR	
17	8-O-18	8018.03c		-	-	O18.ACE	O18.dir	No in JEFF-3.1.1/2
18	9-F-19	9019.03c	-	-	-	F19.ACE	F19.DIR	
19	10-Ne-20	10020.03c	-	-	-	Ne20.ACE	Ne20.dir	No in JEFF-3.1.1/2
20	10-Ne-21	10021.03c	-	-	ptable	Ne21.ACE	Ne21.dir	No in JEFF-3.1.1/2
21	10-Ne-22	10022.03c	-	-	ptable	Ne22.ACE	Ne22.dir	No in JEFF-3.1.1/2
22	11-Na-22	11022.03c	-(a)	(c)	ptable	Na22.ACE	Na22.DIR	
23	11-Na-23	11023.03c	-	-	-	Na23.ACE	Na23.DIR	

24	12-Mg-24	12024.03c	-	-	-	Mg24.ACE	Mg24.DIR	
25	12-Mg-25	12025.03c	-	-	-	Mg25.ACE	Mg25.DIR	
26	12-Mg-26	12026.03c	-	-	-	Mg26.ACE	Mg26.DIR	
27	12-Mg-27	12027.03c	-	-	ptable	Mg27.ACE	Mg27.dir	No in JEFF-3.1.1/2
28	13-Al-27	13027.03c	-	-	-	Al27.ACE	Al27.DIR	
29	14-Si-28	14028.03c	-	-	-	Si28.ACE	Si28.DIR	
30	14-Si-29	14029.03c	-	-	-	Si29.ACE	Si29.DIR	
31	14-Si-30	14030.03c	-	-	-	Si30.ACE	Si30.DIR	
32	14-Si-31	14031.03c	-	-	ptable	Si31.ACE	Si31.dir	No in JEFF-3.1.1/2
33	14-Si-32	14032.03c	-	-	-	Si32.ACE	Si32.dir	No in JEFF-3.1.1/2
34	15-P-31	15031.03c	-	-	-	P31.ACE	P31.DIR	
35	16-S-32	16032.03c	-	-	-	S32.ACE	S32.DIR	
36	16-S-33	16033.03c	-	-	ptable	S33.ACE	S33.DIR	
37	16-S-34	16034.03c	-	-	ptable	S34.ACE	S34.DIR	
38	16-S-36	16036.03c	-	-	(e)	S36.ACE	S36.DIR	
39	17-Cl-35	17035.03c	-	-	-	Cl35.ACE	Cl35.DIR	
40	17-Cl-36	17036.03c	-	-	ptable	Cl36.ACE	Cl36.dir	No in JEFF-3.1.1/2
41	17-Cl-37	17037.03c	-	-	-	Cl37.ACE	Cl37.DIR	
42	18-Ar-36	18036.03c	-(a)	(c)	ptable	Ar36.ACE	Ar36.DIR	
43	18-Ar-38	18038.03c	ptable	ptable	ptable	Ar38.ACE	Ar38.DIR	
44	18-Ar-39	18039.03c	-	-	ptable	Ar39.ACE	Ar39.dir	No in JEFF-3.1.1/2
45	18-Ar-40	18040.03c	-	-	-	Ar40.ACE	Ar40.DIR	
46	18-Ar-41	18041.03c	-	-	ptable	Ar41.ACE	Ar41.dir	No in JEFF-3.1.1/2
47	19-K-39	19039.03c	-	-	(e)	K39.ACE	K39.DIR	
48	19-K-40	19040.03c	-	-	ptable	K40.ACE	K40.DIR	
49	19-K-41	19041.03c	-	-	ptable	K41.ACE	K41.DIR	
50	20-Ca-40	20040.03c	-	-	-	Ca40.ACE	Ca40.DIR	

51	20-Ca-41	20041.03c	-	-	ptable	Ca41.ACE	Ca41.dir	No in JEFF-3.1.1/2
52	20-Ca-42	20042.03c	-	-	-	Ca42.ACE	Ca42.DIR	
53	20-Ca-43	20043.03c	-	-	-	Ca43.ACE	Ca43.DIR	
54	20-Ca-44	20044.03c	-	-	-	Ca44.ACE	Ca44.DIR	
55	20-Ca-45	20045.03c	-	-	ptable	Ca45.ACE	Ca45.dir	No in JEFF-3.1.1/2
56	20-Ca-46	20046.03c	-	-	-	Ca46.ACE	Ca46.DIR	
57	20-Ca-48	20048.03c	-	-	-	Ca48.ACE	Ca48.DIR	
58	21-Sc-45	21045.03c	-	-	-	Sc45.ACE	Sc45.DIR	
59	21-Sc-46	21046.03c	-	-	ptable	Sc46.ACE	Sc46.dir	No in JEFF-3.1.1/2
60	22-Ti-46	22046.03c	-	-	-	Ti46.ACE	Ti46.DIR	
61	22-Ti-47	22047.03c	-	-	-	Ti47.ACE	Ti47.DIR	
62	22-Ti-48	22048.03c	-	-	-	Ti48.ACE	Ti48.DIR	
63	22-Ti-49	22049.03c	-	-	-	Ti49.ACE	Ti49.DIR	
64	22-Ti-50	22050.03c	-	-	-	Ti50.ACE	Ti50.DIR	
65	23-V-0	23000.03c	-	-	-	V0.ACE	V0.DIR	
66	23-V-49	23049.03c	-	-	ptable	V49.ACE	V49.dir	No in JEFF-3.1.1/2
67	24-Cr-50	24050.03c	-	-	-	Cr50.ACE	Cr50.DIR	
68	24-Cr-51	24051.03c	-	-	ptable	Cr51.ACE	Cr51.dir	No in JEFF-3.1.1/2
69	24-Cr-52	24052.03c	-	-	-	Cr52.ACE	Cr52.DIR	
70	24-Cr-53	24053.03c	-	-	-	Cr53.ACE	Cr53.DIR	
71	24-Cr-54	24054.03c	-	-	-	Cr54.ACE	Cr54.DIR	
72	25-Mn-53	25053.03c	-	-	ptable	Mn53.ACE	Mn53.dir	No in JEFF-3.1.1/2
73	25-Mn-54	25054.03c	-	-	ptable	Mn54.ACE	Mn54.dir	No in JEFF-3.1.1/2
74	25-Mn-55	25055.03c	-	-	-	Mn55.ACE	Mn55.DIR	
75	26-Fe-54	26054.03c	-	-	-	Fe54.ACE	Fe54.DIR	
76	26-Fe-56	26056.03c	-	-	-	Fe56.ACE	Fe56.DIR	
77	26-Fe-57	26057.03c	-	-	-	Fe57.ACE	Fe57.DIR	

78	26-Fe-58	26058.03c	ptable	ptable	ptable	Fe58.ACE	Fe58.DIR	
79	27-Co-57	27057.03c	-	-	ptable	Co57.ACE	Co57.dir	No in JEFF-3.1.1/2
80	27-Co-58M	27058.03c	-	-	-	Co58M.ACE	Co58M.DIR	
81	27-Co-58	27058.03c	-	-	-	Co58.ACE	Co58.DIR	
82	27-Co-59	27059.03c	-	-	-	Co59.ACE	Co59.DIR	
83	27-Co-60	27060.03c	-	-	ptable	Co60.ACE	Co60.dir	No in JEFF-3.1.1/2
84	28-Ni-58	28058.03c	-	-	-	Ni58.ACE	Ni58.DIR	
85	28-Ni-59	28059.03c	-	-	-	Ni59.ACE	Ni59.DIR	
86	28-Ni-60	28060.03c	-	-	-	Ni60.ACE	Ni60.DIR	
87	28-Ni-61	28061.03c	-	-	-	Ni61.ACE	Ni61.DIR	
88	28-Ni-62	28062.03c	-	-	-	Ni62.ACE	Ni62.DIR	
89	28-Ni-63	28063.03c	-	-	ptable	Ni63.ACE	Ni63.dir	No in JEFF-3.1.1/2
90	28-Ni-64	28064.03c	-	-	-	Ni64.ACE	Ni64.DIR	
91	29-Cu-63	29063.03c	-	-	-	Cu63.ACE	Cu63.DIR	
92	29-Cu-64	29064.03c	-	-	ptable	Cu64.ACE	Cu64.dir	No in JEFF-3.1.1/2
93	29-Cu-65	29065.03c	-	-	-	Cu65.ACE	Cu65.DIR	
94	29-Cu-66	29066.03c	-	-	ptable	Cu66.ACE	Cu66.dir	No in JEFF-3.1.1/2
95	30-Zn-0	30000.03c	-	-	-	Zn0.ACE	Zn0.DIR	No in JEFF-32T3
96	30-Zn-64	30064.03c	-	-	ptable	Zn64.ACE	Zn64.dir	No in JEFF-3.1.1/2
97	30-Zn-66	30066.03c	-	-	ptable	Zn66.ACE	Zn66.dir	No in JEFF-3.1.1/2
98	30-Zn-67	30067.03c	-	-	-	Zn67.ACE	Zn67.dir	No in JEFF-3.1.1/2
99	30-Zn-68	30068.03c	-	-	ptable	Zn68.ACE	Zn68.dir	No in JEFF-3.1.1/2
100	30-Zn-70	30070.03c	-	-	ptable	Zn70.ACE	Zn70.dir	No in JEFF-3.1.1/2
101	31-Ga-0	31000.03c	-	-	-	Ga0.ACE	Ga0.DIR	No in JEFF-32T3
102	31-Ga-69	31069.03c	-	-	ptable	Ga69.ACE	Ga69.dir	No in JEFF-3.1.1/2
103	31-Ga-71	31071.03c	-	-	ptable	Ga71.ACE	Ga71.dir	No in JEFF-3.1.1/2
104	32-Ge-70	32070.03c	-	-	ptable	Ge70.ACE	Ge70.DIR	

105	32-Ge-72	32072.03c	-	-	ptable	Ge72.ACE	Ge72.DIR	
106	32-Ge-73	32073.03c	-	-	ptable	Ge73.ACE	Ge73.DIR	
107	32-Ge-74	32074.03c	-	-	ptable	Ge74.ACE	Ge74.DIR	
108	32-Ge-76	32076.03c	-	-	ptable	Ge76.ACE	Ge76.DIR	
109	33-As-75	33075.03c	-	-	ptable	As75.ACE	As75.DIR	
110	34-Se-74	34074.03c	-	-	ptable	Se74.ACE	Se74.DIR	
111	34-Se-76	34076.03c	-	-	ptable	Se76.ACE	Se76.DIR	
112	34-Se-77	34077.03c	-	-	ptable	Se77.ACE	Se77.DIR	
113	34-Se-78	34078.03c	-	-	ptable	Se78.ACE	Se78.DIR	
114	34-Se-79	34079.03c	ptable	ptable	ptable	Se79.ACE	Se79.DIR	
115	34-Se-80	34080.03c	-	-	ptable	Se80.ACE	Se80.DIR	
116	34-Se-82	34082.03c	-	-	ptable	Se82.ACE	Se82.DIR	
117	35-Br-79	35079.03c	-	-	ptable	Br79.ACE	Br79.DIR	
118	35-Br-81	35081.03c	-	-	ptable	Br81.ACE	Br81.DIR	
119	36-Kr-78	36078.03c	-	-	ptable	Kr78.ACE	Kr78.DIR	
120	36-Kr-80	36080.03c	-	-	ptable	Kr80.ACE	Kr80.DIR	
121	36-Kr-82	36082.03c	-	-	ptable	Kr82.ACE	Kr82.DIR	
122	36-Kr-83	36083.03c	-	ptable	ptable	Kr83.ACE	Kr83.DIR	
123	36-Kr-84	36084.03c	-	-	ptable	Kr84.ACE	Kr84.DIR	
124	36-Kr-85	36085.03c	-	-	ptable	Kr85.ACE	Kr85.DIR	
125	36-Kr-86	36086.03c	-	-	-	Kr86.ACE	Kr86.DIR	
126	37-Rb-85	37085.03c	-	-	ptable	Rb85.ACE	Rb85.DIR	
127	37-Rb-86	37086.03c	-	-	ptable	Rb86.ACE	Rb86.DIR	
128	37-Rb-87	37087.03c	-	-	ptable	Rb87.ACE	Rb87.DIR	
129	37-Rb-88	37088.03c	-	-	ptable	Rb88.ACE	Rb88.dir	No in JEFF-3.1.1/2
130	38-Sr-84	38084.03c	-	-	ptable	Sr84.ACE	Sr84.DIR	
131	38-Sr-86	38086.03c	-	-	ptable	Sr86.ACE	Sr86.DIR	

132	38-Sr-87	38087.03c	-	-	ptable	Sr87.ACE	Sr87.DIR	
133	38-Sr-88	38088.03c	-	-	ptable	Sr88.ACE	Sr88.DIR	
134	38-Sr-89	38089.03c	-	-	ptable	Sr89.ACE	Sr89.DIR	
135	38-Sr-90	38090.03c	-	-	ptable	Sr90.ACE	Sr90.DIR	
136	39-Y-89	39089.03c	-	-	-	Y89.ACE	Y89.DIR	
137	39-Y-90	39090.03c	-	-	ptable	Y90.ACE	Y90.DIR	
138	39-Y-91	39091.03c	-	-	ptable	Y91.ACE	Y91.DIR	
139	40-Zr-90	40090.03c	-	-	ptable	Zr90.ACE	Zr90.DIR	
140	40-Zr-91	40091.03c	ptable	ptable	ptable	Zr91.ACE	Zr91.DIR	
141	40-Zr-92	40092.03c	ptable	ptable	ptable	Zr92.ACE	Zr92.DIR	
142	40-Zr-93	40093.03c	ptable	ptable	ptable	Zr93.ACE	Zr93.DIR	
143	40-Zr-94	40094.03c	ptable	ptable	ptable	Zr94.ACE	Zr94.DIR	
144	40-Zr-95	40095.03c	ptable	ptable	ptable	Zr95.ACE	Zr95.DIR	
145	40-Zr-96	40096.03c	-	-	-	Zr96.ACE	Zr96.DIR	
146	41-Nb-93	41093.03c	-	-	-	Nb93.ACE	Nb93.DIR	
147	41-Nb-94	41094.03c	ptable	ptable	ptable	Nb94.ACE	Nb94.DIR	
148	41-Nb-95	41095.03c	ptable	ptable	ptable	Nb95.ACE	Nb95.DIR	
149	42-Mo-92	42092.03c	ptable	ptable	ptable	Mo92.ACE	Mo92.DIR	
150	42-Mo-94	42094.03c	ptable	ptable	ptable	Mo94.ACE	Mo94.DIR	
151	42-Mo-95	42095.03c	ptable	(c)	ptable	Mo95.ACE	Mo95.DIR	
152	42-Mo-96	42096.03c	ptable	ptable	ptable	Mo96.ACE	Mo96.DIR	
153	42-Mo-97	42097.03c	ptable	ptable	ptable	Mo97.ACE	Mo97.DIR	
154	42-Mo-98	42098.03c	ptable	ptable	ptable	Mo98.ACE	Mo98.DIR	
155	42-Mo-99	42099.03c	ptable	ptable	ptable	Mo99.ACE	Mo99.DIR	
156	42-Mo-100	42100.03c	ptable	ptable	ptable	Mo100.ACE	Mo100.DIR	
157	43-Tc-98	43098.03c	-	-	ptable	Tc98.ACE	Tc98.dir	No in JEFF-3.1.1/2
158	43-Tc-99	43099.03c	ptable	ptable	ptable	Tc99.ACE	Tc99.DIR	

159	44-Ru-96	44096.03c	-	-	-	Ru96.ACE	Ru96.DIR	
160	44-Ru-98	44098.03c	-	-	-	Ru98.ACE	Ru98.DIR	
161	44-Ru-99	44099.03c	-	-	-	Ru99.ACE	Ru99.DIR	
162	44-Ru-100	44100.03c	-	ptable	ptable	Ru100.ACE	Ru100.DIR	
163	44-Ru-101	44101.03c	-(a)	(c)	ptable	Ru101.ACE	Ru101.DIR	
164	44-Ru-102	44102.03c	-	ptable	ptable	Ru102.ACE	Ru102.DIR	
165	44-Ru-103	44103.03c	ptable	ptable	ptable	Ru103.ACE	Ru103.DIR	
166	44-Ru-104	44104.03c	-	ptable	ptable	Ru104.ACE	Ru104.DIR	
167	44-Ru-105	44105.03c	-	-	-	Ru105.ACE	Ru105.DIR	
168	44-Ru-106	44106.03c	-	-	-	Ru106.ACE	Ru106.DIR	
169	45-Rh-103	45103.03c	ptable	ptable	ptable	Rh103.ACE	Rh103.DIR	
170	45-Rh-104	45104.03c	-	-	ptable	Rh104.ACE	Rh104.dir	No in JEFF-3.1.1/2
171	45-Rh-105	45105.03c	-	ptable	ptable	Rh105.ACE	Rh105.DIR	
172	46-Pd-102	46102.03c	-	-	-	Pd102.ACE	Pd102.DIR	
173	46-Pd-104	46104.03c	-(a)	-	-	Pd104.ACE	Pd104.DIR	
174	46-Pd-105	46105.03c	ptable	(c)	ptable	Pd105.ACE	Pd105.DIR	
175	46-Pd-106	46106.03c	-(a)	-	-	Pd106.ACE	Pd106.DIR	
176	46-Pd-107	46107.03c	-(a)	ptable	ptable	Pd107.ACE	Pd107.DIR	
177	46-Pd-108	46108.03c	-(a)	-	-	Pd108.ACE	Pd108.DIR	
178	46-Pd-110	46110.03c	-(a)	(c)	ptable	Pd110.ACE	Pd110.DIR	
179	47-Ag-107	47107.03c	-	-	-	Ag107.ACE	Ag107.DIR	
180	47-Ag-109	47109.03c	-(a)	(c)	ptable	Ag109.ACE	Ag109.DIR	
181	47-Ag-110M	47110.03c	ptable	ptable	ptable	Ag110M.ACE	Ag110M.DIR	
182	47-Ag-111	47111.03c	-		ptable	Ag111.ACE	Ag111.DIR	
183	48-Cd-106	48106.03c	ptable	ptable	ptable	Cd106.ACE	Cd106.DIR	
184	48-Cd-108	48108.03c	ptable	ptable	ptable	Cd108.ACE	Cd108.DIR	
185	48-Cd-109	48109.03c	-	-	ptable	Cd109.ACE	Cd109.dir	No in JEFF-3.1.1/2

186	48-Cd-110	48110.03c	ptable	ptable	ptable	Cd110.ACE	Cd110.DIR	
187	48-Cd-111	48111.03c	-	-	ptable	Cd111.ACE	Cd111.DIR	
188	48-Cd-112	48112.03c	ptable	ptable	ptable	Cd112.ACE	Cd112.DIR	
189	48-Cd-113	48113.03c	-	-	ptable	Cd113.ACE	Cd113.DIR	
190	48-Cd-114	48114.03c	ptable	ptable	ptable	Cd114.ACE	Cd114.DIR	
191	48-Cd-115	48115.03c	-	-	ptable	Cd115M.ACE	Cd115M.DIR	No in JEFF-3.1.1/2
192	48-Cd-116	48116.03c	ptable	ptable	ptable	Cd116.ACE	Cd116.DIR	
193	49-In-113	49113.03c	ptable	ptable	ptable	In113.ACE	In113.DIR	
194	49-In-115	49115.03c	ptable	ptable	ptable	In115.ACE	In115.DIR	
195	50-Sn-112	50112.03c	ptable	ptable	ptable	Sn112.ACE	Sn112.DIR	
196	50-Sn-113	50113.03c	-	-	ptable	Sn113.ACE	Sn113.dir	No in JEFF-3.1.1/2
197	50-Sn-114	50114.03c	ptable	ptable	ptable	Sn114.ACE	Sn114.DIR	
198	50-Sn-115	50115.03c	ptable	ptable	ptable	Sn115.ACE	Sn115.DIR	
199	50-Sn-116	50116.03c	ptable	ptable	ptable	Sn116.ACE	Sn116.DIR	
200	50-Sn-117	50117.03c	ptable	ptable	ptable	Sn117.ACE	Sn117.DIR	
201	50-Sn-118	50118.03c	ptable	ptable	ptable	Sn118.ACE	Sn118.DIR	
202	50-Sn-119	50119.03c	ptable	ptable	ptable	Sn119.ACE	Sn119.DIR	
203	50-Sn-120	50120.03c	ptable	ptable	ptable	Sn120.ACE	Sn120.DIR	
204	50-Sn-122	50122.03c	ptable	ptable	ptable	Sn122.ACE	Sn122.DIR	
205	50-Sn-123	50123.03c	-	-	-	Sn123.ACE	Sn123.DIR	
206	50-Sn-124	50124.03c	ptable	ptable	ptable	Sn124.ACE	Sn124.DIR	
207	50-Sn-125	50125.03c	-	-	-	Sn125.ACE	Sn125.DIR	
208	50-Sn-126	50126.03c	-	-	-	Sn126.ACE	Sn126.DIR	
209	51-Sb-121	51121.03c	ptable	ptable	ptable	Sb121.ACE	Sb121.DIR	
210	51-Sb-123	51123.03c	ptable	ptable	ptable	Sb123.ACE	Sb123.DIR	
211	51-Sb-124	51124.03c	-	-	-	Sb124.ACE	Sb124.DIR	
212	51-Sb-125	51125.03c	-	-	-	Sb125.ACE	Sb125.DIR	

213	51-Sb-126	51126.03c	-	-	-	Sb126.ACE	Sb126.DIR	
214	52-Te-120	52120.03c	-	-	-	Te120.ACE	Te120.DIR	
215	52-Te-122	52122.03c	-	-	ptable	Te122.ACE	Te122.DIR	
216	52-Te-123	52123.03c	-	-	-	Te123.ACE	Te123.DIR	
217	52-Te-124	52124.03c	-	-	ptable	Te124.ACE	Te124.DIR	
218	52-Te-125	52125.03c	-	-	-	Te125.ACE	Te125.DIR	
219	52-Te-126	52126.03c	-	-	-	Te126.ACE	Te126.DIR	
220	52-Te-127M	52127.03c	-	-	-	Te127M.ACE	Te127M.DIR	
221	52-Te-128	52128.03c	-	-	-	Te128.ACE	Te128.DIR	
222	52-Te-129M	52129.03c	-	-	-	Te129M.ACE	Te129M.DIR	
223	52-Te-130	52130.03c	-	-	-	Te130.ACE	Te130.DIR	
224	52-Te-131M	52131.03c	-	-	ptable	Te131M.ACE	Te131M.dir	No in JEFF-3.1.1/2
225	52-Te-132	52132.03c	-	-	-	Te132.ACE	Te132.DIR	
226	53-I-126	53126.03c	-	-	ptable	I126.ACE	I126.dir	No in JEFF-3.1.1/2
227	53-I-127	53127.03c	ptable	ptable	ptable	I127.ACE	I127.DIR	
228	53-I-128	53128.03c	-	-	ptable	I128.ACE	I128.dir	No in JEFF-3.1.1/2
229	53-I-129	53129.03c	ptable	ptable	ptable	I129.ACE	I129.DIR	
230	53-I-130	53130.03c	-	-	ptable	I130.ACE	I130.DIR	
231	53-I-131	53131.03c	-	ptable	ptable	I131.ACE	I131.DIR	
232	53-I-135	53135.03c	-	-	-	I135.ACE	I135.DIR	
233	54-Xe-123	54123.03c	-	-	-	Xe123.ACE	Xe123.dir	No in JEFF-3.1.1/2
234	54-Xe-124	54124.03c	-	-	-	Xe124.ACE	Xe124.DIR	
235	54-Xe-126	54126.03c	-	-	-	Xe126.ACE	Xe126.DIR	
236	54-Xe-128	54128.03c	-	ptable	ptable	Xe128.ACE	Xe128.DIR	
237	54-Xe-129	54129.03c	-	ptable	ptable	Xe129.ACE	Xe129.DIR	
238	54-Xe-130	54130.03c	-	-	-	Xe130.ACE	Xe130.DIR	
239	54-Xe-131	54131.03c	-	-	-	Xe131.ACE	Xe131.DIR	

240	54-Xe-132	54132.03c	-	ptable	ptable	Xe132.ACE	Xe132.DIR	
241	54-Xe-133	54133.03c	-	ptable	ptable	Xe133.ACE	Xe133.DIR	
242	54-Xe-134	54134.03c	-	ptable	ptable	Xe134.ACE	Xe134.DIR	
243	54-Xe-135	54135.03c	-	-	-	Xe135.ACE	Xe135.DIR	
244	54-Xe-136	54136.03c	-	-	-	Xe136.ACE	Xe136.DIR	
245	55-Cs-133	55133.03c	ptable	ptable	ptable	Cs133.ACE	Cs133.DIR	
246	55-Cs-134	55134.03c	-		-	Cs134.ACE	Cs134.DIR	
247	55-Cs-135	55135.03c	ptable	ptable	ptable	Cs135.ACE	Cs135.DIR	
248	55-Cs-136	55136.03c	-		-	Cs136.ACE	Cs136.DIR	
249	55-Cs-137	55137.03c	ptable	ptable	ptable	Cs137.ACE	Cs137.DIR	
250	56-Ba-130	56130.03c	ptable	ptable	ptable	Ba130.ACE	Ba130.DIR	
251	56-Ba-132	56132.03c	ptable	ptable	ptable	Ba132.ACE	Ba132.DIR	
252	56-Ba-133	56133.03c	-	-	ptable	Ba133.ACE	Ba133.dir	No in JEFF-3.1.1/2
253	56-Ba-134	56134.03c	ptable	ptable	ptable	Ba134.ACE	Ba134.DIR	
254	56-Ba-135	56135.03c	ptable	ptable	ptable	Ba135.ACE	Ba135.DIR	
255	56-Ba-136	56136.03c	ptable	ptable	ptable	Ba136.ACE	Ba136.DIR	
256	56-Ba-137	56137.03c	ptable	ptable	ptable	Ba137.ACE	Ba137.DIR	
257	56-Ba-138	56138.03c	-	-	-	Ba138.ACE	Ba138.DIR	
258	56-Ba-139	56139.03c	-	-	ptable	Ba139.ACE	Ba139.dir	No in JEFF-3.1.1/2
259	56-Ba-140	56140.03c	ptable	ptable	ptable	Ba140.ACE	Ba140.DIR	
260	57-La-138	57138.03c	ptable	ptable	ptable	La138.ACE	La138.DIR	
261	57-La-139	57139.03c	-(a)	ptable	ptable	La139.ACE	La139.DIR	
262	57-La-140	57140.03c	-		ptable	La140.ACE	La140.DIR	
263	58-Ce-136	58136.03c	-	-	ptable	Ce136.ACE	Ce136.dir	No in JEFF-3.1.1/2
264	58-Ce-138	58138.03c	-	-	ptable	Ce138.ACE	Ce138.dir	No in JEFF-3.1.1/2
265	58-Ce-139	58139.03c	-	-	ptable	Ce139.ACE	Ce139.dir	No in JEFF-3.1.1/2
266	58-Ce-140	58140.03c	-	-	-	Ce140.ACE	Ce140.DIR	

267	58-Ce-141	58141.03c	ptable	(c)	ptable	Ce141.ACE	Ce141.DIR	
268	58-Ce-142	58142.03c	ptable	ptable	ptable	Ce142.ACE	Ce142.DIR	
269	58-Ce-143	58143.03c	-	-	ptable	Ce143.ACE	Ce143.DIR	
270	58-Ce-144	58144.03c	ptable	ptable	ptable	Ce144.ACE	Ce144.DIR	
271	59-Pr-141	59141.03c	-(a)	ptable	ptable	Pr141.ACE	Pr141.DIR	
272	59-Pr-142	59142.03c	-	-	-	Pr142.ACE	Pr142.DIR	
273	59-Pr-143	59143.03c	-	ptable	ptable	Pr143.ACE	Pr143.DIR	
274	60-Nd-142	60142.03c	-	-	-	Nd142.ACE	Nd142.DIR	
275	60-Nd-143	60143.03c	ptable	ptable	ptable	Nd143.ACE	Nd143.DIR	
276	60-Nd-144	60144.03c	-(a)	(c)	ptable	Nd144.ACE	Nd144.DIR	
277	60-Nd-145	60145.03c	-(a)	(c)	ptable	Nd145.ACE	Nd145.DIR	
278	60-Nd-146	60146.03c	-(a)	ptable	ptable	Nd146.ACE	Nd146.DIR	
279	60-Nd-147	60147.03c	-	ptable	ptable	Nd147.ACE	Nd147.DIR	
280	60-Nd-148	60148.03c	-(a)	(c)	ptable	Nd148.ACE	Nd148.DIR	
281	60-Nd-150	60150.03c	-	-	-	Nd150.ACE	Nd150.DIR	
282	61-Pm-147	61147.03c	ptable	ptable	ptable	Pm147.ACE	Pm147.DIR	
283	61-Pm-148M	61148.03c	-	-	-	Pm148M.ACE	Pm148M.DIR	
284	61-Pm-148	61148.03c	ptable	ptable	ptable	Pm148.ACE	Pm148.DIR	
285	61-Pm-149	61149.03c	-	ptable	ptable	Pm149.ACE	Pm149.DIR	
286	61-Pm-151	61151.03c	-	ptable	ptable	Pm151.ACE	Pm151.DIR	
287	62-Sm-144	62144.03c	-	(c)	ptable	Sm144.ACE	Sm144.DIR	
288	62-Sm-147	62147.03c	ptable	(c)	ptable	Sm147.ACE	Sm147.DIR	
289	62-Sm-148	62148.03c	-	ptable	ptable	Sm148.ACE	Sm148.DIR	
290	62-Sm-149	62149.03c	ptable	ptable	ptable	Sm149.ACE	Sm149.DIR	
291	62-Sm-150	62150.03c	-		-	Sm150.ACE	Sm150.DIR	
292	62-Sm-151	62151.03c	ptable	ptable	ptable	Sm151.ACE	Sm151.DIR	
293	62-Sm-152	62152.03c	ptable	(c)	ptable	Sm152.ACE	Sm152.DIR	

294	62-Sm-153	62153.03c	-	ptable	ptable	Sm153.ACE	Sm153.DIR	
295	62-Sm-154	62154.03c	-	ptable	ptable	Sm154.ACE	Sm154.DIR	
296	63-Eu-151	63151.03c	ptable	ptable	ptable	Eu151.ACE	Eu151.DIR	
297	63-Eu-152M	63152.03c	-	-	ptable	Eu152M.ACE	Eu152M.dir	No in JEFF-3.1.1/2
298	63-Eu-152	63152.03c	ptable	ptable	ptable	Eu152.ACE	Eu152.DIR	
299	63-Eu-153	63153.03c	ptable	ptable	ptable	Eu153.ACE	Eu153.DIR	
300	63-Eu-154	63154.03c	ptable	ptable	ptable	Eu154.ACE	Eu154.DIR	
301	63-Eu-155	63155.03c	ptable	ptable	ptable	Eu155.ACE	Eu155.DIR	
302	63-Eu-156	63156.03c	-	ptable	ptable	Eu156.ACE	Eu156.DIR	
303	63-Eu-157	63157.03c	-	ptable	ptable	Eu157.ACE	Eu157.DIR	
304	64-Gd-148	64148.03c	-	-	ptable	Gd148.ACE	Gd148.dir	No in JEFF-3.1.1/2
305	64-Gd-152	64152.03c	ptable	ptable	ptable	Gd152.ACE	Gd152.DIR	
306	64-Gd-153	64153.03c	-	-	ptable	Gd153.ACE	Gd153.dir	No in JEFF-3.1.1/2
307	64-Gd-154	64154.03c	-	-	ptable	Gd154.ACE	Gd154.DIR	
308	64-Gd-155	64155.03c	ptable	ptable	ptable	Gd155.ACE	Gd155.DIR	
309	64-Gd-156	64156.03c	ptable	ptable	ptable	Gd156.ACE	Gd156.DIR	
310	64-Gd-157	64157.03c	-	-	-	Gd157.ACE	Gd157.DIR	
311	64-Gd-158	64158.03c	-	-	-	Gd158.ACE	Gd158.DIR	
312	64-Gd-160	64160.03c	-	-	-	Gd160.ACE	Gd160.DIR	
313	64-Gd-161	64161.03c	-	-	ptable	Gd161.ACE	Gd161.dir	No in JEFF-3.1.1/2
314	65-Tb-159	65159.03c	ptable	ptable	ptable	Tb159.ACE	Tb159.DIR	
315	65-Tb-160	65160.03c	-	-	ptable	Tb160.ACE	Tb160.DIR	
316	66-Dy-156	66156.03c	-	-	ptable	Dy156.ACE	Dy156.dir	No in JEFF-3.1.1/2
317	66-Dy-158	66158.03c	-	-	ptable	Dy158.ACE	Dy158.dir	No in JEFF-3.1.1/2
318	66-Dy-160	66160.03c	-	-	ptable	Dy160.ACE	Dy160.DIR	
319	66-Dy-161	66161.03c	ptable	(c)	ptable	Dy161.ACE	Dy161.DIR	
320	66-Dy-162	66162.03c	ptable	ptable	ptable	Dy162.ACE	Dy162.DIR	

321	66-Dy-163	66163.03c	-	ptable	ptable	Dy163.ACE	Dy163.DIR	
322	66-Dy-164	66164.03c	ptable	ptable	ptable	Dy164.ACE	Dy164.DIR	
323	66-Dy-165	66165.03c	-	-	ptable	Dy165.ACE	Dy165.dir	No in JEFF-3.1.1/2
324	67-Ho-165	67165.03c	-	-	-	Ho165.ACE	Ho165.DIR	
325	67-Ho-166M	67166.03c	-	-	ptable	Ho166M.ACE	Ho166M.dir	No in JEFF-3.1.1/2
326	68-Er-162	68162.03c	-	-	-	Er162.ACE	Er162.DIR	
327	68-Er-164	68164.03c	-	-	-	Er164.ACE	Er164.DIR	
328	68-Er-166	68166.03c	-	-	ptable	Er166.ACE	Er166.DIR	
329	68-Er-167	68167.03c	ptable	ptable	ptable	Er167.ACE	Er167.DIR	
330	68-Er-168	68168.03c	-		ptable	Er168.ACE	Er168.DIR	
331	68-Er-169	68169.03c	-	-	ptable	Er169.ACE	Er169.dir	No in JEFF-3.1.1/2
332	68-Er-170	68170.03c	-	-	ptable	Er170.ACE	Er170.DIR	
333	68-Er-171	68171.03c	-	-	ptable	Er171.ACE	Er171.dir	No in JEFF-3.1.1/2
334	68-Er-172	68172.03c	-	-	ptable	Er172.ACE	Er172.dir	No in JEFF-3.1.1/2
335	69-Tm-169	69169.03c	-	-	ptable	Tm169.ACE	Tm169.dir	No in JEFF-3.1.1/2
336	69-Tm-170	69170.03c	-	-	ptable	Tm170.ACE	Tm170.dir	No in JEFF-3.1.1/2
337	69-Tm-171	69171.03c	-	-	ptable	Tm171.ACE	Tm171.dir	No in JEFF-3.1.1/2
338	70-Yb-168	70168.03c	-	-	ptable	Yb168.ACE	Yb168.dir	No in JEFF-3.1.1/2
339	70-Yb-169	70169.03c	-	-	ptable	Yb169.ACE	Yb169.dir	No in JEFF-3.1.1/2
340	70-Yb-170	70170.03c	-	-	ptable	Yb170.ACE	Yb170.dir	No in JEFF-3.1.1/2
341	70-Yb-171	70171.03c	-	-	ptable	Yb171.ACE	Yb171.dir	No in JEFF-3.1.1/2
342	70-Yb-172	70172.03c	-	-	ptable	Yb172.ACE	Yb172.dir	No in JEFF-3.1.1/2
343	70-Yb-173	70173.03c	-	-	ptable	Yb173.ACE	Yb173.dir	No in JEFF-3.1.1/2
344	70-Yb-174	70174.03c	-	-	ptable	Yb174.ACE	Yb174.dir	No in JEFF-3.1.1/2
345	70-Yb-176	70176.03c	-	-	ptable	Yb176.ACE	Yb176.dir	No in JEFF-3.1.1/2
346	71-Lu-175	71175.03c	ptable	ptable	-	Lu175.ACE	Lu175.DIR	
347	71-Lu-176	71176.03c	ptable	ptable	ptable	Lu176.ACE	Lu176.DIR	

348	71-Lu-177	71177.03c	-	-	ptable	Lu177.ACE	Lu177.dir	No in JEFF-3.1.1/2
349	72-Hf-174	72174.03c	ptable	ptable	ptable	Hf174.ACE	Hf174.DIR	
350	72-Hf-176	72176.03c	ptable	ptable	ptable	Hf176.ACE	Hf176.DIR	
351	72-Hf-177	72177.03c	ptable	ptable	ptable	Hf177.ACE	Hf177.DIR	
352	72-Hf-178	72178.03c	ptable	ptable	ptable	Hf178.ACE	Hf178.DIR	
353	72-Hf-179	72179.03c	ptable	ptable	ptable	Hf179.ACE	Hf179.DIR	
354	72-Hf-180	72180.03c	ptable	ptable	ptable	Hf180.ACE	Hf180.DIR	
355	72-Hf-181	72181.03c	-	-	ptable	Hf181.ACE	Hf181.dir	No in JEFF-3.1.1/2
356	73-Ta-180M	73180.03c	-	-	ptable	Ta180M.ACE	Ta180M.dir	No in JEFF-3.1.1/2
357	73-Ta-181	73181.03c	ptable	ptable	ptable	Ta181.ACE	Ta181.DIR	
358	73-Ta-182	73182.03c	ptable	ptable	ptable	Ta182.ACE	Ta182.DIR	
359	74-W-180	74180.03c	-	-	-	W180.ACE	W180.dir	No in JEFF-3.1.1/2
360	74-W-182	74182.03c	-	-	ptable	W182.ACE	W182.DIR	
361	74-W-183	74183.03c	-	-	ptable	W183.ACE	W183.DIR	
362	74-W-184	74184.03c	-	-	ptable	W184.ACE	W184.DIR	
363	74-W-186	74186.03c	-	-	ptable	W186.ACE	W186.DIR	
364	75-Re-185	75185.03c	ptable	(c)	ptable	Re185.ACE	Re185.DIR	
365	75-Re-187	75187.03c	ptable	(c)	ptable	Re187.ACE	Re187.DIR	
366	75-Re-188	75188.03c	-	-	ptable	Re188.ACE	Re188.dir	No in JEFF-3.1.1/2
367	76-Os-0	76000.03c	-	-	-	Os0.ACE	Os0.DIR	No in JEFF-32T3
368	76-Os-184	76184.03c	-	-	ptable	Os184.ACE	Os184.dir	No in JEFF-3.1.1/2
369	76-Os-186	76186.03c	-	-	ptable	Os186.ACE	Os186.dir	No in JEFF-3.1.1/2
370	76-Os-187	76187.03c	-	-	ptable	Os187.ACE	Os187.dir	No in JEFF-3.1.1/2
371	76-Os-188	76188.03c	-	-	ptable	Os188.ACE	Os188.dir	No in JEFF-3.1.1/2
372	76-Os-189	76189.03c	-	-	ptable	Os189.ACE	Os189.dir	No in JEFF-3.1.1/2
373	76-Os-190	76190.03c	-	-	ptable	Os190.ACE	Os190.dir	No in JEFF-3.1.1/2
374	76-Os-191	76191.03c	-	-	ptable	Os191.ACE	Os191.dir	No in JEFF-3.1.1/2

375	76-Os-192	76192.03c	-	-	ptable	Os192.ACE	Os192.dir	No in JEFF-3.1.1/2
376	76-Os-193	76193.03c	-	-	ptable	Os193.ACE	Os193.dir	No in JEFF-3.1.1/2
377	77-Ir-191	77191.03c	ptable	ptable	-	Ir191.ACE	Ir191.DIR	
378	77-Ir-192	77192.03c	-	-	ptable	Ir192.ACE	Ir192.dir	No in JEFF-3.1.1/2
379	77-Ir-193	77193.03c	ptable	ptable	ptable	Ir193.ACE	Ir193.DIR	
380	78-Pt-0	78000.03c	-	-	-	Pt0.ACE	Pt0.DIR	No in JEFF-32T3
381	78-Pt-190	78190.03c	-	-	ptable	Pt190.ACE	Pt190.dir	No in JEFF-3.1.1/2
382	78-Pt-192	78192.03c	-	-	ptable	Pt192.ACE	Pt192.dir	No in JEFF-3.1.1/2
383	78-Pt-194	78194.03c	-	-	ptable	Pt194.ACE	Pt194.dir	No in JEFF-3.1.1/2
384	78-Pt-195	78195.03c	-	-	ptable	Pt195.ACE	Pt195.dir	No in JEFF-3.1.1/2
385	78-Pt-196	78196.03c	-	-	ptable	Pt196.ACE	Pt196.dir	No in JEFF-3.1.1/2
386	78-Pt-198	78198.03c	-	-	ptable	Pt198.ACE	Pt198.dir	No in JEFF-3.1.1/2
387	79-Au-197	79197.03c	-	-	ptable	Au197.ACE	Au197.DIR	
388	80-Hg-196	80196.03c	-	-	-	Hg196.ACE	Hg196.DIR	
389	80-Hg-198	80198.03c	-	-	-	Hg198.ACE	Hg198.DIR	
390	80-Hg-199	80199.03c	-	-	-	Hg199.ACE	Hg199.DIR	
391	80-Hg-200	80200.03c	-	-	-	Hg200.ACE	Hg200.DIR	
392	80-Hg-201	80201.03c	-	-	-	Hg201.ACE	Hg201.DIR	
393	80-Hg-202	80202.03c	-	-	-	Hg202.ACE	Hg202.DIR	
394	80-Hg-204	80204.03c	-	-	-	Hg204.ACE	Hg204.DIR	
395	81-Tl-0	81000.03c	-	-	-	Tl0.ACE	Tl0.DIR	No in JEFF-32T3
396	81-Tl-203	81203.03c	-	-	ptable	Tl203.ACE	Tl203.dir	No in JEFF-3.1.1/2
397	81-Tl-204	81204.03c	-	-	ptable	Tl204.ACE	Tl204.dir	No in JEFF-3.1.1/2
398	81-Tl-205	81205.03c	-	-	-	Tl205.ACE	Tl205.dir	No in JEFF-3.1.1/2
399	82-Pb-204	82204.03c	-	-	-	Pb204.ACE	Pb204.DIR	
400	82-Pb-205	82205.03c	-	-	-	Pb205.ACE	Pb205.dir	No in JEFF-3.1.1/2
401	82-Pb-206	82206.03c	-	-	-	Pb206.ACE	Pb206.DIR	

402	82-Pb-207	82207.03c	-	-	-	Pb207.ACE	Pb207.DIR	
403	82-Pb-208	82208.03c	-	-	-	Pb208.ACE	Pb208.DIR	
404	83-Bi-209	83209.03c	-	-	-	Bi209.ACE	Bi209.DIR	
405	84-Po-209	84209.03c	-	-	ptable	Po209.ACE	Po209.dir	No in JEFF-3.1.1/2
406	88-Ra-223	88223.03c	-	-	-	Ra223.ACE	Ra223.DIR	
407	88-Ra-224	88224.03c	-	-	-	Ra224.ACE	Ra224.DIR	
408	88-Ra-225	88225.03c	-	-	-	Ra225.ACE	Ra225.DIR	
409	88-Ra-226	88226.03c	-	-	-	Ra226.ACE	Ra226.DIR	
410	89-Ac-225	89225.03c	-	-	-	Ac225.ACE	Ac225.DIR	
411	89-Ac-226	89226.03c	-	-	-	Ac226.ACE	Ac226.DIR	
412	89-Ac-227	89227.03c	-	-	-	Ac227.ACE	Ac227.DIR	
413	90-Th-227	90227.03c	-	-	-	Th227.ACE	Th227.DIR	
414	90-Th-228	90228.03c	-	-	-	Th228.ACE	Th228.DIR	
415	90-Th-229	90229.03c	-	-	-	Th229.ACE	Th229.DIR	
416	90-Th-230	90230.03c	-	-	-	Th230.ACE	Th230.DIR	
417	90-Th-232	90232.03c	ptable	ptable	ptable	Th232.ACE	Th232.DIR	
418	90-Th-233	90233.03c	-	-	-	Th233.ACE	Th233.DIR	
419	90-Th-234	90234.03c	-	-	-	Th234.ACE	Th234.DIR	
420	91-Pa-231	91231.03c	ptable	ptable	ptable	Pa231.ACE	Pa231.DIR	
421	91-Pa-232	91232.03c	-	-	ptable	Pa232.ACE	Pa232.DIR	
422	91-Pa-233	91233.03c	ptable	ptable	ptable	Pa233.ACE	Pa233.DIR	
423	92-U-232	92232.03c	ptable	ptable	ptable	U232.ACE	U232.DIR	
424	92-U-233	92233.03c	ptable	ptable	ptable	U233.ACE	U233.DIR	
425	92-U-234	92234.03c	ptable	ptable	ptable	U234.ACE	U234.DIR	
426	92-U-235	92235.03c	ptable	(c)	ptable	U235.ACE	U235.DIR	
427	92-U-236	92236.03c	-	-	-	U236.ACE	U236.DIR	
428	92-U-237	92237.03c	ptable	ptable	ptable	U237.ACE	U237.DIR	

429	92-U-238	92238.03c	ptable	ptable	ptable	U238.ACE	U238.DIR	
430	92-U-239	92239.03c	-	-	ptable	U239.ACE	U239.dir	No in JEFF-3.1.1/2
431	92-U-240	92240.03c	-	-	ptable	U240.ACE	U240.dir	No in JEFF-3.1.1/2
432	92-U-241	92241.03c	-	-	ptable	U241.ACE	U241.dir	No in JEFF-3.1.1/2
433	93-Np-235	93235.03c	-	-	-	Np235.ACE	Np235.DIR	
434	93-Np-236	93236.03c	-	-	-	Np236.ACE	Np236.DIR	
435	93-Np-237	93237.03c	-(a)	-	-	Np237.ACE	Np237.DIR	
436	93-Np-238	93238.03c	-(a)	(c)	ptable	Np238.ACE	Np238.DIR	
437	93-Np-239	93239.03c	-	-	-	Np239.ACE	Np239.DIR	
438	94-Pu-236	94236.03c	ptable	ptable	ptable	Pu236.ACE	Pu236.DIR	
439	94-Pu-237	94237.03c	-	-	-	Pu237.ACE	Pu237.DIR	
440	94-Pu-238	94238.03c	ptable	(d)	(d)	Pu238.ACE	Pu238.DIR	
441	94-Pu-239	94239.03c	ptable	ptable	ptable	Pu239.ACE	Pu239.DIR	
442	94-Pu-240	94240.03c	ptable	(c)	ptable	Pu240.ACE	Pu240.DIR	
443	94-Pu-241	94241.03c	ptable	ptable	ptable	Pu241.ACE	Pu241.DIR	
444	94-Pu-242	94242.03c	ptable	ptable	ptable	Pu242.ACE	Pu242.DIR	
445	94-Pu-243	94243.03c	ptable	(c)	ptable	Pu243.ACE	Pu243.DIR	
446	94-Pu-244	94244.03c	ptable	ptable	ptable	Pu244.ACE	Pu244.DIR	
447	94-Pu-246	94246.03c	-		-	Pu246.ACE	Pu246.DIR	
448	95-Am-241	95241.03c	ptable	(c)	ptable	Am241.ACE	Am241.DIR	
449	95-Am-242M	95242.03c	ptable	ptable	ptable	Am242M.ACE	Am242M.DIR	
450	95-Am-242	95242.03c	ptable	ptable	ptable	Am242G.ACE	Am242G.DIR	
451	95-Am-243	95243.03c	ptable	ptable	ptable	Am243.ACE	Am243.DIR	
452	95-Am-244M	95244.03c	-	-	-	Am244M.ACE	Am244M.DIR	
453	95-Am-244	95244.03c	-	-	-	Am244.ACE	Am244.DIR	
454	96-Cm-240	96240.03c	ptable	ptable	-	Cm240.ACE	Cm240.DIR	
455	96-Cm-241	96241.03c	-	-	-	Cm241.ACE	Cm241.DIR	

456	96-Cm-242	96242.03c	ptable	ptable	ptable	Cm242.ACE	Cm242.DIR	
457	96-Cm-243	96243.03c	ptable	ptable	ptable	Cm243.ACE	Cm243.DIR	
458	96-Cm-244	96244.03c	ptable	ptable	ptable	Cm244.ACE	Cm244.DIR	
459	96-Cm-245	96245.03c	ptable	ptable	ptable	Cm245.ACE	Cm245.DIR	
460	96-Cm-246	96246.03c	ptable	ptable	ptable	Cm246.ACE	Cm246.DIR	
461	96-Cm-247	96247.03c	ptable	ptable	ptable	Cm247.ACE	Cm247.DIR	
462	96-Cm-248	96248.03c	ptable	ptable	ptable	Cm248.ACE	Cm248.DIR	
463	96-Cm-249	96249.03c	ptable	ptable	-	Cm249.ACE	Cm249.DIR	
464	96-Cm-250	96250.03c	ptable	ptable	ptable	Cm250.ACE	Cm250.DIR	
465	97-Bk-247	97247.03c	-	-	-	Bk247.ACE	Bk247.DIR	
466	97-Bk-249	97249.03c	ptable	ptable	ptable	Bk249.ACE	Bk249.DIR	
467	97-Bk-250	97250.03c	ptable	ptable	ptable	Bk250.ACE	Bk250.DIR	
468	98-Cf-249	98249.03c	ptable	ptable	ptable	Cf249.ACE	Cf249.DIR	
469	98-Cf-250	98250.03c	ptable	(c)	ptable	Cf250.ACE	Cf250.DIR	
470	98-Cf-251	98251.03c	ptable	(c)	ptable	Cf251.ACE	Cf251.DIR	
471	98-Cf-252	98252.03c	-(a)	(c)	ptable	Cf252.ACE	Cf252.DIR	
472	98-Cf-253	98253.03c	-	-	-	Cf253.ACE	Cf253.dir	No in JEFF-3.1.1/2
473	98-Cf-254	98254.03c	-	-	-	Cf254.ACE	Cf254.DIR	
474	99-Es-253	99253.03c	-(a)	(c)	ptable	Es253.ACE	Es253.DIR	
475	99-Es-254	99254.03c	-	-	-	Es254.ACE	Es254.DIR	
476	99-Es-255	99255.03c	-	-	-	Es255.ACE	Es255.DIR	
477	100-Fm-255	100255.03c	-	-	-	Fm255.ACE	Fm255.DIR	

(a) Originally, JEFF3.1.1 includes *ptable* option, but it was been eliminated according section 2.3.2.

(c) JEFF3.1.2 includes *ptable* option with some problems according section 2.3.2. This work recommends to use these PTABLES, but it should be revised in future evaluations.

(d) This table has been eliminated due to problems in MCNP code.

(e) This table has been eliminated in JEFF-3.2T3 due to problems in PURR processing.

JEFF-3.2T3 contains some isotopes in ground and isomeric states (see Table 2). These isotopes are processed using the same procedure to obtain “.ace” and “.dir” files.

Table 2. Isotopes in isomeric state (library at 293.6K).

No.	Nuclide	ZAID	JEFF-32T3	ACE filename	XSDIR filename	Comment
1	27-Co-58	27058.03c	-	Co58M.ACE	Co58M.DIR	
2	47-Ag-110M	47110.03c	ptable	Ag110M.ACE	Ag110M.DIR	
3	48-Cd-115	48115.03c	ptable	Cd115M.ACE	Cd115M.DIR	NEW in JEFF-32T3
4	52-Te-127M	52127.03c	-	Te127M.ACE	Te127M.DIR	
5	52-Te-129M	52129.03c	-	Te129M.ACE	Te129M.DIR	
6	52-Te-131M	52131.03c	ptable	Te131M.ACE	Te131M.dir	NEW in JEFF-32T3
7	61-Pm-148M	61148.03c	-	Pm148M.ACE	Pm148M.DIR	
8	63-Eu-152M	63152.03c	ptable	Eu152M.ACE	Eu152M.dir	NEW in JEFF-32T3
9	67-Ho-166M	67166.03c	ptable	Ho166M.ACE	Ho166M.dir	NEW in JEFF-32T3
10	73-Ta-180M	73180.03c	ptable	Ta180M.ACE	Ta180M.dir	NEW in JEFF-32T3
11	95-Am-242M	95242.03c	ptable	Am242M.ACE	Am242M.DIR	
12	95-Am-244M	95244.03c	-	Am244M.ACE	Am244M.DIR	

2.6 Processing a multi-temperature ACE format

A multi-temperature ACE-format neutron library for a wide range of up to ten temperatures depending on the application needs: 293.6, 300, 400, 500, 600, 700, 800, 900, 1000, 1200, 1500 and 1800 degrees Kelvin.

General format is <MAT>.<ZAID>, where ZAID is given in Table 3, and MAT is =h1 for hydrogen, h2 for deuterium, h3 for tritium... Fe56 for iron-56 ... etc ...

Table 3. Multi-temperature ACE library

#	Temperature (K)	ZAID suffix
0	293.6	.03c
1	300	.03c
2	400	.04c
3	500	.05c
4	600	.06c
5	700	.07c
6	800	.08c
7	900	.09c
8	1000	.10c
9	1200	.12c
10	1500	.15c
11	1800	.18c

See ANNEX 6.2 for the complete information of multi-temperature ACE format.

2.7 Processing Scattering Thermal Libraries in ACE format

Several *Scattering Thermal Libraries* (STL) have been processed using special NJOY inputs. **[NDC(NDS)-0470]**

Figure 4. NJOY input to generate ACE Thermal Scattering library for H bound in CH₂.

```
moder / Extract thermal Scattering Law
1 -61
' H-CH2      from JEFF3.1.1'/
60 37
0/
moder / Extract/convert neutron evaluated data
1 -21
'1-H-1 from JEFF3.2'/
20 125
0/
reconr / Reconstruct XS for neutrons
-21 -22
'JEFF3.2 PENDF for 1-H-1'/
125 2/
0.001 0. 0.001/ err tempr errmax
'JEFF3.2: 1-H-1 from JEFF-3.2'/
'Processed by NJOY99.364,NEA_JUL2013'/
0/
broadr / Doppler broaden XS
-21 -22 -23
125 1 0 0 0./
0.001 2.0e+6 0.001/ errthn thnmax errmax
293.6
0/
thermr / Add thermal scattering data (free gas)
0 -23 -62
0 125 12 1 1 11 1 221 1/
293.6
0.001 4.0
thermr / Add thermal scattering data (bound)
-61 -62 -27
37 125 16 1 4 11 2 223 1/
293.6
0.001 4.0
acer / Prepare ACE files
-21 -27 0 28 29
2 0 1 .32/
'H-CH2      293.6 K from (JEFF-3.2) NJOY99.364, NEA_JUL2013'/
125 293.6 'pol00 ' /
1001      0      0 /
223 64 224 1 1 4.0 0/
acer / Check ACE files
0 28 0 71 81
7 1 1 -1/
/
stop
```

For hydrogen bound in polyethylene:

Type of ACER run option	IOPT: 2 (THERMAL DATA)
Print control	IPRINT: 0 (MINIMUM)
ACE output type	NTYPE: 1
ID suffix for ZAID	SUFF: .32
Material to be processed	MATD: 125
Temperature desired	NTEMPD: 293.6K
Thermal ZAID name	TNAME: 'pol00'
MT for thermal incoherent data*	MTI: 223
Number of bins for incoherent scattering ⁺	NBINT: 64
MT for thermal elastic data*	MTE: 224
COHERENT/INCOHERENT ELASTIC	IELAS 0/1
Number of atom types in mixed moderator	NMIX: 2
Max. energy ⁺	EMAX: 4.0 eV
Weight option	IWT: 0/1 VARIABLE/CONSTANT

* MTI and MTE values from Table 3 included in section XVII-22 (ACER module) in NJOY manual.

+ Private communication, M.Mattes, IKE.

Table 4. Temperatures for Thermal Scattering Libraries.

* Beryllium	- Thermal Neutron Scattering Law Data in MF=7	* 26 1451	17
*	T=293.6 400 500 600 700 800 1000 1200 K	* 26 1451	19
Graphite IKE	EVAL-JAN05 Keinert, Mattes	31 1451	5
* Temperatures (K) =	293.6, 400, 500, 600, 700, 800, 1000,	* 31 1451	17
*	1200, 1600, 2000, 3000	* 31 1451	18
D(D2O) IKE	EVAL-FEB04 Keinert, Mattes	11 1451	5
* Temperatures:	293.6 323.6 373.6 423.6 473.6 523.6 573.6 643.9 K	* 11 1451	17
H(ZrH) IKE	EVAL-JAN05 Keinert	7 1451	5
* TEMPERATURES =	293.6 400 500 600 700 800 1000 1200 DEG K.	* 7 1451	16
H(H2O) IKE	EVAL-JAN04 Keinert, Mattes	1 1451	5
* Temperatures (K)=	293.6 323.6 373.6 423.6 473.6 523.6	* 1 1451	17
*	573.6 623.6 647.2 800 1000	* 1 1451	18
* Polyethylene	- Thermal Neutron Scattering Law Data in MF=7	* 37 1451	22
* H (CH2)	are given for the temperatures	* 37 1451	23
*	T= 293.6 and 350 K	* 37 1451	24
H(CaH2) CEA, ILL	EVAL-OCT04 O.SEROT CEA Cadarache	8 1451	5
Temperatures =	296. 400. 500. 600. 700. 800. 1000. 1200. K.	8 1451	16
Ca(CaH2) CEA, ILL	EVAL-OCT04 O.SEROT CEA Cadarache	59 1451	5
Temperatures =	296. 400. 500. 600. 700. 800. 1000. 1200. K.	59 1451	16
24-Mg CEA	EVAL-SEP03 C.MOUNIER	52 1451	5
TEMPERATURES =	20 100 296 773 DEG K.	52 1451	16

To identify these libraries a label is defined for each isotope, see Table 2.5.

Table 5. Information on the JEFF-3.2T3 Thermal Scattering ACE library at 293.6K.

No.	Nuclide	ZAID	ACE filename	XSDIR filename
1	pol00.32t	Hydrogen bound in polyethylene	CH2-293.ace	CH2-293.dir
2	lw00.32t	Hydrogen bound in water	H2O-293.ace	H2O-293.dir
3	h zr00.32t	Hydrogen bound in ZrH	HZr-293.ace	HZr-293.dir
4	gra00.32t	Graphite	Gra-293.ace	Gra-293.dir
5	hw00.32t	D bound in D2O	D2O-293.ace	D2O-293.dir
6	be00.32t	Be	Be-293.ace	Be-293.dir
7	beo00.32t	Be in BeO	BeO-293.ace	BeO-293.ace
8	mg00.32t	Mg-24	Mg-20.ace	Mg-20.dir
9	hca00.32t	H in CaH2	H-CaH2-296.ace	H-CaH2-296.dir
10	cah00.32t	Ca in CaH2	Ca-CaH2-296.ace	Ca-CaH2-296.dir

To take into account different temperatures in the STLs, the identification format will change according: “<mm><xx>.32t”, where <mm>=lw, pol, h zr, ... is the the associated identification to material, and <xx>=00,01,02,03, ..., is the associated identification to temperature given in Table 6.

See ANNEX 6.3 for the complete information of multi-temperature STLs in ACE format.

Table 6. Information on the JEFF-3.2 Thermal Scattering ACE library at different temperatures

Temp (K)	Hydrogen bound in water	Hydrogen bound in polyethylene	Hydrogen bound in ZrH	Graphite	D bound in D2O	Be	Mg	Hydrogen in CaH2	Ca in CaH2
20.0							mg00.32t		
100.0							mg01.32t		
293.6	lw00.32t	pol00.32t	h zr00.32t	gr00.32t	hw00.32t	be00.32t			
296							mg02.32t	hca00.32t	cah00.32t
323	lw01.32t				hw01.32t				
350		pol01.32t							
373	lw02.32t				hw02.32t				
400			h zr01.32t	gr01.32t		be01.32t		hca01.32t	cah01.32t
423	lw03.32t				hw03.32t				
473	lw04.32t				hw04.32t				
500			h zr02.32t	gr02.32t		be02.32t		hca02.32t	cah02.32t
523	lw05.32t				hw05.32t				
573	lw06.32t				hw06.32t				
600			h zr03.32t	gr03.32t		be03.32t		hca03.32t	cah03.32t
623	lw07.32t								
643					hw07.32t				
647	lw08.32t								
700			h zr04.32t	gr04.32t		be04.32t		hca04.32t	cah04.32t
773							mg04.32t		
800	lw09.32t		h zr05.32t	gr05.32t		be05.32t		hca05.32t	cah05.32t
1000	lw10.32t		h zr06.32t	gr06.32t		be06.32t		hca06.32t	cah06.32t
1200			h zr07.32t	gr07.32t		be07.32t		hca07.32t	cah07.32t
1600				gr08.32t					
2000				gr09.32t					
3000				gr10.32t					

ACER (thermal scattering libraries)

- For hydrogen bound in polyethylene

```
acer / Prepare ACE files
-21 -27 0 28 29
2 0 1 .32/
'H-CH2    293.6 K from (JEFF-3.2) NJOY99.364, NEA_JUL2013' /
125 293.6 'pol00 ' /
1001      0      0 /
223 64 224 1 1 4.0 0/
```

- For hydrogen bound in water

```
acer / Prepare ACE files
-21 -27 0 28 29
2 0 1 .32/
'H-H2O    293.6 K from (JEFF-3.2) NJOY99.364, NEA_JUL2013' /
125 293.6 'lw00 ' /
1001      0      0 /
222 64 0 0 1 4.0 0/
```

- For hydrogen bound in ZrH

```
acer / Prepare ACE files
-21 -27 0 28 29
2 0 1 .32/
'H-ZrH    293.6 K from (JEFF-3.2) NJOY99.364, NEA_JUL2013' /
125 293.6 'h zr00 ' /
1001      0      0 /
225 64 226 1 1 4.0 0/
```

- Graphite

```
acer / Prepare ACE files
-21 -27 0 28 29
2 0 1 .32/
'Graphi   293.6 K from (JEFF-3.2) NJOY99.364, NEA_JUL2013' /
600 293.6 'gr00 ' /
6000      0      0 /
229 64 230 0 1 4.0 0/
```

- For D bound in D2O

```
acer / Prepare ACE files
-21 -27 0 28 29
2 0 1 .32/
'D-D2O    293.6 K from (JEFF-3.2) NJOY99.364, NEA_JUL2013' /
128 293.6 'hw00 ' /
1002      0      0 /
228 64 0 0 1 4.0 0/
```

- For Be

```
acer / Prepare ACE files
-21 -27 0 28 29
2 0 1 .32/
'4-Be      293.6 K from (JEFF-3.2) NJOY99.364, NEA_JUL2013'/
425 293.6 'be00 ' /
  4009      0      0 /
  231 64 232  0  1 4.0 0/
```

- For Mg

```
acer / Prepare ACE files
-21 -27 0 28 29
2 0 1 .32/
'24-Mg     20.0 K from (JEFF-3.2) NJOY99.364, NEA_JUL2013'/
1225 20.0 'mg01 ' /
12024      0      0 /
  249 64 250  1  1 4.0 0/
```

- For Hydrogen in CaH2

```
acer / Prepare ACE files
-21 -27 0 28 29
2 0 1 .32/
'H-CaH2    296.0 K from (JEFF-3.2) NJOY99.364, NEA_JUL2013'/
125 296.0 'hca01 ' /
  1001      0      0 /
  249 64 250  1  1 4.0 0/
```

- For Ca in CaH2

```
acer / Prepare ACE files
-21 -27 0 28 29
2 0 1 .32/
'Ca-CaH2   296.0 K from (JEFF-3.2) NJOY99.364, NEA_JUL2013'/
2025 296.0 'cah01 ' /
20040      0      0 /
  249 64 250  1  1 4.0 0/
```

2.8 Processing JEFF-3.2T3 in BOXER format

JEFF-3.2T3 has been processed using ERRORR/COVR NJOY modules. Table 7 shows covariance data to be processed.

Table 7. List of 220 isotopes with uncertainty information (MF31,..., MF40)

MAT	MF31 17 cases	MF32/33 218 cases	MF34 157 cases	MF35 3 cases	MF40 137 cases
Am241					X
Ar39		X	X		X
Ar41		X	X		X
As75		X	X		X
Au197		X			
B10		X			
B11		X			
Ba133		X	X		X
Ba139		X	X		X
Be9		X			
Bi209		X			
Br79		X	X		X
Br81		X	X		X
C0		X			
C13		X	X		
Ca41		X	X		X
Ca45		X	X		
Cd109		X	X		X
Ce136		X	X		X
Ce138		X	X		X
Ce139		X	X		X
Ce143	X	X	X	X	X
Cf253		X	X		
Cl36		X	X		X
Cm240	X	X			
Cm241	X	X			
Cm242	X	X			
Cm243	X	X			
Cm244	X	X			
Cm245	X	X			
Cm246	X	X			
Cm247	X	X			
Cm248	X	X			

Cm249	X	X			
Cm250	X	X			
Co57		X	X		X
Co59		X			
Co60		X	X		X
Cr50		X			X
Cr51		X	X		X
Cr52		X			
Cr53		X			X
Cr54		X			X
Cu63		X			
Cu64		X	X		X
Cu65		X			
Cu66		X	X		X
Dy156		X	X		
Dy158		X	X		X
Dy160		X	X		X
Dy165		X	X		X
Er166		X	X		X
Er167		X	X		X
Er168		X	X		X
Er169		X	X		X
Er170		X	X		X
Er171		X	X		X
Er172		X	X		X
Eu152M		X	X		X
F19		X			
Fe54		X			
Fe56		X	X		
Fe57		X			
Fe58		X			
Ga69		X	X		X
Ga71		X	X		X
Gd148		X	X		X
Gd152		X			
Gd153		X	X		X
Gd154		X			
Gd161		X	X		
Ge70		X	X		
Ge72		X	X		X
Ge73		X	X		X

Ge74		X	X		X
Ge76		X	X		X
H1		X			
Hf181		X	X		X
Ho166M		X	X		X
I126		X	X		X
I128		X	X		X
Ir191		X			
Ir192		X	X		X
K39		X	X		X
K40		X	X		X
K41		X	X		X
Kr78		X	X		X
Kr80		X	X		X
Kr82		X	X		X
Kr83		X	X		X
Kr84		X	X		X
Kr85		X	X		X
Kr86		X	X		X
La138		X	X		X
La140		X	X		X
Li6		X			
Lu175		X	X		X
Lu176		X	X		X
Lu177		X	X		X
Mg27		X	X		
Mn53		X	X		X
Mn54		X	X		X
Mn55		X			
N15		X			
Na23		X			
Nb93					X
Ne20		X	X		
Ne21		X	X		
Ne22		X	X		
Ni58		X	X		
Ni60		X	X		
Ni61		X	X		
Ni62		X			
Ni63		X			X
Ni64		X			

O17		X	X		
O18		X	X		
Os184		X	X		X
Os186		X	X		X
Os187		X	X		X
Os188		X	X		X
Os189		X	X		X
Os190		X	X		X
Os191		X	X		X
Os192		X	X		X
Os193		X	X		X
P31		X	X		X
Pa232	X	X	X	X	
Pb204		X			
Pb205		X			
Pb206		X			
Pb207		X			
Pb208		X			
Po209		X	X		X
Pt190		X	X		
Pt192		X	X		X
Pt194		X	X		X
Pt195		X	X		X
Pt196		X	X		X
Pt198		X	X		X
Rb85		X	X		X
Rb86		X	X		X
Rb87		X	X		X
Rb88		X	X		X
Re185		X	X		X
Re187		X	X		X
Re188		X	X		X
Rh104		X	X		X
S32		X	X		
S33		X	X		
S34		X	X		
S36		X	X		
Sc46		X	X		X
Se74		X	X		X
Se76		X	X		X
Se77		X	X		X

Se78		X	X		X
Se79		X	X		X
Se80		X	X		X
Se82		X	X		X
Si28		X			
Si29		X			
Si30		X			
Si31		X	X		
Si32		X	X		
Sn122		X	X		X
Sn124		X	X		X
Sr84		X	X		X
Sr86		X	X		X
Sr87		X	X		X
Sr88		X	X		X
Sr89		X	X		X
Sr90		X	X		X
Ta180M		X	X		X
Tb160		X	X		X
Tc98		X	X		X
Te122		X	X		X
Te124		X	X		X
Te131M		X	X		X
Th232	X	X	X		
Ti46		X			
Ti47		X			
Ti48		X			
Ti49		X			
Ti50		X			
Tl203		X			X
Tl204		X			X
Tl205		X	X		X
Tm169		X	X		X
Tm170		X	X		X
Tm171		X	X		X
U232	X	X	X	X	
U233	X	X			
U234	X	X			
U238		X			
V0		X			
V49		X	X		X

W182		X			
W183		X			
W184		X			
W186		X			
Y89		X			
Y90		X	X		X
Y91		X	X		X
Yb168		X	X		X
Yb169		X	X		X
Yb170		X	X		X
Yb171		X	X		X
Yb172		X	X		X
Yb173		X	X		X
Yb174		X	X		X
Yb176		X	X		X
Zn64		X	X		X
Zn66		X	X		X
Zn67		X	X		X
Zn68		X	X		X
Zn70		X	X		X
Zr90		X	X		X
Zr92		X	X		X
Zr94		X	X		X

However, some problems when processing MF31,...MF40 files with NJOY99.364 have been identified. Table 8 shows a list of errors.

Table 8. List of 141 isotopes in JEFF-3.2T3 with problems to process covariance data with NJOY99.393.

MAT	Problem in MF33	Problem in MF34	Problem in MF40
Ar39			***error in grid***illegal mt1=0.
Ar41			***error in grid***illegal mt1=0.
As75	Stop in ERRORR		***error in grid***illegal mt1=0.
Ba133			***error in grid***illegal mt1=0.
Ba139			***error in grid***illegal mt1=0.
Be9	ERRORR: ***error in errorr***illegal mt gt 870		
Br79			***error in grid***illegal mt1=0.
Br81			***error in grid***illegal mt1=0.

Ca41			***error in covcal***
Cd109			***error in grid***illegal mt1=0.
Ce136			***error in grid***illegal mt1=0.
Ce138			***error in grid***illegal mt1=0.
Ce139			***error in grid***illegal mt1=0.
Ce143	Stop in ERRORR		***error in grid***illegal mt1=0.
Cl36			***error in covcal***
Co57			***error in grid***illegal mt1=0.
Co60			***error in grid***illegal mt1=0.
Cr50			***error in grid***illegal mt1=0.
Cr51			***error in grid***illegal mt1=0.
Cr53			***error in grid***illegal mt1=0.
Cr54			***error in grid***illegal mt1=0.
Cu64			***error in grid***illegal mt1=0.
Cu66			***error in grid***illegal mt1=0.
Dy158			***error in grid***illegal mt1=0.
Dy160			***error in grid***illegal mt1=0.
Dy165			***error in grid***illegal mt1=0.
Er166			***error in grid***illegal mt1=0.
Er167			***error in grid***illegal mt1=0.
Er168			***error in grid***illegal mt1=0.
Er169			***error in grid***illegal mt1=0.
Er170			***error in grid***illegal mt1=0.
Er171			***error in grid***illegal mt1=0.
Er172			***error in grid***illegal mt1=0.
Eu152M		null covariance matrix	***error in grid***illegal mt1=0.
Ga69	Stop in ERRORR		***error in grid***illegal mt1=0.
Ga71	Stop in ERRORR		***error in grid***illegal mt1=0.
Gd148			***error in grid***illegal mt1=0.
Gd152	ERRORR: --- message from resprx_rrr_lcomp12- --no scattering radius uncertainty		
Gd153			***error in grid***illegal mt1=0.
Gd154	ERRORR: '--- message from resprx_rrr_lcomp12- --no scattering radius uncertainty		
Ge72			***error in grid***illegal mt1=0.
Ge73			***error in grid***illegal mt1=0.
Ge74			***error in grid***illegal mt1=0.
Ge76			***error in grid***illegal mt1=0.

Hf181			***error in grid***illegal mt1=0.
Ho166M		null covariance matrix	***error in grid***illegal mt1=0.
I126			***error in grid***illegal mt1=0.
I128			***error in grid***
Ir192			***error in grid***
K39			***error in grid***illegal mt1=0.
K40			***error in grid***illegal mt1=0.
K41			***error in grid***illegal mt1=0.
Kr78			***error in grid***illegal mt1=0.
Kr80			***error in grid***illegal mt1=0.
Kr82			***error in grid***illegal mt1=0.
Kr83	Stop in COVR		***error in grid***illegal mt1=0.
Kr84	COVR: ***error in press***matrix not symmetric		***error in grid***illegal mt1=0.
Kr85	Stop in COVR		***error in grid***illegal mt1=0.
Kr86			***error in grid***illegal mt1=0.
La138	Stop in COVR		***error in grid***illegal mt1=0.
La140	Stop in COVR		***error in grid***illegal mt1=0.
Lu175			***error in grid***illegal mt1=0.
Lu176			***error in grid***illegal mt1=0.
Lu177			***error in grid***illegal mt1=0.
Mn53			***error in grid***illegal mt1=0.
Mn54			***error in covcal***
Ni63			***error in grid***illegal mt1=0.
Os184			***error in grid***illegal mt1=0.
Os186			***error in grid***illegal mt1=0.
Os187			***error in grid***illegal mt1=0.
Os188	COVR: ***error in press***matrix not symmetric		***error in grid***illegal mt1=0.
Os189			***error in grid***illegal mt1=0.
Os190			***error in grid***illegal mt1=0.
Os191			***error in grid***illegal mt1=0.
Os192			***error in grid***illegal mt1=0.
Os193			***error in grid***illegal mt1=0.
P31			***error in covcal***
Pb206	ERRORR: --- message from resprx_rrr_lcomp12- --no scattering radius uncertainty		

Pb207	ERRORR: --- message from resprx_rrr_lcomp12- --no scattering radius uncertainty		
Po209			***error in grid***illegal mt1=0.
Pt192			***error in grid***illegal mt1=0.
Pt194			***error in grid***illegal mt1=0.
Pt195			***error in grid***illegal mt1=0.
Pt196			***error in grid***illegal mt1=0.
Pt198			***error in grid***illegal mt1=0.
Rb85			***error in grid***illegal mt1=0.
Rb86			***error in grid***illegal mt1=0.
Rb87	Stop in ERRORR		***error in grid***illegal mt1=0.
Rb88			***error in grid***illegal mt1=0.
Re185			***error in grid***illegal mt1=0.
Re187			***error in grid***illegal mt1=0.
Re188			***error in grid***illegal mt1=0.
Rh104	ERRORR: ***error in resprx***number of pointwise xsec of resonance exceeded. please increase the maxe parameter.		***error in grid***illegal mt1=0.
Sc46			***error in grid***illegal mt1=0.
Se74			***error in grid***illegal mt1=0.
Se76			***error in grid***illegal mt1=0.
Se77			***error in grid***illegal mt1=0.
Se78			***error in grid***illegal mt1=0.
Se79			***error in grid***illegal mt1=0.
Se80			***error in grid***illegal mt1=0.
Se82			***error in grid***illegal mt1=0.
Si28	ERRORR: ***error in findex***id lmt not defined		
Sn122			***error in grid***illegal mt1=0.
Sn124			***error in grid***illegal mt1=0.
Sr84			***error in grid***illegal mt1=0.
Sr86			***error in grid***illegal mt1=0.
Sr87			***error in grid***illegal mt1=0.
Sr88			***error in grid***illegal mt1=0.
Sr89			***error in grid***illegal mt1=0.
Sr90			***error in grid***illegal mt1=0.

Ta180M	COVR: ***error in press***matrix not symmetric	null covariance matrix	***error in grid***illegal mt1=0.
Tb160			***error in grid***illegal mt1=0.
Tc98			***error in grid***illegal mt1=0.
Te122			***error in grid***illegal mt1=0.
Te124			***error in grid***illegal mt1=0.
Te131M		null covariance matrix	***error in grid***illegal mt1=0.
Th232		***error in gridd*** (This problem has been reported to A.Trkov as evaluator)	
Tl203			***error in grid***illegal mt1=0.
Tl205			***error in grid***illegal mt1=0.
Tm169			***error in grid***illegal mt1=0.
Tm170			***error in grid***illegal mt1=0.
Tm171			***error in grid***illegal mt1=0.
V49			***error in grid***illegal mt1=0.
Y90			***error in grid***illegal mt1=0.
Y91			***error in grid***illegal mt1=0.
Yb168			***error in grid***illegal mt1=0.
Yb169			***error in grid***illegal mt1=0.
Yb170			***error in grid***illegal mt1=0.
Yb171			***error in grid***illegal mt1=0.
Yb172			***error in grid***illegal mt1=0.
Yb173			***error in grid***illegal mt1=0.
Yb174	COVR: ***error in press***matrix not symmetric		***error in grid***illegal mt1=0.
Yb176			***error in grid***illegal mt1=0.
Zn64			***error in grid***illegal mt1=0.
Zn66			***error in grid***illegal mt1=0.
Zn67			***error in grid***illegal mt1=0.
Zn68			***error in grid***illegal mt1=0.
Zn70			***error in grid***illegal mt1=0.
Zr90			***error in grid***illegal mt1=0.
Zr92			***error in grid***illegal mt1=0.
Zr94			***error in grid***illegal mt1=0.

2.8.1 Problems in Nb-93 processing MF40

According with the problem found in the processing of Nb-93 in JEFF-3.2, it has been solved:

- Updating NJOY with uposc5

```
*ident uposc5
*/ groupr -- nov2011
*/ - processing JEFF-3.1.2 with VDF6.6A in WindowsXP
*i up347.64
      if (mfd.gt.100000000) lfs=mod(mfd,10)
```

- Updating: JEFF32T3N4125.ASC

Original File

```
...
...
4.109300+4 9.210510+1      0      0      1      4125 0 0 0
0.000000+0-3.082000+4      0      1      0      0412540 4 1
1.000000+1 1.000000+0      0      4      0      1412540 4 2
0.000000+0 0.000000+0      1      5      528      1412540 4 3
0.000000+0 0.000000+0      1      5      528      32412540 4 4
1.000000-5 4.000000+4 5.000000+4 6.000000+4 8.000000+4 1.000000+5412540 4 5
1.500000+5 2.000000+5 3.000000+5 4.000000+5 5.000000+5 6.000000+5412540 4 6
...
...
```

Updated File:

```
...
...
4.109300+4 9.210510+1      0      0      1      4125 0 0 0
0.000000+0-3.082000+4      0      1      0      0412540 4 1
1.000000+1 1.000000+0      0      4      0      1412540 4 2
0.000000+0 0.000000+0      1      5      528      1412540 4 3
0.000000+0 0.000000+0      1      5      528      32412540 4 4
1.000000-5 4.000000+4 5.000000+4 6.000000+4 8.000000+4 1.000000+5412540 4 5
1.500000+5 2.000000+5 3.000000+5 4.000000+5 5.000000+5 6.000000+5412540 4 6
...
...
```

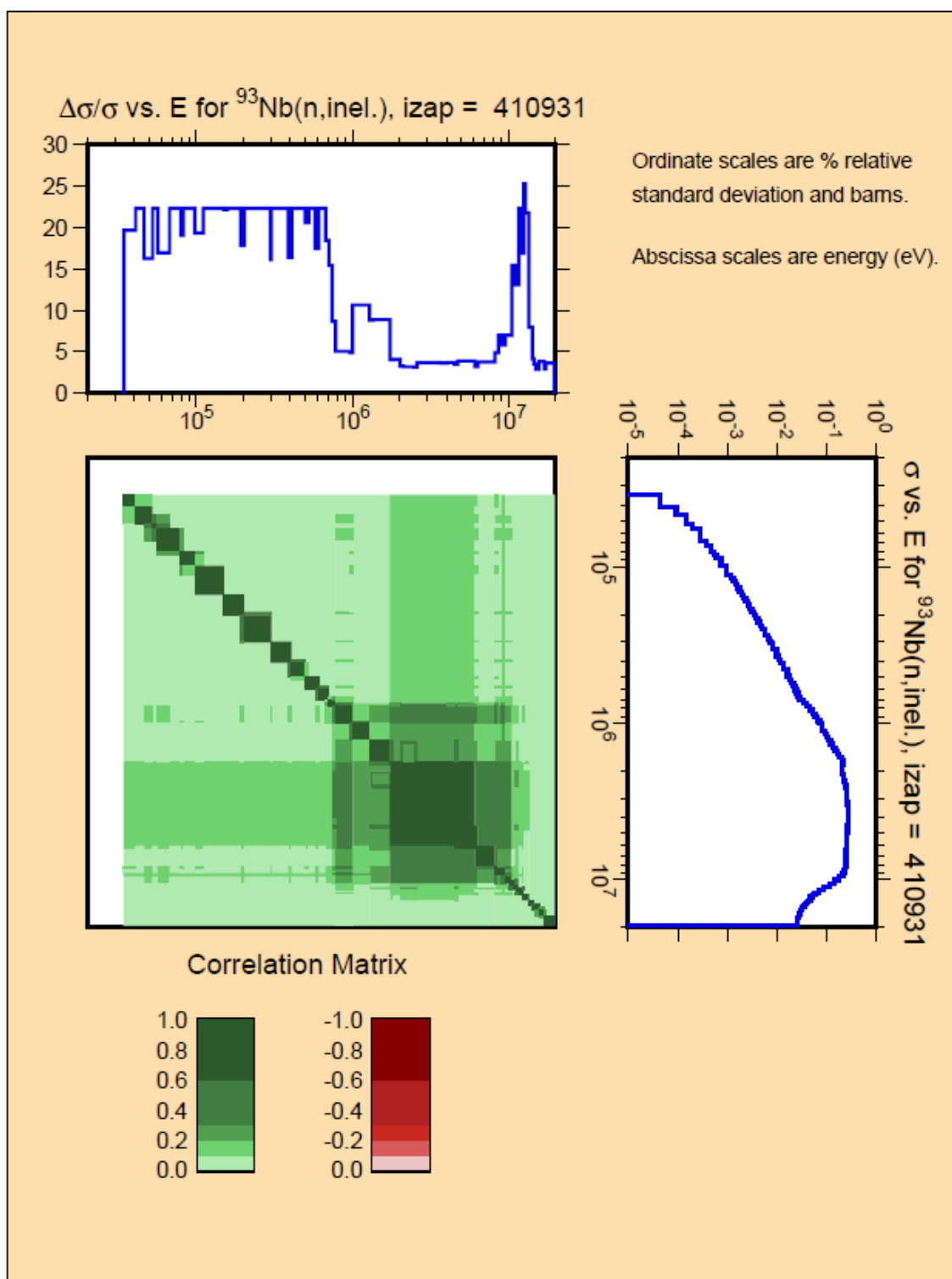
Figure 5. NJOY input to process Nb93-MF40

```
moder / Extract/convert neutron evaluated data
1 21
'41-Nb-93 from JEFF3.2T3'/
20 4125
0/
reconr / Reconstruct XS for neutrons
21 22
'JEFF3.2T3 PENDF for 41-Nb-93'/
4125 2/
0.001 0.0 0.003/ err tempr errmax
'JEFF3.2T3: 41-Nb-93'/
'Processed by NJOY99.364, NEA_Dec2011'/
0/
broadr / Doppler broaden XS
21 22 23
4125 1 0 0 0./
```

```

0.001 2.0e+6 0.003/ errthn thnmax errmax
300.
0/
grouprr / Prepare multigroup data for neutrons
21 23 0 24
4125 17 0 2 6 1 1 1/
'(JEFF3.2T3) NJOY99.364 NEA DEC2011 '/
300.
1.E+10
3 /
40410931 4 /
0/
0/
errorrr
21 0 24 77/
4125 17 2 1 1/
0 40 /Procesa Lib 33 de incertidumbres
covr
77 78/
3 1
'NEA JEFF-3.2T3 Dec 2011'/
'Processing BOXER NJOY99.364'/
4125 0 0 0 /
covr
77 0 79/
1
1.0E-5
1 1 0 1 1 / irelco(0=absol/1=relative)
4125 0 0 0 /
viewrr
79 80/
stop

```

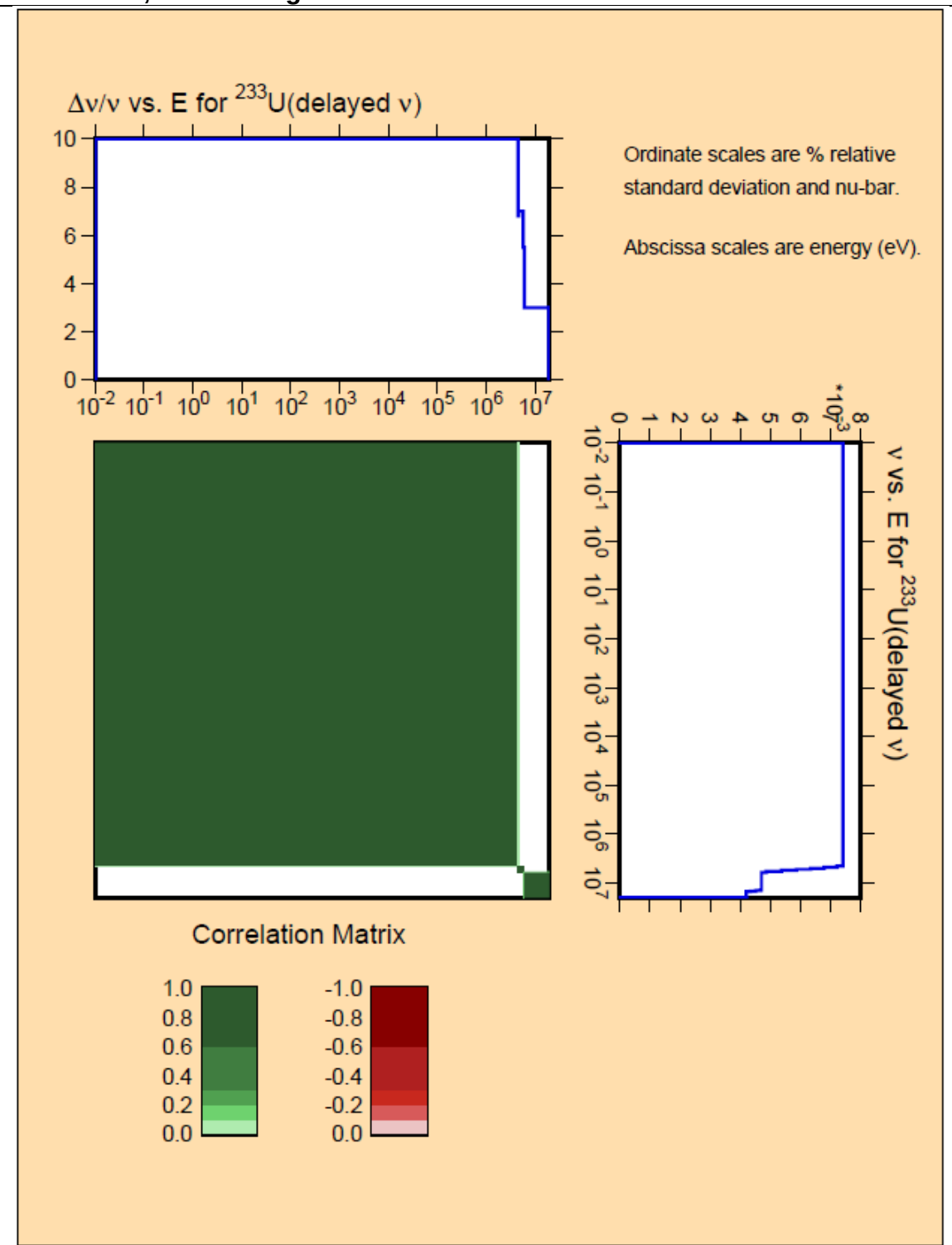
Figure 6. Processing Nb93-MF40

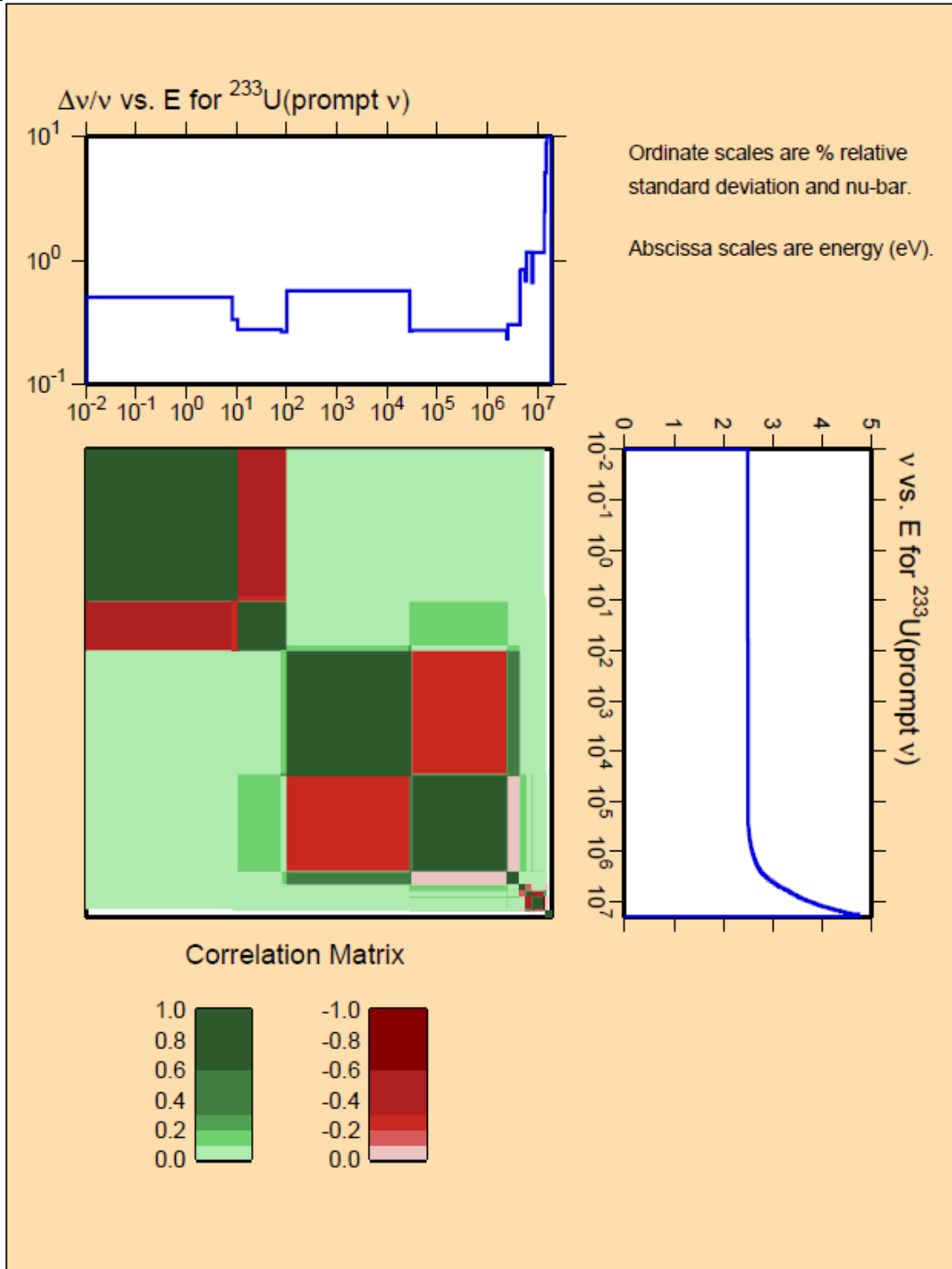
2.8.2 Example of Processing MF31

Figure 7. NJOY input to process MF31

```
moder / Extract/convert neutron evaluated data
1 21
'92-U-233 from JEFF3.2T3'/
20 9222
0/
reconr / Reconstruct XS for neutrons
21 22
'JEFF3.2T3 PENDF for 92-U-233'/
9222 2/
0.001 0.0 0.003/ err tempr errmax
'JEFF3.2T3: 92-U-233'/
'Processed by NJOY99.364, NEA_Dec2011'/
0/
broadr / Doppler broaden XS
21 22 23
9222 1 0 0 0./
0.001 2.0e+6 0.001/ errthn thnmax errmax
300.
0/
groupr / Prepare multigroup data for neutrons
21 23 0 24
9222 17 0 2 6 1 1 1/
'(JEFF3.2T3) NJOY99.364 NEA DEC2011 '/
300.
1.E+10
3/
3 452/
3 455/
3 456/
5 455/
0/
0/
errorr
21 0 24 77/
9222 17 2 1 1/
0 31 /Procesa Lib 33 de incertidumbres
covr
77 78/
3 1
'NEA JEFF-3.2T3 Dec 2011'/
'Processing BOXER NJOY99.364'/
9222 0 0 0 /
covr
77 0 79/
1
1.0E-5
1 1 0 1 1 / irelco(0=absol/1=relative)
9222 0 0 0 /
viewr
79 80/
stop
```

JEFF-3.1.2; Processing U233-MF31



JEFF-3.1.2; Processing U233-MF31

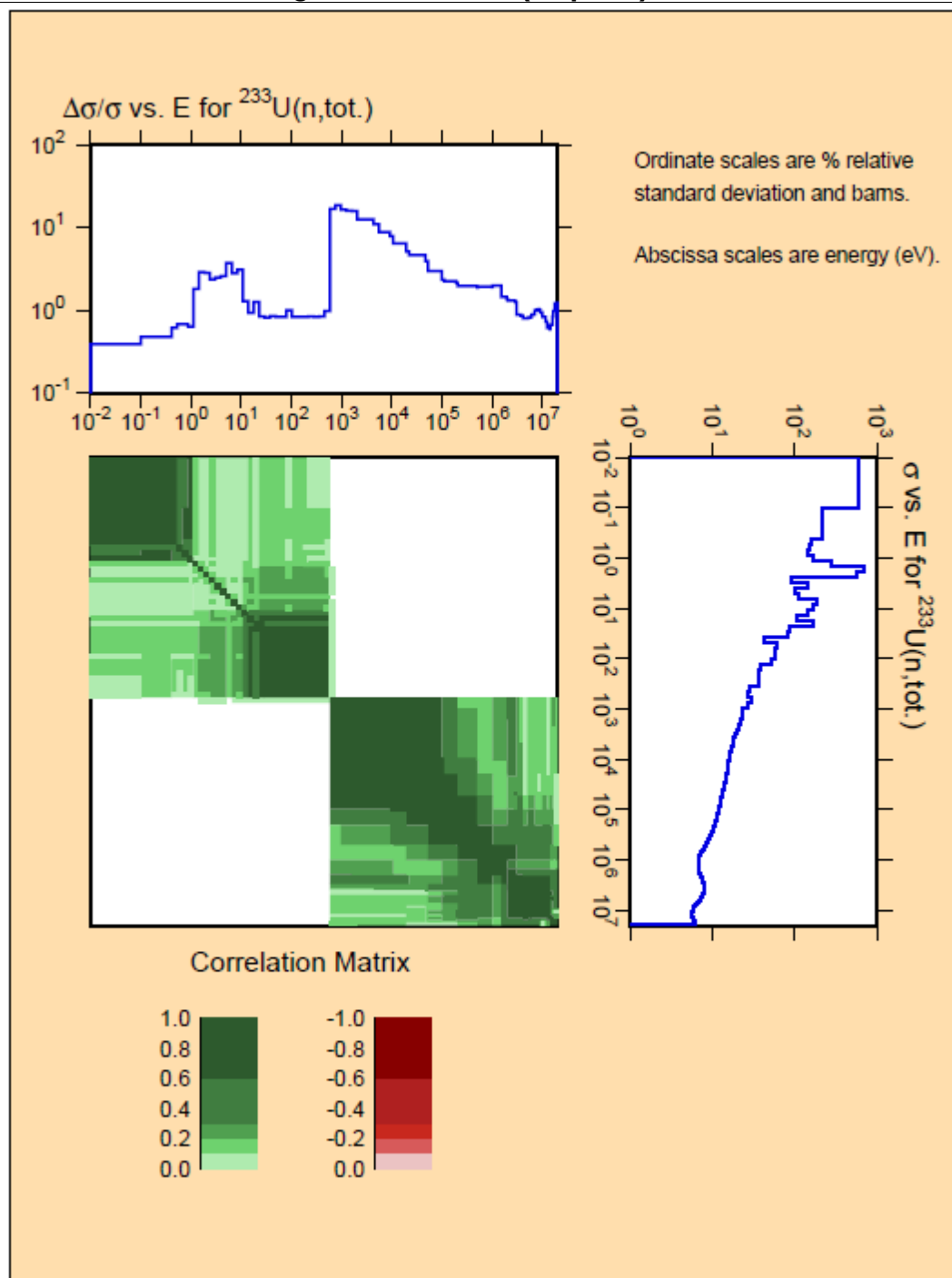
See ANNEX 6.4 : “COV_PROCESS_JEFF32T3”

2.8.3 Example of Processing MF32/33

Figure 8. NJOY input to process U233.

```
moder / Extract/convert neutron evaluated data
1 21
'92-U-233 from JEFF3.2T3'/
20 9222
0/
reconr / Reconstruct XS for neutrons
21 22
'JEFF3.2T3 PENDF for 92-U-233'/
9222 2/
0.001 0.0 0.003/ err tempr errmax
'JEFF3.2T3: 92-U-233'/
'Processed by NJOY99.364, NEA_Dec2011'/
0/
broadr / Doppler broaden XS
21 22 23
9222 1 0 0 0./
0.001 2.0e+6 0.003/ errthn thnmax errmax
300.
0/
errorr
21 23 0 77/
9222 17 2 1 1/
1 300.0 / mprint temp
0 33 /Procesa Lib 33 de incertidumbres
covr
77 78/
3 1
'NEA JEFF-3.2T3 Dec 2011'/
'Processing BOXER NJOY99.364'/
9222 0 0 0 /
covr
77 0 79/
1
1.0E-5
1 1 0 1 1 / irelco(0=absol/1=relative)
9222 0 0 0 /
viewr
79 80/
stop
```

See ANNEX 6.4 : “COV_PROCESS_JEFF32T3”

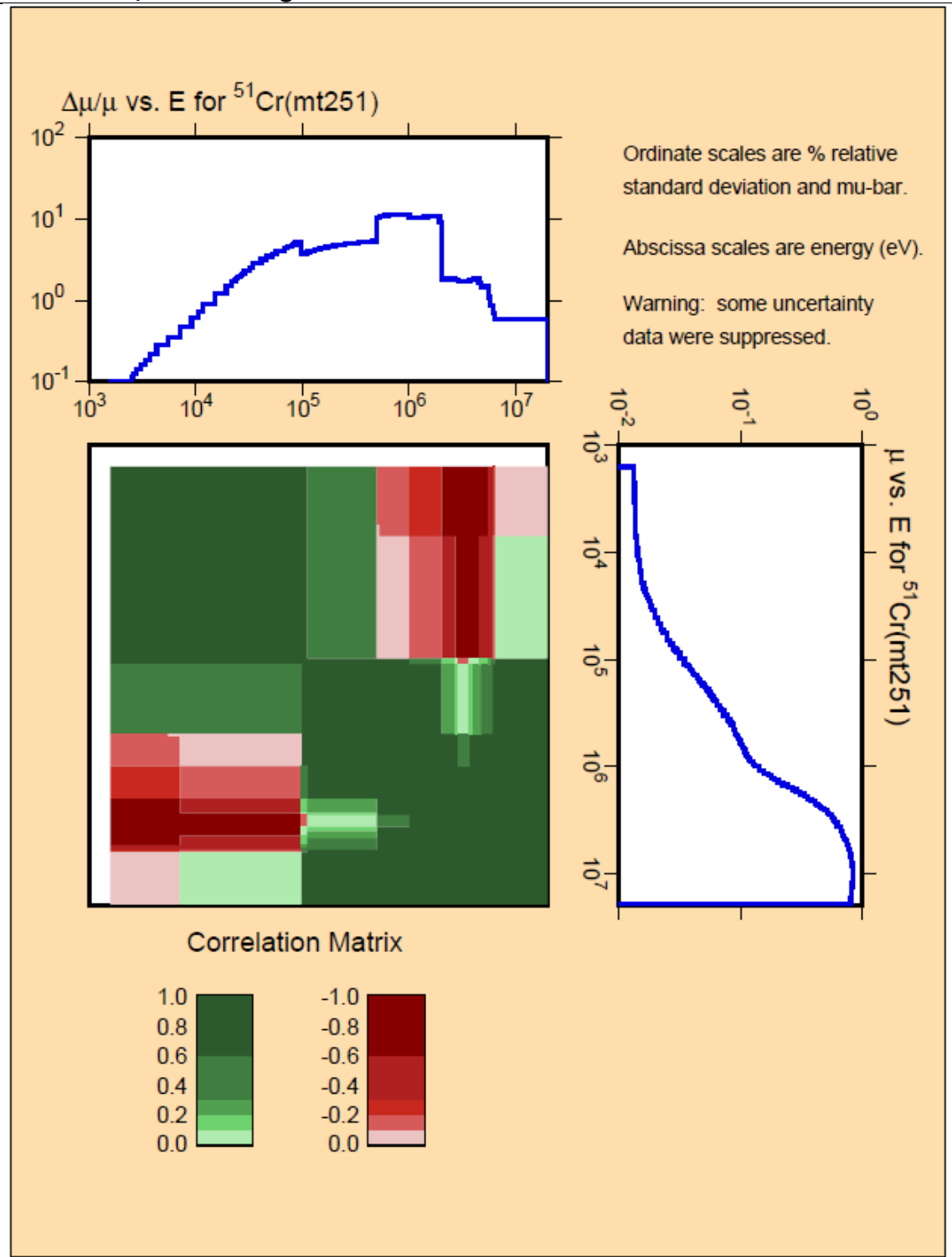
JEFF-3.1.2; Processing U233-MF32/33 (17 plots)

2.8.4 Example of Processing MF34

Figure 9. NJOY input to process MF34

```
moder / Extract/convert neutron evaluated data
1 21
'24-Cr-51 from JEFF3.2T3'/
20 2428
0/
reconr / Reconstruct XS for neutrons
21 22
'JEFF3.2T3 PENDF for 24-Cr-51'/
2428 2/
0.001 0.0 0.003/ err tempr errmax
'JEFF3.2T3: 24-Cr-51'/
'Processed by NJOY99.364, NEA_Dec2011'/
0/
broadr / Doppler broaden XS
21 22 23
2428 1 0 0 0./
0.001 2.0e+6 0.003/ errthn thnmax errmax
300.
0/
errorr
21 23 0 77/
2428 17 2 1 1/
1 300.0 / mprint temp
0 34 /Procesa Lib 33 de incertidumbres
covr
77 78/
3 1
'NEA JEFF-3.2T3 Dec 2011'/
'Processing BOXER NJOY99.364'/
2428 0 0 0 /
covr
77 0 79/
1
1.0E-5
1 1 0 1 1 / irelco(0=absol/1=relative)
2428 0 0 0 /
viewr
79 80/
stop
```

See ANNEX 6.4 : “COV_PROCESS_JEFF32T3”

JEFF-3.1.2; Processing Cr51-MF34

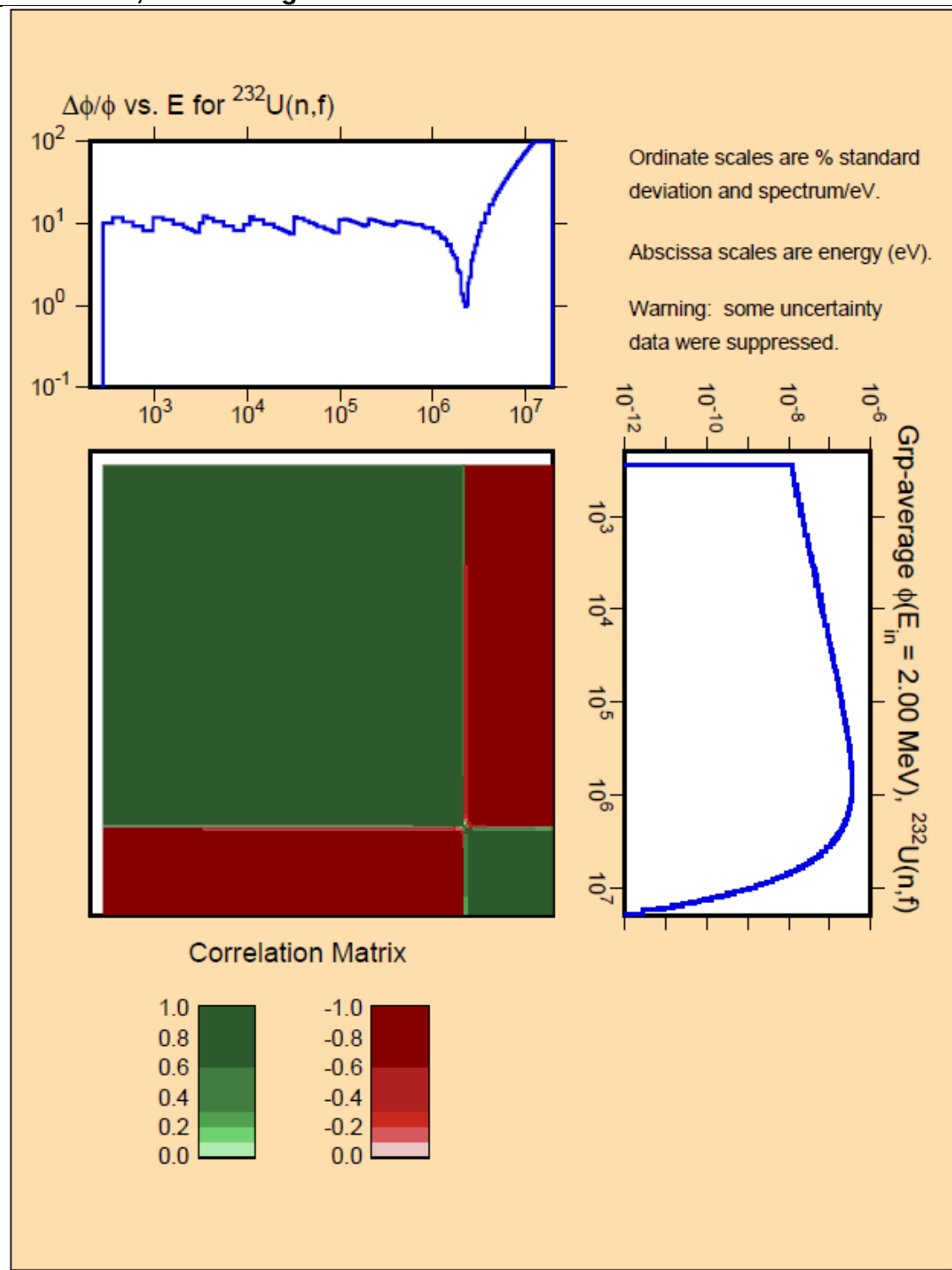
2.8.5 Example of Processing MF35

Figure 10. NJOY input to process MF35

```
moder / Extract/convert neutron evaluated data
1 21
'92-U-232 from JEFF3.2T3'/
20 9219
0/
reconr / Reconstruct XS for neutrons
21 22
'JEFF3.2T3 PENDF for 92-U-232'/
9219 2/
0.001 0.0 0.003/ err tempr errmax
'JEFF3.2T3: 92-U-232'/
'Processed by NJOY99.364, NEA_Dec2011'/
0/
broadr / Doppler broaden XS
21 22 23
9219 1 0 0 0./
0.001 2.0e+6 0.003/ errthn thnmax errmax
300.
0/
groupr / Prepare multigroup data for neutrons
21 23 0 24
9219 17 0 2 6 1 1 1/
'(JEFF3.2T3) NJOY99.364 NEA DEC2011 '/
300.
1.E+10
3/
3 452/
3 455/
3 456/
5 18/
0/
0/
errorr
21 0 24 77/
9219 17 2 1 1/
0 35 /Procesa Lib 33 de incertidumbres
covr
77 78/
3 1
'NEA JEFF-3.2T3 Dec 2011'/
'Processing BOXER NJOY99.364'/
9219 0 0 0 /
covr
77 0 79/
1
1.0E-5
1 1 0 1 1 / irelco(0=absol/1=relative)
9219 0 0 0 /
viewr
79 80/
stop
```

See ANNEX 6.4 : “COV_PROCESS_JEFF32T3”

JEFF-3.1.2; Processing U232-MF35

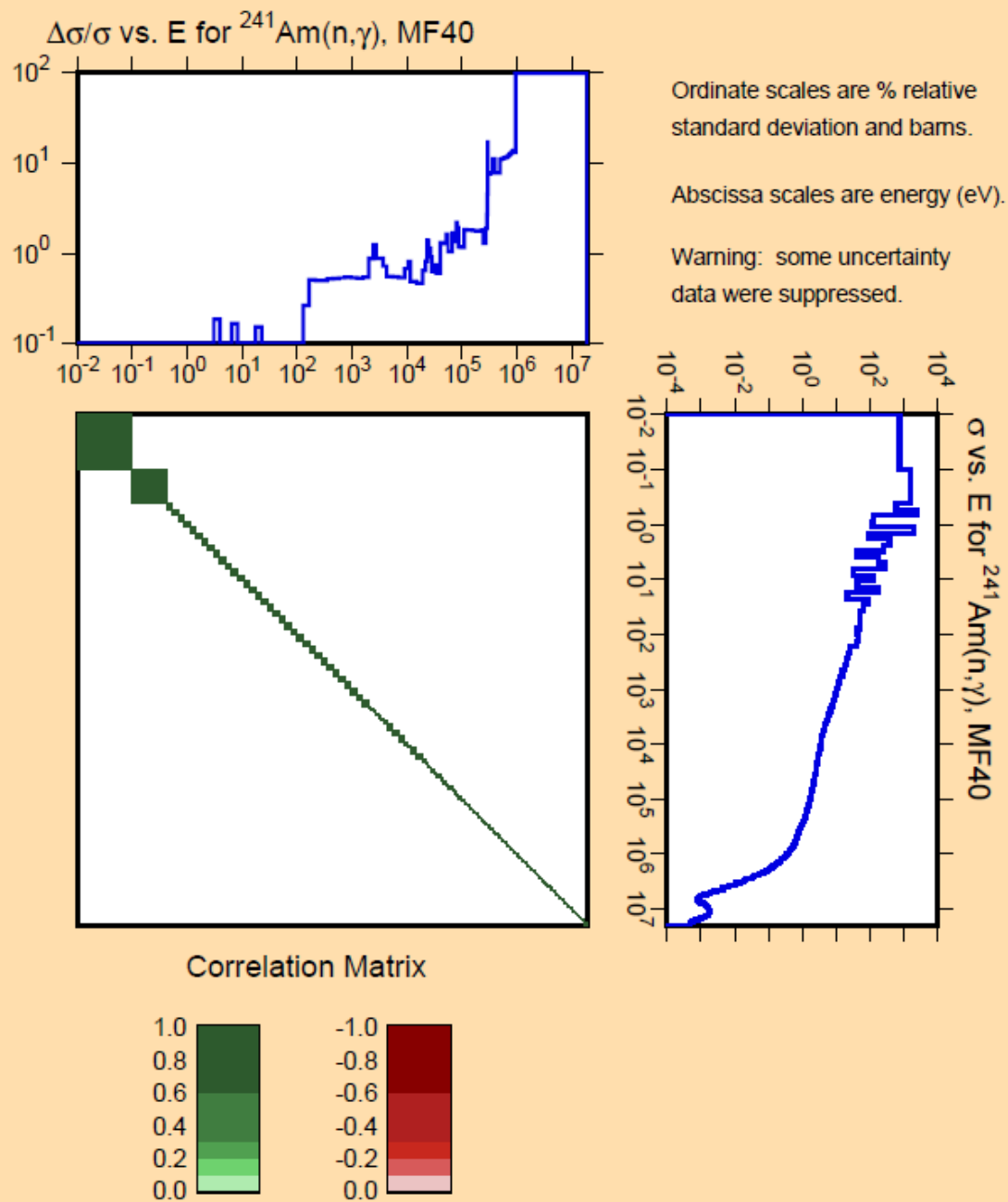


2.8.6 Example of Processing MF40

Figure 11. NJOY input to process MF40

```
moder / Extract/convert neutron evaluated data
1 21
'95-Am-241 from JEFF3.2T3'/
20 9543
0/
reconr / Reconstruct XS for neutrons
21 22
'JEFF3.2T3 PENDF for 95-Am-241'/
9543 2/
0.001 0.0 0.003/ err tempr errmax
'JEFF3.2T3: 95-Am-241'/
'Processed by NJOY99.364, NEA_Dec2011'/
0/
broadr / Doppler broaden XS
21 22 23
9543 1 0 0 0./
0.001 2.0e+6 0.003/ errthn thnmax errmax
300.
0/
groupr / Prepare multigroup data for neutrons
21 23 0 24
9543 17 0 2 6 1 1 1/
'(JEFF3.2T3) NJOY99.364 NEA DEC2011 '/
300.
1.E+10
3/
3 452/
3 455/
3 456/
5 18/
0/
0/
errorr
21 0 24 77/
9543 17 2 1 1/
0 40 /Procesa Lib 33 de incertidumbres
covr
77 78/
3 1
'NEA JEFF-3.2T3 Dec 2011'/
'Processing BOXER NJOY99.364'/
9543 0 0 0 /
covr
77 0 79/
1
1.0E-5
1 1 0 1 1 / irelco(0=absol/1=relative)
9543 0 0 0 /
viewr
79 80/
stop
```

See ANNEX 6.4 : “COV_PROCESS_JEFF32T3”

JEFF-3.1.2; Processing Am241-MF40

2.9 Problems processing URR with PURR

Problems in JEFF32T3:

- NJOY99.393 cannot process S36 and K39 with PURR/NJOY module
- Pu238 is processed with PURR module. But, MCNP stops when Pu238 uses “ptable” option processed with PURR module.

In this work, S36, K39 and Pu238 are processed without PURR/NJOY module.

2.10 Problems processing in GENDF format

One problem has been found in:

- 1) Es253 in GROUPR module:

<pre>---message from getunr--- Warning, negative URR cross sections found, check unresr</pre>

3. Criticality Validation

An extensive criticality validation suite can be used by the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* from the OECD-NEA project ICSBEP, September 2010 Edition **[ICSBEP]**.

An expanded Criticality Validation Suite presented by R.D. Mosteller, F.B. Broewn and B.C. Kiedrowski containing **119 cases** **[LA-UR-11-04170]** for a variety of fuels is used in this work. A comparison with **[NEA/JEFF-3.1.1]** is also performed:

➤ ²³³ U	: 18
➤ highly enriched uranium (HEU)	: 40
➤ intermediate-enriched uranium (IEU)	: 17
➤ low-enriched uranium (LEU)	: 8
➤ plutonium	: 36

For each type of fuel, there are cases with a variety of:

- moderators
- reflectors
- spectra
- geometries

In addition, 4 cases also included in ICSBEP are included for testing purposes:

- Np237
- heavy-Water solutions
- very thermal Pu solution
- unmoderated ZEUS benchmark

MCNP inputs uses (`kcode 10000 1.0 100 600`). A statistical uncertainty between 0.00020 and 0.00040 is obtained. For simplicity, this statistical uncertainty is not shown in the following tables.

See ANNEX 6.5 including 123 MCNP inputs used in this Criticality Validation Suite.

Table 9. ^{233}U Benchmarks

Spectrum	Form	Shape	Moderator and/or Reflector	ICSBEP Benchmark name	Benchmark	keff			
						This work			
						ENDF/B-VII.1 293.6K	JEFF-3.1.2 293.6K	JEFF-3.2T2 300K	JEFF-3.2T3 293.6K
Fast	Metal	Spheres	Unreflected	u233-met-fast-001	1.0000±0.0010	0.99994	1.00444	0.99961	0.99961
				u233-met-fast-002-CASE_1	1.0000±0.0010	0.99850	1.00252	0.99902	0.99902
			HEU	u233-met-fast-002-CASE_2	1.0000±0.0011	1.00014	1.00379	1.00061	1.00061
				u233-met-fast-003-CASE_1	1.0000±0.0010	0.99808	1.00528	0.99881	0.99881
			Normal Uranium	u233-met-fast-003-CASE_2	1.0000±0.0010	0.99778	1.00466	0.99977	0.99977
				u233-met-fast-006	1.0000±0.0014	0.99902	1.00586	1.00105	1.00105
			Tungsten	u233-met-fast-004-CASE_1	1.0000±0.0007	0.99895	1.00584	0.99945	0.99924
				u233-met-fast-004-CASE_2	1.0000±0.0008	0.99505	1.00466	0.99804	0.99713
			Beryllium	u-233-met-fast-005-CASE_1	1.0000±0.0030	0.99626	BeO STL+	BeO STL+	BeO STL+
				u-233-met-fast-005-CASE_2	1.0000±0.0030	0.99504	BeO STL+	BeO STL+	BeO STL+
Intermediate	Solution	Sphere	Beryllium	u233-sol-inter-001-case1	1.0000±0.0083	0.98521	0.98438	0.98586	0.98563
Thermal	UO2+ZrO2	Lattice	Water	u233-comp-therm-001-case3	1.0000±0.0024	1.00163	0.99795	1.00381	1.00348
	Solution	Sphere	Unreflected	u233-sol-therm-001-case1	1.0000±0.0031	1.00137	0.99844	1.00173	1.00195
				u233-sol-therm-001-case2	1.0000±0.0033	1.00101	0.99846	1.00160	1.00192
				u233-sol-therm-001-case3	1.0000±0.0033	1.00039	0.99835	1.00165	1.00114
				u233-sol-therm-001-case4	1.0000±0.0033	1.00016	0.99806	1.00135	1.00146
				u233-sol-therm-001-case5	1.0000±0.0033	1.00026	0.99802	1.00079	1.00005
				u233-sol-therm-008	1.0000±0.0029	1.00136	0.99805	1.00133	1.00121

$$\sigma < |\Delta k| \leq 2\sigma \quad 2\sigma < |\Delta k| \leq 3\sigma \quad 3\sigma < |\Delta k|$$

Table 10. HEU Benchmarks

Spectrum	Form	Shape	Moderator and/or Reflector	ICSBEP Benchmark name	Benchmark	keff			
						This work			
						ENDF/B-VII.1 293.6K	JEFF-3.1.2 293.6K	JEFF-3.2T2 300K	JEFF-3.2T3 293.6K
Fast	Metal	Spheres	Unreflected	heu-met-fast-001	1.0000±0.0010	0.99983	0.99612	0.99985	0.99985
				heu-met-fast-008	0.9989±0.0016	0.99522	0.99246	0.99570	0.99585
				heu-met-fast-018-case2	1.0000±0.0014	0.99950	0.99565	0.99966	0.9993
			Normal Uranium	heu-met-fast-003-case1	1.0000±0.0050	0.99476	0.99366	0.99614	0.99614
				heu-met-fast-003-case2	1.0000±0.0050	0.99440	0.99300	0.99570	0.9957
				heu-met-fast-003-case3	1.0000±0.0050	0.99868	0.99723	0.99993	0.99993
				heu-met-fast-003-case4	1.0000±0.0030	0.99738	0.99627	0.99928	0.99928
				heu-met-fast-003-case5	1.0000±0.0030	1.00097	1.00010	1.00402	1.00402
				heu-met-fast-003-case6	1.0000±0.0030	1.00129	0.99980	1.00369	1.00369
				heu-met-fast-003-case7	1.0000±0.0030	1.00194	1.00167	1.00486	1.00486
				heu-met-fast-028	1.0000±0.0030	1.00259	1.00161	1.00512	1.00512
			Depleted Uranium	heu-met-fast-014	0.9989±0.0017	0.99798	0.99613	0.99849	0.99905
			Tungsten carbide	heu-met-fast-003-case8	1.0000±0.0050	1.00167	1.00144	1.00239	1.0028
				heu-met-fast-003-case9	1.0000±0.0050	1.00190	1.00254	1.00398	1.00417
				heu-met-fast-003-case10	1.0000±0.0050	1.00560	1.00820	1.00823	1.00747
				heu-met-fast-003-case11	1.0000±0.0050	1.01019	1.01385	1.01319	1.0137
			Nickel	heu-met-fast-003-case12	1.0000±0.0030	1.00879	1.00174	1.00523	1.00523
			Steel	heu-met-fast-013	0.9990±0.0015	0.99734	0.99314	0.99540	0.99528
				heu-met-fast-021-case2	1.0000±0.0024	0.99744	0.99328	0.99670	0.99629
			Duralumin	heu-met-fast-022-case2	1.0000±0.0019	0.99755	0.99427	0.99717	0.9969
			Aluminium	heu-met-fast-012	0.9992±0.0018	0.99839	0.99494	0.99792	0.99816
			Graphite	heu-met-fast-019-case2	1.0000±0.0028	1.00740	1.00282	1.00693	1.00663
			Beryllium	heu-met-fast-009-case1	0.9992±0.0015	0.99745	0.99385	0.99695	0.99699
			Beryllium Oxide	heu-met-fast-009-case2	0.9992±0.0015	0.99684	0.99257	0.99536	0.99522
			Polyethylene	heu-met-fast-011	0.9989±0.0015	0.99826	0.99510	0.99835	0.99884
				heu-met-fast-020-case2	1.0000±0.0028	1.00080	0.99738	1.00106	1.00103
			Water	heu-met-fast-004-case1	1.0020±0.0010	1.00050	0.99536	0.99806	0.99806
		Cylinder	Unreflected	heu-met-fast-015	0.9996±0.0017	0.99409	0.99069	0.99368	0.99449
		Lattice	Paraffin	heu-met-fast-026-case9	1.0000±0.0038	0.99036	0.98730	0.98906	0.98902
Intermediate	UH3	Cylinder	Natural U	heu-comp-inter-003-case7	1.0000±0.0047	0.99666	0.99556	0.99989	0.99951
	Metal	Cylinder	Graphite, copper	heu-met-inter-006-case1	0.9977±0.0008	0.99422	0.99293	1.00968	0.99696
				heu-met-inter-006-case2	0.9997±0.0008	0.99665	0.99481	1.01436	1.00034

				heu-met-inter-006-case3	1.0015±0.0009	0.99926	0.99843	1.01978	1.00372
				heu-met-inter-006-case4	1.0016±0.0008	1.00777	1.00479	1.03244	1.01115
Thermal	UO2+ZrO2	Lattice	Water, ThO2	u233-comp-therm-001-case6	1.0015±0.0028	0.99889	0.99755	1.00312	1.00276
	Solution	Sphere	Unreflected	heu-sol-therm-013-case1	1.0012±0.0026	0.99828	0.99903	0.99824	0.99959
				heu-sol-therm-013-case2	1.0007±0.0036	0.99709	0.99819	0.99768	0.9977
				heu-sol-therm-013-case3	1.0009±0.0036	0.99475	0.99502	0.99420	0.99384
				heu-sol-therm-013-case4	1.0003±0.0036	0.99626	0.99638	0.99521	0.99578
				heu-sol-therm-032	1.0015±0.0026	0.99921	0.99924	0.99900	0.99936

$$\sigma < |\Delta k| \leq 2\sigma \quad 2\sigma < |\Delta k| \leq 3\sigma \quad 3\sigma < |\Delta k|$$

Table 11. IEU Benchmarks

Spectrum	Form	Shape	Moderator and/or Reflector	ICSBEP Benchmark name	Benchmark	keff			
						This work			
						ENDF/B-VII.1 293.6K	JEFF-3.1.2 293.6K	JEFF-3.2T2 300K	JEFF-3.2T3 293.6K
Fast	Metal	Spheres	Unreflected	ieu-met-fast-003-case2	1.0000±0.0017	1.00255	0.99983	1.00233	1.00281
			Steel	ieu-met-fast-005-case2	1.0000±0.0021	1.00193	0.99787	1.00195	1.00092
			Duralumin	ieu-met-fast-006-case2	1.0000±0.0023	0.99659	0.99230	0.99502	0.99482
			Graphite	ieu-met-fast-004-case2	1.0000±0.0030	1.00739	1.00424	1.00720	1.00706
		Cylinder	Unreflected	ieu-met-fast-001-case1	0.9989±0.0010	0.99997	0.99756	1.00049	1.00134
				ieu-met-fast-001-case2	0.9997±0.0010	1.00053	0.99750	1.00077	1.00152
				ieu-met-fast-001-case3	0.9993±0.0005	1.00109	0.99802	1.00067	1.00043
				ieu-met-fast-001-case4	1.0002±0.0005	1.00130	0.99799	1.00119	1.00122
			Normal U	ieu-met-fast-002	1.0000±0.0030	0.99872	0.99192	0.99711	0.99711
			Depleted U	ieu-met-fast-007-case1	1.0049±0.0008	1.00463	0.99820	1.00417	1.00443
Intermediate	Plate	Lattice	Normal U, steel	mix-met-fast-008-case7	1.0030±0.0025	1.01911	1.01594	1.02341	1.02326
Thermal	UO2	Lattice	Water	ieu-comp-therm-002-CASE_3	1.0017±0.0044	1.00451	1.00114	1.00076	1.00078
	Solution	Cylinder	Unreflected	ieu-sol-therm-007-CASE14	0.9961±0.0009	0.99473	0.99558	0.99539	0.99551
				ieu-sol-therm-007-CASE30	0.9973±0.0009	0.99724	0.99816	0.99765	0.99691
				ieu-sol-therm-007-CASE32	0.9985±0.0010	0.99611	0.99654	0.99622	0.99672
				ieu-sol-therm-007-CASE36	0.9988±0.0011	0.99860	0.99867	0.99848	0.99848
				ieu-sol-therm-007-CASE49	0.9983±0.0011	0.99746	0.99742	0.99740	0.9974

$$\sigma < |\Delta k| \leq 2\sigma \quad 2\sigma < |\Delta k| \leq 3\sigma \quad 3\sigma < |\Delta k|$$

Table 12. LEU Benchmarks

Spectrum	Form	Shape	Moderator and/or Reflector	ICSBEP Benchmark name	Benchmark	keff			
						This work			
						ENDF/B-VII.1 293.6K	JEFF-3.1.2 293.6K	JEFF-3.2T2 300K	JEFF-3.2T3 293.6K
Thermal	UO2	Lattice	UO2 rods, Water	leu-comp-ther-008-CASE_1	1.0007±0.0016	1.00152	1.00040	1.00030	1.00088
				leu-comp-therm-008-CASE_2	1.0007±0.0016	1.00122	1.00085	1.00028	1.00038
				leu-comp-therm-008-CASE_5	1.0007±0.0016	1.00149	1.00111	0.99943	1.00049
				leu-comp-therm-008-CASE_7	1.0007±0.0016	1.00105	1.00028	0.99992	0.99996
				leu-comp-therm-008-CASE_8	1.0007±0.0016	1.00094	1.00014	0.99965	0.99937
				leu-comp-therm-008-CASE_11	1.0007±0.0016	1.00179	1.00135	1.00042	1.00153
	Solution	Sphere	Water	leu-sol-therm-002-case1	1.0038±0.0040	1.00020	1.00040	0.99932	0.99977
			Unreflected	leu-sol-therm-002-case2	1.0024±0.0037	0.99590	0.99661	0.99541	0.9963

$$\sigma < |\Delta k| \leq 2\sigma \quad 2\sigma < |\Delta k| \leq 3\sigma \quad 3\sigma < |\Delta k|$$

Table 13. Plutonium Benchmarks

Spectrum	Form	Shape	Moderator and/or Reflector	ICSBEP Benchmark name	Benchmark	Keff			
						This work			
Spectrum	Form	Shape	Moderator and/or Reflector	ICSBEP Benchmark name	Benchmark	ENDF/B-VII.1 293.6K	JEFF-3.1.2 293.6K	JEFF-3.2T2 300K	JEFF-3.2T3 293.6K
Fast	Metal	Spheres	Unreflected	pu-met-fast-001-CASE_1	1.0000±0.0020	0.99982	0.99999	1.00012	1.00012
				pu-met-fast-002-CASE_1	1.0000±0.0020	0.99984	1.00413	1.00249	1.00249
				pu-met-fast-022	1.0000±0.0021	0.99841	0.99778	0.99888	0.9989
			HEU	mix-met-fast-001-CASE_1	1.0000±0.0016	0.99885	0.99837	0.99905	0.99905
				mix-met-fast-003	0.9993±0.0016	1.00105	1.00059	1.00113	1.00099
			Normal Uranium	pu-met-fast-006	1.0000±0.0030	1.00083	1.00237	1.00275	1.00275
				pu-met-fast-010-CASE_1	1.0000±0.0018	0.99969	1.00109	1.00102	1.00102
			Depleted Uranium	pu-met-fast-020	0.9993±0.0017	0.99852	0.99998	0.99977	0.99974
			Thorium	pu-met-fast-008-case2	1.0000±0.0006	0.99744	1.00234	0.99731	0.99731
			Tungsten	pu-met-fast-005-CASE_1	1.0000±0.0013	0.99993	1.00395	1.00315	1.00183
			Steel	pu-met-fast-025	1.0000±0.0020	0.99832	0.99729	0.99735	0.99712
				pu-met-fast-026	1.0000±0.0024	0.99983	0.99806	0.99908	0.99886
			Aluminium	pu-met-fast-009-CASE_1	1.0000±0.0027	1.00027	0.99917	0.99936	0.99936
			Graphite	pu-met-fast-023	1.0000±0.0020	1.00037	0.99863	0.99897	0.99896
			Beryllium	pu-met-fast-018-CASE_1	1.0000±0.0030	0.99908	BeO STL+	BeO STL+	BeO STL+
				pu-met-fast-019	0.9992±0.0015	1.00117	0.99941	0.99840	0.99852
			Polyethylene	pu-met-fast-024	1.0000±0.0020	1.00208	0.99958	1.00037	1.00038
			Water	pu-met-fast-011-CASE_1	1.0000±0.0010	0.99998	0.99688	0.99786	0.99786
		Cylinder	Beryllium	pu-met-fast-021-case1	1.0000±0.0026	1.00417	1.00311	1.00369	1.00333
			Beryllium Oxide	pu-met-fast-021-case2	1.0000±0.0026	0.99387	BeO STL+	BeO STL+	BeO STL+
		Lattice	Unreflected	pu-met-fast-003-case103	1.0000±0.0030	0.99568	0.99679	0.99625	0.99614
Intermediate	Mixture	Homog	Hydrogen, graphite	pu-comp-inter-001	1.0000±0.0110	1.01127	1.00735	1.00577	1.00577
Thermal	MOX	Lattice	Water	mix-comp-therm-002-case-pnl30	1.0024±0.0060	1.00181	0.99945	1.00035	1.00055
				mix-comp-therm-002-case-pnl31	1.0009±0.0047	1.00252	1.00225	1.00268	1.00297
				mix-comp-therm-002-case-pnl32	1.0042±0.0031	1.00323	1.00137	1.00186	1.00255
				mix-comp-therm-002-case-pnl33	1.0024±0.0021	1.00703	1.00612	1.00642	1.00683
				mix-comp-therm-002-case-pnl34	1.0038±0.0025	1.00427	1.00255	1.00309	1.00268
				mix-comp-therm-002-case-pnl35	1.0029±0.0027	1.00648	1.00480	1.00544	1.00515
	Solution	Sphere	Unreflected	pu-sol-therm-009-case3a	1.0000±0.0033	1.01870	1.01414	1.01613	1.01551
				pu-sol-therm-011-CASE_5.16	1.0000±0.0052	1.00669	1.00244	1.00290	1.0027

				pu-sol-therm-011-CASE_1.18	1.0000±0.0052	0.99372	0.99082	0.99196	0.99196
				pu-sol-therm-011-CASE_6.18	1.0000±0.0052	1.00000	0.99755	0.99778	0.99759
				pu-sol-therm-021-case_1.t9a	1.0000±0.0032	1.00550	1.00224	1.00168	1.00168
				pu-sol-therm-021-CASE_3.T9A	1.0000±0.0065	1.00458	1.00424	1.00183	1.00337
		Cylinder	Water	pu-sol-therm-018-case_9	1.0000±0.0034	1.00343	1.00262	1.00175	1.00168
				pu-sol-therm-034-case_01	1.0000±0.0062	1.00002	0.99817	0.99731	0.99818

$$\sigma < |\Delta k| \leq 2\sigma \quad 2\sigma < |\Delta k| \leq 3\sigma \quad 3\sigma < |\Delta k|$$

Table 14. Additional criticality validation tests taken from ICSBEP.

		Case	Benchmark	This work			
				ENDF/B-VII.1 293.6K	JEFF-3.1.2 293.6K	JEFF-3.2T2 300K	JEFF-3.2T3 293.6K
PU	Thermal	PU-SOL-THERM-009 (48-inch sphere of plutonium nitrate solution)	1.00030 (330)	1.01528	1.01072	1.01157	1.01157
			- Same sphere as for ORNL-10 (HEU) and ORNL-11 (U233) Benchmarks - Very thermal spectra with very little leakage - Cross sections for Pu239 should be re-examined in the deep thermal range				
HEU	Fast	HEU-MET-FAST-73 (Unmoderated ZEUS benchmark)	1.00120 (150)	1.01152	1.00840	1.04404	1.01042
			- Benchmark contains no moderator and therefore has a fast spectrum - Fast cross sections for Cu should be reviewed				
HEU	Thermal	HEU-SOL-THERM-004_case1 (Heavy water solutions, reflected spheres)	1.00000 (330)	0.98590	0.98500	0.99361	0.99438
			Improvement for cases with deuterium				
SPEC	Thermal	SPEC-MET-FAST-08 (Neptunium sphere reflected by HEU)	1.00190 (360)	0.99493	0.98912	0.99061	0.99129
			Fast cross sections for Np-237 should be reviewed				

Table 15. Isotopes/materials in ^{233}U Benchmarks

u233-comp-therm-001-case3					
B10.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	Fe54.ACE
Fe56.ACE	Fe57.ACE	Fe58.ACE	H1.ACE	H2O-293.ACE	Mn55.ACE
Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE	O16.ACE
Sn112.ACE	Sn114.ACE	Sn115.ACE	Sn116.ACE	Sn117.ACE	Sn118.ACE
Sn119.ACE	Sn120.ACE	Sn122.ACE	Sn124.ACE	U233.ACE	U234.ACE
U238.ACE	Zr90.ACE	Zr91.ACE	Zr92.ACE	Zr94.ACE	Zr96.ACE
u233-met-fast-001					
U233.ACE	U234.ACE	U235.ACE	U238.ACE		
u233-met-fast-002-CASE_1					
U233.ACE	U234.ACE	U235.ACE	U238.ACE		
u233-met-fast-002-CASE_2					
U233.ACE	U234.ACE	U235.ACE	U238.ACE		
u233-met-fast-003-CASE_1					
U233.ACE	U234.ACE	U235.ACE	U238.ACE		
u233-met-fast-003-CASE_2					
U233.ACE	U234.ACE	U235.ACE	U238.ACE		
u233-met-fast-004-CASE_1					
Cu63.ACE	Cu65.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE
Ni64.ACE	U233.ACE	U234.ACE	U238.ACE	W182.ACE	W183.ACE
W184.ACE	W186.ACE	Zr90.ACE	Zr91.ACE	Zr92.ACE	Zr94.ACE
Zr96.ACE					
u233-met-fast-004-CASE_2					
Cu63.ACE	Cu65.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE
Ni64.ACE	U233.ACE	U234.ACE	U238.ACE	W182.ACE	W183.ACE
W184.ACE	W186.ACE	Zr90.ACE	Zr91.ACE	Zr92.ACE	Zr94.ACE
Zr96.ACE					
u-233-met-fast-005-CASE_1					
Be9.ACE	BeO-293.ACE	O16.ACE	U233.ACE	U234.ACE	U238.ACE
u-233-met-fast-005-CASE_2					
Be9.ACE	BeO-293.ACE	O16.ACE	U233.ACE	U234.ACE	U238.ACE
u233-met-fast-006					
U233.ACE	U234.ACE	U235.ACE	U238.ACE		
u233-sol-inter-001-case1					
Be-293.ACE	Be9.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE
F19.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	H1.ACE
H2O-293.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE
O16.ACE	U232.ACE	U233.ACE	U234.ACE	U235.ACE	U238.ACE
u233-sol-therm-001-case1					
Al27.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE
Fe58.ACE	H1.ACE	H2O-293.ACE	Mn55.ACE	N14.ACE	O16.ACE
Si28.ACE	Si29.ACE	Si30.ACE	Th232.ACE	U233.ACE	U234.ACE
U235.ACE	U238.ACE				

u233-sol-therm-001-case2					
Al27.ACE	B10.ACE	B11.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE
Fe56.ACE	Fe57.ACE	Fe58.ACE	H1.ACE	H2O-293.ACE	Mn55.ACE
N14.ACE	O16.ACE	Si28.ACE	Si29.ACE	Si30.ACE	Th232.ACE
U233.ACE	U234.ACE	U235.ACE	U238.ACE		
u233-sol-therm-001-case3					
Al27.ACE	B10.ACE	B11.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE
Fe56.ACE	Fe57.ACE	Fe58.ACE	H1.ACE	H2O-293.ACE	Mn55.ACE
N14.ACE	O16.ACE	Si28.ACE	Si29.ACE	Si30.ACE	Th232.ACE
U233.ACE	U234.ACE	U235.ACE	U238.ACE		
u233-sol-therm-001-case4					
Al27.ACE	B10.ACE	B11.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE
Fe56.ACE	Fe57.ACE	Fe58.ACE	H1.ACE	H2O-293.ACE	Mn55.ACE
N14.ACE	O16.ACE	Si28.ACE	Si29.ACE	Si30.ACE	Th232.ACE
U233.ACE	U234.ACE	U235.ACE	U238.ACE		
u233-sol-therm-001-case5					
Al27.ACE	B10.ACE	B11.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE
Fe56.ACE	Fe57.ACE	Fe58.ACE	H1.ACE	H2O-293.ACE	Mn55.ACE
N14.ACE	O16.ACE	Si28.ACE	Si29.ACE	Si30.ACE	Th232.ACE
U233.ACE	U234.ACE	U235.ACE	U238.ACE		
u233-sol-therm-008					
Al27.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE
Fe58.ACE	H1.ACE	H2O-293.ACE	Mn55.ACE	N14.ACE	O16.ACE
Si28.ACE	Si29.ACE	Si30.ACE	Th232.ACE	U233.ACE	U234.ACE
U235.ACE	U238.ACE				

Table 16. Isotopes/materials in Pu Benchmarks

mix-comp-therm-002-case-pn130					
Al27.ACE	Am241.ACE	B10.ACE	B11.ACE	Cr50.ACE	Cr52.ACE
Cr53.ACE	Cr54.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	H1.ACE	H2O-293.ACE	Mg24.ACE	Mg25.ACE
Mg26.ACE	Mn55.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE
Ni64.ACE	O16.ACE	Pb204.ACE	Pb206.ACE	Pb207.ACE	Pb208.ACE
Pu238.ACE	Pu239.ACE	Pu240.ACE	Pu241.ACE	Pu242.ACE	Si28.ACE
Si29.ACE	Si30.ACE	Sn112.ACE	Sn114.ACE	Sn115.ACE	Sn116.ACE
Sn117.ACE	Sn118.ACE	Sn119.ACE	Sn120.ACE	Sn122.ACE	Sn124.ACE
Ti46.ACE	Ti47.ACE	Ti48.ACE	Ti49.ACE	Ti50.ACE	U234.ACE
U235.ACE	U236.ACE	U238.ACE	Zr90.ACE	Zr91.ACE	Zr92.ACE
Zr94.ACE	Zr96.ACE				
mix-comp-therm-002-case-pn131					
Al27.ACE	Am241.ACE	B10.ACE	B11.ACE	Cr50.ACE	Cr52.ACE
Cr53.ACE	Cr54.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	H1.ACE	H2O-293.ACE	Mg24.ACE	Mg25.ACE
Mg26.ACE	Mn55.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE
Ni64.ACE	O16.ACE	Pb204.ACE	Pb206.ACE	Pb207.ACE	Pb208.ACE
Pu238.ACE	Pu239.ACE	Pu240.ACE	Pu241.ACE	Pu242.ACE	Si28.ACE
Si29.ACE	Si30.ACE	Sn112.ACE	Sn114.ACE	Sn115.ACE	Sn116.ACE
Sn117.ACE	Sn118.ACE	Sn119.ACE	Sn120.ACE	Sn122.ACE	Sn124.ACE
Ti46.ACE	Ti47.ACE	Ti48.ACE	Ti49.ACE	Ti50.ACE	U234.ACE
U235.ACE	U236.ACE	U238.ACE	Zr90.ACE	Zr91.ACE	Zr92.ACE
Zr94.ACE	Zr96.ACE				
mix-comp-therm-002-case-pn132					
Al27.ACE	Am241.ACE	B10.ACE	B11.ACE	Cr50.ACE	Cr52.ACE
Cr53.ACE	Cr54.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	H1.ACE	H2O-293.ACE	Mg24.ACE	Mg25.ACE
Mg26.ACE	Mn55.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE
Ni64.ACE	O16.ACE	Pb204.ACE	Pb206.ACE	Pb207.ACE	Pb208.ACE
Pu238.ACE	Pu239.ACE	Pu240.ACE	Pu241.ACE	Pu242.ACE	Si28.ACE
Si29.ACE	Si30.ACE	Sn112.ACE	Sn114.ACE	Sn115.ACE	Sn116.ACE
Sn117.ACE	Sn118.ACE	Sn119.ACE	Sn120.ACE	Sn122.ACE	Sn124.ACE
Ti46.ACE	Ti47.ACE	Ti48.ACE	Ti49.ACE	Ti50.ACE	U234.ACE
U235.ACE	U236.ACE	U238.ACE	Zr90.ACE	Zr91.ACE	Zr92.ACE
Zr94.ACE	Zr96.ACE				
mix-comp-therm-002-case-pn133					
Al27.ACE	Am241.ACE	B10.ACE	B11.ACE	Cr50.ACE	Cr52.ACE
Cr53.ACE	Cr54.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	H1.ACE	H2O-293.ACE	Mg24.ACE	Mg25.ACE
Mg26.ACE	Mn55.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE
Ni64.ACE	O16.ACE	Pb204.ACE	Pb206.ACE	Pb207.ACE	Pb208.ACE
Pu238.ACE	Pu239.ACE	Pu240.ACE	Pu241.ACE	Pu242.ACE	Si28.ACE
Si29.ACE	Si30.ACE	Sn112.ACE	Sn114.ACE	Sn115.ACE	Sn116.ACE
Sn117.ACE	Sn118.ACE	Sn119.ACE	Sn120.ACE	Sn122.ACE	Sn124.ACE
Ti46.ACE	Ti47.ACE	Ti48.ACE	Ti49.ACE	Ti50.ACE	U234.ACE
U235.ACE	U236.ACE	U238.ACE	Zr90.ACE	Zr91.ACE	Zr92.ACE
Zr94.ACE	Zr96.ACE				
mix-comp-therm-002-case-pn134					

Al27.ACE	Am241.ACE	B10.ACE	B11.ACE	Cr50.ACE	Cr52.ACE
Cr53.ACE	Cr54.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	H1.ACE	H2O-293.ACE	Mg24.ACE	Mg25.ACE
Mg26.ACE	Mn55.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE
Ni64.ACE	O16.ACE	Pb204.ACE	Pb206.ACE	Pb207.ACE	Pb208.ACE
Pu238.ACE	Pu239.ACE	Pu240.ACE	Pu241.ACE	Pu242.ACE	Si28.ACE
Si29.ACE	Si30.ACE	Sn112.ACE	Sn114.ACE	Sn115.ACE	Sn116.ACE
Sn117.ACE	Sn118.ACE	Sn119.ACE	Sn120.ACE	Sn122.ACE	Sn124.ACE
Ti46.ACE	Ti47.ACE	Ti48.ACE	Ti49.ACE	Ti50.ACE	U234.ACE
U235.ACE	U236.ACE	U238.ACE	Zr90.ACE	Zr91.ACE	Zr92.ACE
Zr94.ACE	Zr96.ACE				
mix-comp-therm-002-case-pn135					
Al27.ACE	Am241.ACE	B10.ACE	B11.ACE	Cr50.ACE	Cr52.ACE
Cr53.ACE	Cr54.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	H1.ACE	H2O-293.ACE	Mg24.ACE	Mg25.ACE
Mg26.ACE	Mn55.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE
Ni64.ACE	O16.ACE	Pb204.ACE	Pb206.ACE	Pb207.ACE	Pb208.ACE
Pu238.ACE	Pu239.ACE	Pu240.ACE	Pu241.ACE	Pu242.ACE	Si28.ACE
Si29.ACE	Si30.ACE	Sn112.ACE	Sn114.ACE	Sn115.ACE	Sn116.ACE
Sn117.ACE	Sn118.ACE	Sn119.ACE	Sn120.ACE	Sn122.ACE	Sn124.ACE
Ti46.ACE	Ti47.ACE	Ti48.ACE	Ti49.ACE	Ti50.ACE	U234.ACE
U235.ACE	U236.ACE	U238.ACE	Zr90.ACE	Zr91.ACE	Zr92.ACE
Zr94.ACE	Zr96.ACE				
mix-met-fast-001-CASE_1					
Ga0.ACE	Pu239.ACE	Pu240.ACE	Pu241.ACE	U235.ACE	U238.ACE
mix-met-fast-003					
Al27.ACE	C0.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	Ga0.ACE	Mg24.ACE	Mg25.ACE	Mg26.ACE
Mn55.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE
Pu239.ACE	Pu240.ACE	Pu241.ACE	U234.ACE	U235.ACE	U236.ACE
U238.ACE	W182.ACE	W183.ACE	W184.ACE	W186.ACE	
pu-comp-inter-001					
B10.ACE	B11.ACE	C0.ACE	Ca40.ACE	Ca42.ACE	Ca43.ACE
Ca44.ACE	Ca46.ACE	Ca48.ACE	Gra-293.ACE	H1.ACE	O16.ACE
Pu239.ACE	Pu240.ACE	Pu241.ACE	Pu242.ACE		
pu-met-fast-001-CASE_1					
Ga0.ACE	Pu239.ACE	Pu240.ACE	Pu241.ACE		
pu-met-fast-002-CASE_1					
Ga0.ACE	Pu239.ACE	Pu240.ACE	Pu241.ACE	Pu242.ACE	
pu-met-fast-003-case103					
Al27.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	Pu239.ACE
Pu240.ACE	Pu241.ACE	Pu242.ACE			
pu-met-fast-005-CASE_1					
Cu63.ACE	Cu65.ACE	Ga0.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE
Ni62.ACE	Ni64.ACE	Pu239.ACE	Pu240.ACE	Pu241.ACE	W182.ACE
W183.ACE	W184.ACE	W186.ACE	Zr90.ACE	Zr91.ACE	Zr92.ACE
Zr94.ACE	Zr96.ACE				
pu-met-fast-006					
Ga0.ACE	Pu239.ACE	Pu240.ACE	Pu241.ACE	U234.ACE	U235.ACE
U238.ACE					

pu-met-fast-008-case2					
Ga0.ACE	Pu239.ACE	Pu240.ACE	Pu241.ACE	Th232.ACE	
pu-met-fast-009-CASE_1					
Al27.ACE	Ga0.ACE	Pu239.ACE	Pu240.ACE	Pu241.ACE	
pu-met-fast-010-CASE_1					
Ga0.ACE	Pu239.ACE	Pu240.ACE	Pu241.ACE	U235.ACE	U238.ACE
pu-met-fast-011-CASE_1					
H1.ACE	H2O-293.ACE	O16.ACE	Pu239.ACE	Pu240.ACE	Pu241.ACE
Pu242.ACE					
pu-met-fast-018-CASE_1					
Be9.ACE	BeO-293.ACE	Ga0.ACE	O16.ACE	Pu239.ACE	Pu240.ACE
Pu241.ACE					
pu-met-fast-019					
Be-293.ACE	Be9.ACE	C0.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE
Fe56.ACE	Fe57.ACE	Fe58.ACE	Ga0.ACE	Ni58.ACE	Ni60.ACE
Ni61.ACE	Ni62.ACE	Ni64.ACE	O16.ACE	Pu239.ACE	Pu240.ACE
Pu241.ACE	W182.ACE	W183.ACE	W184.ACE	W186.ACE	
pu-met-fast-020					
Al27.ACE	C0.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	Ga0.ACE	Mg24.ACE	Mg25.ACE	Mg26.ACE
Mn55.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE
Pu239.ACE	Pu240.ACE	Pu241.ACE	U235.ACE	U238.ACE	W182.ACE
W183.ACE	W184.ACE	W186.ACE			
pu-met-fast-021-case1					
Al27.ACE	Be-293.ACE	Be9.ACE	C0.ACE	Cr50.ACE	Cr52.ACE
Cr53.ACE	Cr54.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	Mg24.ACE	Mg25.ACE	Mg26.ACE	Mn55.ACE
Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE	O16.ACE
Pu239.ACE	Pu240.ACE	Pu241.ACE	Si28.ACE	Si29.ACE	Si30.ACE
Ti46.ACE	Ti47.ACE	Ti48.ACE	Ti49.ACE	Ti50.ACE	
pu-met-fast-021-case2					
Al27.ACE	Be9.ACE	BeO-293.ACE	C0.ACE	Cr50.ACE	Cr52.ACE
Cr53.ACE	Cr54.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	Mg24.ACE	Mg25.ACE	Mg26.ACE	Mn55.ACE
Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE	O16.ACE
Pu239.ACE	Pu240.ACE	Pu241.ACE	Si28.ACE	Si29.ACE	Si30.ACE
Ti46.ACE	Ti47.ACE	Ti48.ACE	Ti49.ACE	Ti50.ACE	
pu-met-fast-022					
C0.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	Ga0.ACE
Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE	Pu239.ACE
Pu240.ACE					
pu-met-fast-023					
C0.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	Ga0.ACE
Gra-293.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE
Pu239.ACE	Pu240.ACE				
pu-met-fast-024					

C0.ACE	CH2-293.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE
Ga0.ACE	H1.ACE	H2.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE
Ni62.ACE	Ni64.ACE	Pu239.ACE	Pu240.ACE		
pu-met-fast-025					
C0.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	Cu63.ACE
Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	Ga0.ACE
Mn55.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE
Pu239.ACE	Pu240.ACE	Si28.ACE	Si29.ACE	Si30.ACE	
pu-met-fast-026					
C0.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	Cu63.ACE
Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	Ga0.ACE
Mn55.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE
Pu239.ACE	Pu240.ACE	Si28.ACE	Si29.ACE	Si30.ACE	
pu-sol-therm-009-case3a					
Al27.ACE	Cu63.ACE	Cu65.ACE	H1.ACE	H2O-293.ACE	Mn55.ACE
N14.ACE	O16.ACE	Pu238.ACE	Pu239.ACE	Pu240.ACE	Pu241.ACE
Pu242.ACE	Si28.ACE	Si29.ACE	Si30.ACE		
pu-sol-therm-011-CASE_1.18					
Cd106.ACE	Cd108.ACE	Cd110.ACE	Cd111.ACE	Cd112.ACE	Cd113.ACE
Cd114.ACE	Cd116.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE
Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	H1.ACE	H2O-293.ACE
N14.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE
O16.ACE	Pu239.ACE	Pu240.ACE			
pu-sol-therm-011-CASE_5.16					
Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	H1.ACE	H2O-293.ACE	N14.ACE	Ni58.ACE
Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE	O16.ACE	Pu239.ACE
Pu240.ACE					
pu-sol-therm-011-CASE_6.18					
Cd106.ACE	Cd108.ACE	Cd110.ACE	Cd111.ACE	Cd112.ACE	Cd113.ACE
Cd114.ACE	Cd116.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE
Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	H1.ACE	H2O-293.ACE
N14.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE
O16.ACE	Pu239.ACE	Pu240.ACE			
pu-sol-therm-018-case_9					
Am241.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	Fe54.ACE
Fe56.ACE	Fe57.ACE	Fe58.ACE	Gd152.ACE	Gd154.ACE	Gd155.ACE
Gd156.ACE	Gd157.ACE	Gd158.ACE	Gd160.ACE	H1.ACE	H2O-293.ACE
N14.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE
O16.ACE	Pu238.ACE	Pu239.ACE	Pu240.ACE	Pu241.ACE	Pu242.ACE
pu-sol-therm-021-case_1.t9a					
Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	H1.ACE	H2O-293.ACE	Mn55.ACE	N14.ACE
Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE	O16.ACE
Pu238.ACE	Pu239.ACE	Pu240.ACE	Pu241.ACE	Pu242.ACE	
pu-sol-therm-021-CASE_3.T9A					

Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	H1.ACE	H2O-293.ACE	Mn55.ACE	N14.ACE
Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE	O16.ACE
Pu238.ACE	Pu239.ACE	Pu240.ACE	Pu241.ACE	Pu242.ACE	
pu-sol-therm-034-case_01					
Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	Gd152.ACE	Gd154.ACE	Gd155.ACE	Gd156.ACE
Gd157.ACE	Gd158.ACE	Gd160.ACE	H1.ACE	H2O-293.ACE	N14.ACE
Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE	O16.ACE
Pu238.ACE	Pu239.ACE	Pu240.ACE	Pu241.ACE	Pu242.ACE	

Table 17. Isotopes/materials in HEU Benchmarks

heu-comp-inter-003-case7					
Al27.ACE	Au197.ACE	Be9.ACE	C0.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	H1.ACE	Mn55.ACE	N14.ACE	O16.ACE
U234.ACE	U235.ACE	U236.ACE	U238.ACE		
heu-met-fast-001					
N14.ACE	O16.ACE	U234.ACE	U235.ACE	U238.ACE	
heu-met-fast-003-case1					
U234.ACE	U235.ACE	U238.ACE			
heu-met-fast-003-case10					
C0.ACE	U234.ACE	U235.ACE	U238.ACE	W182.ACE	W183.ACE
W184.ACE	W186.ACE				
heu-met-fast-003-case11					
C0.ACE	U234.ACE	U235.ACE	U238.ACE	W182.ACE	W183.ACE
W184.ACE	W186.ACE				
heu-met-fast-003-case12					
Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE	U234.ACE
U235.ACE	U238.ACE				
heu-met-fast-003-case2					
U234.ACE	U235.ACE	U238.ACE			
heu-met-fast-003-case3					
U234.ACE	U235.ACE	U238.ACE			
heu-met-fast-003-case4					
U234.ACE	U235.ACE	U238.ACE			
heu-met-fast-003-case5					
U234.ACE	U235.ACE	U238.ACE			
heu-met-fast-003-case6					
U234.ACE	U235.ACE	U238.ACE			
heu-met-fast-003-case7					
U234.ACE	U235.ACE	U238.ACE			
heu-met-fast-003-case8					
C0.ACE	U234.ACE	U235.ACE	U238.ACE	W182.ACE	W183.ACE
W184.ACE	W186.ACE				
heu-met-fast-003-case9					
C0.ACE	U234.ACE	U235.ACE	U238.ACE	W182.ACE	W183.ACE
W184.ACE	W186.ACE				
heu-met-fast-004-case1					
H1.ACE	H20-293.ACE	O16.ACE	U234.ACE	U235.ACE	U236.ACE
U238.ACE					
heu-met-fast-008					

Al27.ACE	C0.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE
Ni64.ACE	U234.ACE	U235.ACE	U236.ACE	U238.ACE	W182.ACE
W183.ACE	W184.ACE	W186.ACE			
heu-met-fast-009-case1					
Be-293.ACE	Be9.ACE	C0.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE
Fe56.ACE	Fe57.ACE	Fe58.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE
Ni62.ACE	Ni64.ACE	O16.ACE	U234.ACE	U235.ACE	U236.ACE
U238.ACE	W182.ACE	W183.ACE	W184.ACE	W186.ACE	
heu-met-fast-009-case2					
Be9.ACE	BeO-293.ACE	C0.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE
Fe56.ACE	Fe57.ACE	Fe58.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE
Ni62.ACE	Ni64.ACE	O16.ACE	U234.ACE	U235.ACE	U236.ACE
U238.ACE	W182.ACE	W183.ACE	W184.ACE	W186.ACE	
heu-met-fast-011					
C0.ACE	CH2-293.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	H1.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE
Ni62.ACE	Ni64.ACE	U234.ACE	U235.ACE	U236.ACE	U238.ACE
W182.ACE	W183.ACE	W184.ACE	W186.ACE		
heu-met-fast-012					
Al27.ACE	C0.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE
Ni64.ACE	U234.ACE	U235.ACE	U236.ACE	U238.ACE	W182.ACE
W183.ACE	W184.ACE	W186.ACE			
heu-met-fast-013					
C0.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	Cu63.ACE
Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	Mn55.ACE
Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE	Si28.ACE
Si29.ACE	Si30.ACE	U234.ACE	U235.ACE	U236.ACE	U238.ACE
W182.ACE	W183.ACE	W184.ACE	W186.ACE		
heu-met-fast-014					
Al27.ACE	C0.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	Mg24.ACE	Mg25.ACE	Mg26.ACE	Mn55.ACE
Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE	U234.ACE
U235.ACE	U236.ACE	U238.ACE	W182.ACE	W183.ACE	W184.ACE
W186.ACE					
heu-met-fast-015					
C0.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	U234.ACE
U235.ACE	U238.ACE	W182.ACE	W183.ACE	W184.ACE	W186.ACE
heu-met-fast-018-case2					
C0.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	U234.ACE
U235.ACE	U238.ACE	W182.ACE	W183.ACE	W184.ACE	W186.ACE
heu-met-fast-019-case2					
C0.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	Gra-
293.ACE					
U234.ACE	U235.ACE	U238.ACE	W182.ACE	W183.ACE	W184.ACE
W186.ACE					
heu-met-fast-020-case2					

C0.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	H1.ACE
H2.ACE	U234.ACE	U235.ACE	U238.ACE	W182.ACE	W183.ACE
W184.ACE	W186.ACE	CH2-293.ACE			
heu-met-fast-021-case2					
C0.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	Cu63.ACE
Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	Mn55.ACE
Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE	Si28.ACE
Si29.ACE	Si30.ACE	U234.ACE	U235.ACE	U238.ACE	W182.ACE
W183.ACE	W184.ACE	W186.ACE			
heu-met-fast-022-case2					
Al27.ACE	C0.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	U234.ACE	U235.ACE	U238.ACE	W182.ACE
W183.ACE	W184.ACE	W186.ACE			
heu-met-fast-026-case9					
Al27.ACE	C0.ACE	Ca40.ACE	Ca42.ACE	Ca43.ACE	Ca44.ACE
Ca46.ACE	Ca48.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE
Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	H1.ACE	Mg24.ACE
Mg25.ACE	Mg26.ACE	Mn55.ACE	Na23.ACE	Ni58.ACE	Ni60.ACE
Ni61.ACE	Ni62.ACE	Ni64.ACE	O16.ACE	Si28.ACE	Si29.ACE
Si30.ACE	U234.ACE	U235.ACE	U236.ACE	U238.ACE	CH2-293.ACE
heu-met-fast-028					
U234.ACE	U235.ACE	U238.ACE			
heu-met-inter-006-case1					
Al27.ACE	C0.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE
Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE
Gra-293.ACE	Mg24.ACE	Mg25.ACE	Mg26.ACE	Mn55.ACE	Si28.ACE
Si29.ACE	Si30.ACE	Ti46.ACE	Ti47.ACE	Ti48.ACE	Ti49.ACE
Ti50.ACE	U234.ACE	U235.ACE	U236.ACE	U238.ACE	
heu-met-inter-006-case2					
Al27.ACE	C0.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE
Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE
Gra-293.ACE	Mg24.ACE	Mg25.ACE	Mg26.ACE	Mn55.ACE	Si28.ACE
Si29.ACE	Si30.ACE	Ti46.ACE	Ti47.ACE	Ti48.ACE	Ti49.ACE
Ti50.ACE	U234.ACE	U235.ACE	U236.ACE	U238.ACE	
heu-met-inter-006-case3					
Al27.ACE	C0.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE
Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE
Gra-293.ACE	Mg24.ACE	Mg25.ACE	Mg26.ACE	Mn55.ACE	Si28.ACE
Si29.ACE	Si30.ACE	Ti46.ACE	Ti47.ACE	Ti48.ACE	Ti49.ACE
Ti50.ACE	U234.ACE	U235.ACE	U236.ACE	U238.ACE	
heu-met-inter-006-case4					
Al27.ACE	C0.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE
Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE
Gra-293.ACE	Mg24.ACE	Mg25.ACE	Mg26.ACE	Mn55.ACE	Si28.ACE
Si29.ACE	Si30.ACE	Ti46.ACE	Ti47.ACE	Ti48.ACE	Ti49.ACE
Ti50.ACE	U234.ACE	U235.ACE	U236.ACE	U238.ACE	
heu-sol-therm-013-case1					

Al27.ACE	Cu63.ACE	Cu65.ACE	H1.ACE	H2O-293.ACE	Mn55.ACE
N14.ACE	O16.ACE	Si28.ACE	Si29.ACE	Si30.ACE	U234.ACE
U235.ACE	U236.ACE	U238.ACE			
heu-sol-therm-013-case2					
Al27.ACE	B10.ACE	B11.ACE	Cu63.ACE	Cu65.ACE	H1.ACE
H2O-293.ACE	Mn55.ACE	N14.ACE	O16.ACE	Si28.ACE	Si29.ACE
Si30.ACE	U234.ACE	U235.ACE	U236.ACE	U238.ACE	
heu-sol-therm-013-case3					
Al27.ACE	B10.ACE	B11.ACE	Cu63.ACE	Cu65.ACE	H1.ACE
H2O-293.ACE	Mn55.ACE	N14.ACE	O16.ACE	Si28.ACE	Si29.ACE
Si30.ACE	U234.ACE	U235.ACE	U236.ACE	U238.ACE	
heu-sol-therm-013-case4					
Al27.ACE	B10.ACE	B11.ACE	Cu63.ACE	Cu65.ACE	H1.ACE
H2O-293.ACE	Mn55.ACE	N14.ACE	O16.ACE	Si28.ACE	Si29.ACE
Si30.ACE	U234.ACE	U235.ACE	U236.ACE	U238.ACE	
heu-sol-therm-032					
Al27.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE
Fe58.ACE	H1.ACE	Mn55.ACE	N14.ACE	O16.ACE	Si28.ACE
Si29.ACE	Si30.ACE	U233.ACE	U234.ACE	U235.ACE	U236.ACE
U238.ACE	H2O-293.ACE				
u233-comp-therm-001-case6					
B10.ACE	C0.ACE	CH2-293.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE
Cr54.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	Gd152.ACE
Gd154.ACE	Gd155.ACE	Gd156.ACE	Gd157.ACE	Gd158.ACE	Gd160.ACE
H1.ACE	H2O-293.ACE	Mn55.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE
Ni62.ACE	Ni64.ACE	O16.ACE	Sn112.ACE	Sn114.ACE	Sn115.ACE
Sn116.ACE	Sn117.ACE	Sn118.ACE	Sn119.ACE	Sn120.ACE	Sn122.ACE
Sn124.ACE	Th232.ACE	U234.ACE	U235.ACE	U238.ACE	Zr90.ACE
Zr91.ACE	Zr92.ACE	Zr94.ACE	Zr96.ACE		

Table 18. Isotopes/materials in IEU Benchmarks

ieu-comp-therm-002-CASE 3					
Al27.ACE	C0.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE
Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	Gd152.ACE	Gd154.ACE
Gd155.ACE	Gd156.ACE	Gd157.ACE	Gd158.ACE	Gd160.ACE	H1.ACE
H2O-293.ACE	Mn55.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE
Ni64.ACE	O16.ACE	Si28.ACE	Si29.ACE	Si30.ACE	Ti46.ACE
Ti47.ACE	Ti48.ACE	Ti49.ACE	Ti50.ACE	U234.ACE	U235.ACE
U238.ACE					
ieu-met-fast-001-case1					
Al27.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	Cu63.ACE
Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	Mg24.ACE
Mg25.ACE	Mg26.ACE	Mn55.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE
Ni62.ACE	Ni64.ACE	U234.ACE	U235.ACE	U238.ACE	
ieu-met-fast-001-case2					
Al27.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	Cu63.ACE
Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	Mg24.ACE
Mg25.ACE	Mg26.ACE	Mn55.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE
Ni62.ACE	Ni64.ACE	U234.ACE	U235.ACE	U238.ACE	
ieu-met-fast-001-case3					
Al27.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	Cu63.ACE
Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	Mg24.ACE
Mg25.ACE	Mg26.ACE	Mn55.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE
Ni62.ACE	Ni64.ACE	U234.ACE	U235.ACE	U238.ACE	
ieu-met-fast-001-case4					
Al27.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	Cu63.ACE
Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	Mg24.ACE
Mg25.ACE	Mg26.ACE	Mn55.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE
Ni62.ACE	Ni64.ACE	U234.ACE	U235.ACE	U238.ACE	
ieu-met-fast-002					
U234.ACE	U235.ACE	U238.ACE			
ieu-met-fast-003-case2					
C0.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE
Fe58.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE
U234.ACE	U235.ACE	U238.ACE	W182.ACE	W183.ACE	W184.ACE
W186.ACE					
ieu-met-fast-004-case2					
C0.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	Gra-
293.ACE					
U234.ACE	U235.ACE	U238.ACE	W182.ACE	W183.ACE	W184.ACE
W186.ACE					
ieu-met-fast-005-case2					
C0.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	Cu63.ACE
Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	Mn55.ACE
Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE	Si28.ACE
Si29.ACE	Si30.ACE	U234.ACE	U235.ACE	U238.ACE	W182.ACE
W183.ACE	W184.ACE	W186.ACE			
ieu-met-fast-006-case2					

Al27.ACE	C0.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE
Ni64.ACE	U234.ACE	U235.ACE	U238.ACE	W182.ACE	W183.ACE
W184.ACE	W186.ACE				
ieu-met-fast-007-case1					
Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	Mn55.ACE	Nb93.ACE	Ni58.ACE	Ni60.ACE
Ni61.ACE	Ni62.ACE	Ni64.ACE	Si28.ACE	Si29.ACE	Si30.ACE
U234.ACE	U235.ACE	U236.ACE	U238.ACE		
leu-sol-therm-007-CASE14					
Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	H1.ACE	H20-293.ACE	Mn55.ACE	N14.ACE
Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE	O16.ACE
P31.ACE	S32.ACE	S33.ACE	S34.ACE	S36.ACE	Si28.ACE
Si29.ACE	Si30.ACE	U234.ACE	U235.ACE	U236.ACE	U238.ACE
C0.ACE					
leu-sol-therm-007-CASE30					
Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	H1.ACE	H20-293.ACE	Mn55.ACE	N14.ACE
Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE	O16.ACE
P31.ACE	S32.ACE	S33.ACE	S34.ACE	S36.ACE	Si28.ACE
Si29.ACE	Si30.ACE	U234.ACE	U235.ACE	U236.ACE	U238.ACE
C0.ACE					
leu-sol-therm-007-CASE32					
Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	H1.ACE	H20-293.ACE	Mn55.ACE	N14.ACE
Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE	O16.ACE
P31.ACE	S32.ACE	S33.ACE	S34.ACE	S36.ACE	Si28.ACE
Si29.ACE	Si30.ACE	U234.ACE	U235.ACE	U236.ACE	U238.ACE
C0.ACE					
leu-sol-therm-007-CASE36					
Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	H1.ACE	H20-293.ACE	Mn55.ACE	N14.ACE
Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE	O16.ACE
P31.ACE	S32.ACE	S33.ACE	S34.ACE	S36.ACE	Si28.ACE
Si29.ACE	Si30.ACE	U234.ACE	U235.ACE	U236.ACE	U238.ACE
C0.ACE					
leu-sol-therm-007-CASE49					
Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	Fe54.ACE	Fe56.ACE
Fe57.ACE	Fe58.ACE	H1.ACE	H20-293.ACE	Mn55.ACE	N14.ACE
Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE	O16.ACE
P31.ACE	S32.ACE	S33.ACE	S34.ACE	S36.ACE	Si28.ACE
Si29.ACE	Si30.ACE	U234.ACE	U235.ACE	U236.ACE	U238.ACE
C0.ACE					
mix-met-fast-008-case7					
Al27.ACE	C0.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE
Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE
H1.ACE	Mn55.ACE	Mo100.ACE	Mo92.ACE	Mo94.ACE	Mo95.ACE
Mo96.ACE	Mo97.ACE	Mo98.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE
Ni62.ACE	Ni64.ACE	O16.ACE	Si28.ACE	Si29.ACE	Si30.ACE
Ti46.ACE	Ti47.ACE	Ti48.ACE	Ti49.ACE	Ti50.ACE	U235.ACE
U238.ACE	V0.ACE				

Table 19. Isotopes/materials in LEU Benchmarks

leu-comp-ther-008-CASE 1					
Al27.ACE	B10.ACE	B11.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE
Cr54.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE
Fe58.ACE	H1.ACE	H20-293.ACE	Mg24.ACE	Mg25.ACE	Mg26.ACE
Mn55.ACE	O16.ACE	Si28.ACE	Si29.ACE	Si30.ACE	Ti46.ACE
Ti47.ACE	Ti48.ACE	Ti49.ACE	Ti50.ACE	U234.ACE	U235.ACE
U238.ACE					
leu-comp-therm-008-CASE 11					
Al27.ACE	B10.ACE	B11.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE
Cr54.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE
Fe58.ACE	H1.ACE	H20-293.ACE	Mg24.ACE	Mg25.ACE	Mg26.ACE
Mn55.ACE	O16.ACE	Si28.ACE	Si29.ACE	Si30.ACE	Ti46.ACE
Ti47.ACE	Ti48.ACE	Ti49.ACE	Ti50.ACE	U234.ACE	U235.ACE
U238.ACE					
leu-comp-therm-008-CASE 2					
Al27.ACE	B10.ACE	B11.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE
Cr54.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE
Fe58.ACE	H1.ACE	H20-293.ACE	Mg24.ACE	Mg25.ACE	Mg26.ACE
Mn55.ACE	O16.ACE	Si28.ACE	Si29.ACE	Si30.ACE	Ti46.ACE
Ti47.ACE	Ti48.ACE	Ti49.ACE	Ti50.ACE	U234.ACE	U235.ACE
U238.ACE					
leu-comp-therm-008-CASE 5					
Al27.ACE	B10.ACE	B11.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE
Cr54.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE
Fe58.ACE	H1.ACE	H20-293.ACE	Mg24.ACE	Mg25.ACE	Mg26.ACE
Mn55.ACE	Na23.ACE	O16.ACE	Si28.ACE	Si29.ACE	Si30.ACE
Ti46.ACE	Ti47.ACE	Ti48.ACE	Ti49.ACE	Ti50.ACE	U234.ACE
U235.ACE	U238.ACE				
leu-comp-therm-008-CASE 7					
Al27.ACE	B10.ACE	B11.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE
Cr54.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE
Fe58.ACE	H1.ACE	H20-293.ACE	Mg24.ACE	Mg25.ACE	Mg26.ACE
Mn55.ACE	Na23.ACE	O16.ACE	Si28.ACE	Si29.ACE	Si30.ACE
Ti46.ACE	Ti47.ACE	Ti48.ACE	Ti49.ACE	Ti50.ACE	U234.ACE
U235.ACE	U238.ACE				
leu-comp-therm-008-CASE 8					
Al27.ACE	B10.ACE	B11.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE
Cr54.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE
Fe58.ACE	H1.ACE	H20-293.ACE	Mg24.ACE	Mg25.ACE	Mg26.ACE
Mn55.ACE	Na23.ACE	O16.ACE	Si28.ACE	Si29.ACE	Si30.ACE
Ti46.ACE	Ti47.ACE	Ti48.ACE	Ti49.ACE	Ti50.ACE	U234.ACE
U235.ACE	U238.ACE				
leu-sol-therm-002-case1					
Al27.ACE	Cu63.ACE	Cu65.ACE	F19.ACE	H1.ACE	H20-293.ACE
Mn55.ACE	O16.ACE	Si28.ACE	Si29.ACE	Si30.ACE	U234.ACE
U235.ACE	U238.ACE				
leu-sol-therm-002-case2					

Al27.ACE	Cu63.ACE	Cu65.ACE	F19.ACE	H1.ACE	H2O-
293.ACE					
Mn55.ACE	O16.ACE	Si28.ACE	Si29.ACE	Si30.ACE	U234.ACE
U235.ACE	U238.ACE				

Table 20. Isotopes/materials in additional Benchmarks

heu-met-fast-73					
Al27.ACE	C0.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE
Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE
Mg24.ACE	Mg25.ACE	Mg26.ACE	Mn55.ACE	Mo100.ACE	Mo92.ACE
Mo94.ACE	Mo95.ACE	Mo96.ACE	Mo97.ACE	Mo98.ACE	N14.ACE
N15.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE
P31.ACE	S32.ACE	S33.ACE	S34.ACE	S36.ACE	Ti46.ACE
Ti47.ACE	Ti48.ACE	Ti49.ACE	Ti50.ACE	U234.ACE	U235.ACE
U236.ACE	U238.ACE	Si28.ACE	Si29.ACE	Si30.ACE	
heu-sol-therm-004					
Cr50.ACE	Cr52.ACE	Cr53.ACE	Cr54.ACE	D2O-293.ACE	F19.ACE
Fe54.ACE	Fe56.ACE	Fe57.ACE	Fe58.ACE	H1.ACE	H2.ACE
Mn55.ACE	Ni58.ACE	Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE
O16.ACE	Si28.ACE	Si29.ACE	Si30.ACE	U234.ACE	U235.ACE
U238.ACE					
pu-sol-therm-009					
Al27.ACE	Cu63.ACE	Cu65.ACE	H1.ACE	H2O-293.ACE	Mn55.ACE
N14.ACE	O16.ACE	Pu238.ACE	Pu239.ACE	Pu240.ACE	Pu241.ACE
Pu242.ACE	Si28.ACE	Si29.ACE	Si30.ACE		
spec-met-fast-008					
Al27.ACE	Am241.ACE	Am243.ACE	Cr50.ACE	Cr52.ACE	Cr53.ACE
Cr54.ACE	Cu63.ACE	Cu65.ACE	Fe54.ACE	Fe56.ACE	Fe57.ACE
Fe58.ACE	Mg24.ACE	Mg25.ACE	Mg26.ACE	Mn55.ACE	Ni58.ACE
Ni60.ACE	Ni61.ACE	Ni62.ACE	Ni64.ACE	Np237.ACE	Pu238.ACE
Pu239.ACE	Pu240.ACE	Pu241.ACE	Pu242.ACE	Ti46.ACE	Ti47.ACE
Ti48.ACE	Ti49.ACE	Ti50.ACE	U233.ACE	U234.ACE	U235.ACE
U236.ACE	U238.ACE	W182.ACE	W183.ACE	W184.ACE	W186.ACE
Si28.ACE	Si29.ACE	Si30.ACE			

3.1. *Problems found in this criticality study*

- Problems in “ptables” from file Pu238.ACE are found with a fatal error in the unresolved table interpolation. This problem is solved using a 238Pu ACE file without ptable option. No PURR module is used in this case.

```
...
fatal error. error in unresolved table interpolation.
94238.03c 147626 94-Pu-238 from JEFF3.1.2, NJOY99.364, NEA_Dec2011 total nu mat9434 12/21/11
probability tables used from 5.0000E-04 to 1.5000E-01 mev.
temperature = 2.5850E-08 adjusted to 2.5300E-08
...
```

This problem occurs in these cases:

- mix-comp-therm-002-case-pnl30
- mix-comp-therm-002-case-pnl31
- mix-comp-therm-002-case-pnl32
- mix-comp-therm-002-case-pnl33
- mix-comp-therm-002-case-pnl34
- mix-comp-therm-002-case-pnl35

- pu-sol-therm-009-case3a

- pu-sol-therm-018-case_9
- pu-sol-therm-021-case_1.t9a
- pu-sol-therm-021-CASE_3.T9A
- pu-sol-therm-034-case_01

- pu-sol-therm-009
- spec-met-fast-008

-
- Using the original inputs provided in ICSBEP-2012, a problem running with MCNP5_1.5 is found. This problem is solved changing the neutron source in the input at the origin coordinates (0.0000). Instead of “0.00000” a value of “0.00015” is used in the input. It solves the problem of neutron losses.

ksrc	0.00015	0.0001	-70.0	1.63576	0.0001	-70.0
	3.27152	0.0001	-70.0	4.90728	0.0001	-70.0
	6.54304	0.0001	-70.0	8.17880	0.0001	-70.0
	9.81456	0.0001	-70.0	11.45032	0.0001	-70.0
	13.08608	0.0001	-70.0	14.72184	0.0001	-70.0
	16.35760	0.0001	-70.0	17.99336	0.0001	-70.0
	19.62912	0.0001	-70.0	21.26488	0.0001	-70.0
	22.90064	0.0001	-70.0	24.53640	0.0001	-70.0
	26.17216	0.0001	-70.0	27.80792	0.0001	-70.0
	29.44368	0.0001	-70.0	31.07944	0.0001	-70.0
	32.71520	0.0001	-70.0	34.35096	0.0001	-70.0
	35.98672	0.0001	-70.0	37.62248	0.0001	-70.0
	39.25824	0.0001	-70.0	40.89400	0.0001	-70.0
	42.52976	0.0001	-70.0	44.16552	0.0001	-70.0
	45.80128	0.0001	-70.0	47.43704	0.0001	-70.0
	49.07280	0.0001	-70.0			
	0.00015	0.0001	0.0	1.63576	0.0001	0.0
	3.27152	0.0001	0.0	4.90728	0.0001	0.0
	6.54304	0.0001	0.0	8.17880	0.0001	0.0
	9.81456	0.0001	0.0	11.45032	0.0001	0.0
...						
...						

This problem takes place in these cases:

- leu-comp-ther-008-CASE_1
- leu-comp-therm-008-CASE_11
- leu-comp-therm-008-CASE_2
- leu-comp-therm-008-CASE_5
- leu-comp-therm-008-CASE_7
- leu-comp-therm-008-CASE_8

➤ Problems found and solved in ICSBEP September 2010 Edition inputs

- **u233-sol-therm-001-case1**

A problem defining the 3rd region is found.

```
U233-SOL-THERM-001 #3, 1.0274 g/l Unreflected 27.24" Sphere ENDF/B-V
1 0.10026 -1 $ Spherical Solution U(NO3)2-H2O
2 0.060275 1 -2 $ Spherical Shell of Al-1100
0 2

1 so 34.595 $ Inner Radius of Al-1100 Sphell
2 so 34.915 $ Outer RAdius of Al-1100 Sphell

mode n
imp:n 1 1 0
...
...
```

And, it should be changed by :

```
U233-SOL-THERM-001 #3, 1.0274 g/l Unreflected 27.24" Sphere ENDF/B-V
1 1 0.10026 -1 $ Spherical Solution U(NO3)2-H2O
2 2 0.060275 1 -2 $ Spherical Shell of Al-1100
3 0 2

1 so 34.595 $ Inner Radius of Al-1100 Sphell
2 so 34.915 $ Outer RAdius of Al-1100 Sphell

mode n
imp:n 1 1 0
...
...
```

- **u233-sol-therm-008-case1**

A typo-error is found in surface "1201".

B&W	Criticals	Core	XI	Load	1	1511	PPM	Axially	Uniform	Octant	ENDF/B-VI
c	Central Assembly										
1	1	0.068525	1	-2	3	4	-88				\$ Fuel
2	2	0.055323	1	-2	3	4	88	-89			\$ Clad
3	3	0.10019	1	-2	3	4	89	-47			\$ Water
4	1	0.068525	1	-2	3	-90					\$ Fuel
...											
...											
1200	c/z	44.16552	27.80792		0.514858						
1201	c/z	44.16552	27.80792		0.602996						
1202	c/z	45.80128	27.80792		0.514858						
...											
...											

4. QA procedure: warnings & messages

4.1. Checking NJOY output messages for each material

The total number of messages was compiled. All messages were understood, most of them are related to incomplete evaluations.

(1) RECONR Output messages

- Message – non positive elastic cross section.

Some evaluations uses old single-level Breit-Wigner resonance parameters. This representation occasionally goes negative. NJOY fixes this by setting the cross section to a small positive value.

```
---message from emerge---nonpositive elastic cross sections found.  
Ar40  Gd152 Gd157 Ni61  S36   Si32  Te128 U240
```

- The initial value of a threshold reaction cross section is different from zero. NJOY has corrected this by using a jump in the cross section at the threshold energy.

```
---message from lunion---xsec nonzero at threshold for mt= XX  
Am243 Cl35  Cl37  Eu155 F19   Nd150 O16  Pb204
```

- This message can be ignored

```
---message from rdf2bw---calculation of angular distribution not installed
```

```
Al27  Ar39  Ar41  As75  Ba133 Ba139 Br79  Br81  C13   Ca41  
Ca45  Cd106 Cd108 Cd109 Cd110 Cd111 Cd112 Cd114 Cd116 Ce136  
Ce138 Ce139 Ce143 Cl36  Cl37  Co57  Co60  Cr50  Cr51  Cr52  
Cr53  Cr54  Cu63  Cu64  Cu65  Cu66  Dy156 Dy158 Dy160 Dy165  
Er166 Er167 Er168 Er169 Er170 Er171 Er172 Eu152M Fe54  
Fe58  Ga69  Ga71  Gd148 Gd152 Gd153 Gd154 Gd161 Ge70  Ge72  
Ge73  Ge74  Ge76  Hf181 Ho166M I126  I127  I128  I129  
Ir192 K39   K40   K41   Kr78  Kr80  Kr82  Kr83  Kr84  Kr85  
Kr86  La138 La140 Lu175 Lu176 Lu177 Mg27  Mn53  Mn54  Ne20  
Ne21  Ne22  Ni58  Ni60  Ni63  O17   O18   Os184 Os186 Os187  
Os188 Os189 Os190 Os191 Os192 Os193 P31   Pa231 Pa233 Pb204  
Pb205 Pb206 Pb207 Pb208 Po209 Pt190 Pt192 Pt194 Pt195 Pt196  
Pt198 Rb85  Rb86  Rb87  Rb88  Re185 Re187 Re188 Rh104 S32  
S33   S34   S36   Sc46  Se74  Se76  Se77  Se78  Se79  Se80  
Se82  Si28  Si29  Si30  Si31  Si32  Sn122 Sn124 Sr84  Sr86  
Sr87  Sr88  Sr89  Sr90  Ta180M Tb160 Tc98  Tc99  Te122  
Te124 Te131M Th232 Tl203 Tl204 Tl205 Tm169 Tm170 Tm171  
V49   W182  W183  W184  W186  Y90   Y91   Yb168 Yb169 Yb170  
Yb171 Yb172 Yb173 Yb174 Yb176 Zn64  Zn66  Zn67  Zn68  Zn70  
Zr92  Zr94
```

(2) HEATR Output messages

- File 12 (multiplicities for photon production) is missing from the ENDF file.

```
---message from gheat---no file 12 for this material.  
Mo100 Mo96 Mo97 Mo98 N15
```

•

```
---message from h6ddx---vertical segment(s) in distribution  
Cd115M Cf253 Cm240 Cm241 Cm242 Cm243 Cm244 Cm245 Cm246 Cm247  
Cm248 Cm249 Cm250 Eu157 Fe56 Gd152 Gd154 I130 Pa231 Pa232 Pa233  
Pm151 Sn113 Th232 U232 W180
```

- No angular distribution is given for the secondary mt in the evaluation. HEATR assumes isotropic distribution

```
---message from hinit---mf4 and 6 missing, isotropy assumed for mt =XX  
B10 N14
```

- The energy-angle distribution for the specified particle is missing in file 6. NJOY requires energy distributions for all secondary particles from a reaction to compute the energy deposition. In this case, NJOY has to make an assumption and generate an approximate to the data needed.

```
---message from hinit---mf6, mtXX does not give recoil za=YY  
Ag107 Ag109 Ag111 Am241 Ar39 Ar41 As75 B11 Ba133 Ba134 Ba139  
Be9 Bi209 Br79 Br81 Cl3 Ca40 Ca41 Ca42 Ca43 Ca44 Ca45  
Ca46 Ca48 Cd109 Cd110 Cd111 Cd113 Cd115M Ce136 Ce138 Ce139  
Ce141 Ce142 Ce143 Ce144 Cf253 Cl36 Cm240 Cm241 Cm242 Cm243 Cm244  
Cm245 Cm246 Cm247 Cm248 Cm249 Cm250 Co57 Co60 Cr50 Cr51 Cr52  
Cr53 Cr54 Cs133 Cs134 Cs135 Cs137 Cu64 Cu66 Dy156 Dy158 Dy160  
Dy161 Dy162 Dy163 Dy164 Dy165 Er166 Er167 Er168 Er169 Er170 Er171  
Er172 Eu152M Eu153 Eu154 Eu155 Eu156 Eu157 Fe54 Fe56 Fe57  
Fe58 Ga69 Ga71 Gd148 Gd152 Gd153 Gd154 Gd155 Gd156 Gd157 Gd158  
Gd161 Ge70 Ge72 Ge73 Ge74 Ge76 H1 H2 Hf174 Hf177 Hf178  
Hf179 Hf180 Hf181 Ho166M I126 I127 I128 I129 I130 I131  
I135 In113 In115 Ir191 Ir192 K39 K40 K41 Kr78 Kr80 Kr82  
Kr83 Kr84 Kr85 Kr86 La138 La139 La140 Li7 Lu175 Lu176 Lu177  
Mg27 Mn53 Mn54 Mn55 Mo100 Mo92 Mo94 Mo95 Mo96 Mo97 Mo98  
N14 Na23 Nb95 Nd143 Nd144 Nd145 Nd146 Nd147 Nd148 Nd150 Ne20  
Ne21 Ne22 Ni63 Np237 O17 O18 Os184 Os186 Os187 Os188 Os189  
Os190 Os191 Os192 Os193 P31 Pa231 Pa232 Pa233 Pb204 Pb205 Pb206  
Pb207 Pb208 Pd104 Pd105 Pd106 Pd107 Pd108 Pm147 Pm148 Pm148M  
Pm149 Pm151 Po209 Pr141 Pr143 Pt190 Pt192 Pt194 Pt195 Pt196 Pt198  
Pu239 Pu240 Rb85 Rb86 Rb87 Rb88 Re185 Re187 Re188 Rh103 Rh104  
Rh105 Ru100 Ru101 Ru102 Ru103 Ru104 Ru105 S32 S33 S34 S36  
Sb121 Sb123 Sc45 Sc46 Se74 Se76 Se77 Se78 Se79 Se80 Se82  
Si31 Si32 Sm144 Sm147 Sm148 Sm149 Sm150 Sm151 Sm152 Sm153 Sm154  
Sn113 Sn122 Sn124 Sr84 Sr86 Sr87 Sr88 Sr89 Sr90 Ta180M  
Ta181 Tb159 Tb160 Tc98 Tc99 Te122 Te124 Te131M Th232 Ti46  
Ti47 Ti48 Ti49 Ti50 Tl203 Tl204 Tl205 Tm169 Tm170 Tm171 U232  
U233 U234 U235 U236 U237 U238 U239 V49 W180 W182 W183  
W184 W186 Xe123 Xe128 Xe129 Xe130 Xe131 Xe132 Xe133 Xe134 Xe135
```

```

Xe136 Y89   Y90   Y91   Yb168 Yb169 Yb170 Yb171 Yb172 Yb173 Yb174
Yb176 Zn64  Zn66  Zn67  Zn68  Zn70  Zr90  Zr91  Zr92  Zr93  Zr94
Zr95   Zr96

```

- In the ENDF format, mt18 (total fission) is the sum of mt19, mt20, mt21 and mt38

```

---message from hinit---mt18 is redundant
      Am242 Pu237 Pu244 U234   U240

```

- The partial contribution to the total fission, mt19, has no spectrum. NJOY will use the mt18 spectrum

```

---message from hinit---mt19 has no spectrum
      Cf253 Np237 Pa232 U232   U233

```

- No partial components of the fission energy released are given in the evaluation

```

---message from hinit---mt458 is missing for this mat
Ac227 Am242 Am244 Am244M      Bk247 Bk249 Bk250 Cf249 Cf250 Cf251
Cf252 Cf254 Cm240 Cm241 Cm247 Cm249 Cm250 Es254 Es255 Fm255 Np235
Np236 Np238 Np239 Pa231 Pa233 Pu243 Pu246 Ra223 Ra226 Th227 Th228
Th229 Th233 Th234 U237

```

- NJOY does not include energy from delayed emission in the prompt heating. The fission Q-value is changed from the total value given in file 3 to a prompt value using the delayed neutron energy from mf1, mt458.

```

---message from nheat---changed q from   E1 to   E2
Am241 Am242M      Am243 Cf253 Cm242 Cm243 Cm244 Cm245 Cm246 Cm248
Np237 Pa232 Pu236 Pu237 Pu238 Pu239 Pu240 Pu241 Pu242 Pu244 Th230
Th232 U232   U233   U234   U235   U236   U238   U239   U240   U241

```

- The ENDF6 format allows an evaluator to describe a subsection of file 6 using LAW=0 (no distribution given). This is fine for particle yields for gas production, . . . but they are not adequate for computing heating and damage.

```

---message from sixbar---no distribution for mt 5 particle **
Bi209 Ca40  Ca42  Ca43  Ca44  Ca46  Ca48  Fe54  Fe56  Fe57  Fe58
Pb204 Pb205 Pb206 Pb207 Pb208 Pu239 Pu240 Sc45  Tc99  U235  U238

```

- Warning in HEATR


```

---message from hconvr---mf3, mt** is missing
Be9

```

- Warning in HEATR


```

---message from hconvr---mf12, mtXX may be missing
Hg199 Ir193 Li6

```

(3) PURR Output messages

- When a material has no resonance parameters associated with it, this message will be issued.

---message from purr---mat XXXX has no resonance parameters

Ac225 Ac226 Ac227 Bi209 Hg196 Hg198 Hg199 Hg200 Hg201 Hg202 Hg204
Pb204 Pb205 Pb206 Pb207 Pb208 Ra223 Ra224 Ra225 Ra226 Tl205

- The entire resolved energy range seems to overlap the unresolved energy range for this material. NJOY deals with this but no probability tables will be generated by purr as there won't be any unresolved resonance parameters left (they are removed from the file). Another possibility is that the material has no unresolved resonances and that purr was run.

---message from purr---mat 4725 has no unresolved parameters

- Warning in PURR

---message from rdf2un---resolved-unresolved overlap energies

Ar39 Co57 Mg27 Ne22 S34 Si31 Sr88 Zr90

(4) ACER Output messages

- The second acer run provides a consistency check of the ACE file produced by the first acer run. Whenever something abnormal is found, this message will be printed.

---message from consis---consistency problems found

Al27 Am241 Ar39 Ar41 As75 Ba133 Ba139 Be9 Bi209 Br79 Br81
C0 C13 Ca40 Ca41 Ca42 Ca43 Ca44 Ca45 Ca46 Ca48 Cd109
Cd110 Cd111 Cd113 Ce136 Ce138 Ce139 Ce143 Cl36 Co57 Co60 Cr50
Cr51 Cr52 Cr53 Cr54 Cr63 Cu64 Cu65 Cu66 Dy156 Dy158 Dy160
Dy165 Er166 Er167 Er168 Er169 Er170 Er171 Er172 Eu152M Fe54
Fe56 Fe57 Fe58 Ga69 Ga71 Gd148 Gd153 Gd161 Ge70 Ge72 Ge73
Ge74 Ge76 Hf181 Hg196 Hg198 Hg199 Hg200 Hg201 Hg202 Hg204 Ho166M
I126 I128 Ir192 K39 K40 K41 Kr78 Kr80 Kr82 Kr83 Kr84
Kr85 Kr86 La138 La140 Lu175 Lu176 Lu177 Mg27 Mn53 Mn54 Mo100
Mo97 N14 Nb93 Ne20 Ne21 Ne22 Ni61 Ni62 Ni63 Ni64 O16
O17 O18 Os184 Os186 Os187 Os188 Os189 Os190 Os191 Os192 Os193
P31 Pb204 Pb205 Pb206 Pb207 Pb208 Po209 Pt190 Pt192 Pt194 Pt195
Pt196 Pt198 Pu239 Pu240 Rb85 Rb86 Rb87 Rb88 Re185 Re187 Re188
Rh104 S32 S33 S34 S36 Sb121 Sb123 Sc45 Sc46 Se74 Se76
Se77 Se78 Se79 Se80 Se82 Si29 Si30 Si31 Si32 Sn122 Sn124
Sr84 Sr86 Sr87 Sr88 Sr89 Sr90 Ta180M Ta181 Tb160 Tc98
Tc99 Te122 Te124 Te131M Tl203 Tl204 Tl205 Tm169 Tm170 Tm171
U235 U236 U237 U238 V49 W182 W183 W184 W186 Y90 Y91
Yb168 Yb169 Yb170 Yb171 Yb172 Yb173 Yb174 Yb176 Zn64 Zn66 Zn67
Zn68 Zn70 Zr90 Zr92 Zr94 Zr96

-
- This message indicates that a negative PDF value was found, NJOY sets the value to zero and renormalizes the distribution

```

---message from ptleg2---negative probs found
Ac225 Ac227 Ag109 Am244 Am244M Au197 B10 B11 Bk250 Cf254
Co58 Dy164 Es254 Es255 Fm255 Hf177 Hf179 Hg196 Hg198 Ho165 Ir191
Np237 Pa231 Pa233 Pd110 Pu238 Pu240 Pu244 Pu246 Ra223 Ra224 Ra225
Ra226 Rh105 Ru101 Sm151 Th229 Th230 U234 U239 U240 U241 W180
Xe136 Y89

```

- The ptleg subroutine of the acer module translates ENDF Legendre angular distributions into tabulated form with equal probability m intervals. In this routine the cosine interval $m = -1$ to 1 is divided into 1000 intervals and integrated. When the integral of the angular distribution over such an interval is negative, we receive this message. This is caused by the fact that the Legendre polynomial series can lead to negative values.

```

---message from ptleg---negative area between mu= XX and YY
O16

```

- This error normally surfaces when there is an inconsistency between the threshold energy of a reaction in the ENDF file and the value calculated by NJOY. This is already checked and corrected in reconr so this error should never occur. However, NJOY uses ENDF files to transfer information between modules in which any number is rounded to 6 significant digits. In the case of the above mentioned nuclides, the difference between the calculated value and the one in the ENDF file occurs in the 7th significant digit (which is lost due to rounding).

```

---message from unionx---threshold error
Be9 Cl37 U237 Xe123

```

- Warning in ACER

```

---message from convr---discrete anisotropic photon
H1

```

4.2. Checking PREPRO output messages for each material

In order to compare PREPRO-2004 and NJOY99, ACEQA code runs LINEAR+RECENT+SIGMA1 codes.

Warnings and messages from these codes are useful to complete an additional check. **ANNEX 6.6 includes the complete set of Warnings obtained with PREPRO.**

Table 21. Example of “RECENT.LST” messages/warnings for ⁹⁰Y.

Nuclide	Codes	Warnings
Y- 90	LINEAR	None
	RECENT	WARNING RECENT ----- L= 1 J = 1.500 Corresponds to 2 Resonance Sequences. L= 1 J = 2.500 Corresponds to 2 Resonance Sequences. WARNING RECENT ----- FOR L = 1 Expect Sum of Statistical Weights (GJ) to Equal (2*L + 1) = 3.000 Found = 2.000 Corrective Action Will be Taken to Correctly Calculate the Potential Scattering Cross Section - This Procedure is Based on the Decision of the National Nuclear Data Center, Brookhaven National Laboratory, Private Communication, Charles Dunford, (April 1991) WARNING RECENT ----- L= 2 J = 0.500 Corresponds to 2 Resonance Sequences. L= 2 J = 1.500 Corresponds to 2 Resonance Sequences. L= 2 J = 2.500 Corresponds to 2 Resonance Sequences. L= 2 J = 3.500 Corresponds to 2 Resonance Sequences. WARNING RECENT ----- for L= 2 The Following J Sequences are Missing. J = 1.50 J = 2.50 J = 3.50 J = 4.50 WARNING RECENT ----- FOR L = 2 Expect Sum of Statistical Weights (GJ) to Equal (2*L + 1) = 5.000 Found = 0.200 Corrective Action Will be Taken to Correctly Calculate the Potential Scattering Cross Section - This Procedure is Based on the Decision of the National Nuclear Data Center, Brookhaven National Laboratory, Private Communication, Charles Dunford, (April 1991) WARNING RECENT ----- Note, LSSF= 1 Indicates that the Resonance Contribution has Already been Added to the Cross Sections. This Section will be Read, but Ignored in ALL Resonance Calculations.
	SIGMA1	None

For only Pa233 warnings/messages are obtained when running LINEAR-RECENT-SIGMA1 codes. See table 22.

Table 22. List of warnings for JEFF-3.1.2 library processed with LINEAR-RECENT-SIGMA1 codes. Only materials with SIGMA1 warnings are shown.

Nuclide	Codes	Warnings
Pa- 233	LINEAR	
	RECENT	WARNING RECENT -- ----- Note, LSSF= 1 Indicates that the Resonance Contribution has Already been Added to the Cross Sections. This Section will be Read, but Ignored in ALL Resonance Calculations. WARNING RECENT -- ----- Above Cross Section is NOT Positive at

		ANY E									
		Capture	22070	85	22151	WARNING SIGMA1 --					
SIGMA1		-----									
	n	91-Pa-233	9137	19	VI	0.0	-5249000.00	45	37		
	n	91-Pa-233	9137	41	VI	0.0	-11686000.0	38	37		
	n	91-Pa-233	9137	51	VI	0.0	-6650.00000	42	42		
	n	91-Pa-233	9137	52	VI	0.0	-57100.0000	49	49		
	n	91-Pa-233	9137	53	VI	0.0	-70490.0000	46	46		
	n	91-Pa-233	9137	54	VI	0.0	-86480.0000	39	39		
	n	91-Pa-233	9137	91	VI	0.0	-86480.0000	67	67		
	n	91-Pa-233	9137	102	VI	0.0	5219000.00	22151	5199		
	n	91-Pa-233	9137	600	VI	0.0	-463000.000	20	19		
	n	91-Pa-233	9137	601	VI	0.0	-469040.000	21	20		
	n	91-Pa-233	9137	602	VI	0.0	-469060.000	21	20		
	n	91-Pa-233	9137	603	VI	0.0	-479860.000	21	20		
	n	91-Pa-233	9137	604	VI	0.0	-513380.000	21	20		
	n	91-Pa-233	9137	605	VI	0.0	-517550.000	21	20		
	n	91-Pa-233	9137	606	VI	0.0	-556620.000	20	19		
	n	91-Pa-233	9137	607	VI	0.0	-570340.000	20	19		
	n	91-Pa-233	9137	608	VI	0.0	-622000.000	20	19		
	n	91-Pa-233	9137	609	VI	0.0	-641000.000	20	19		
	n	91-Pa-233	9137	610	VI	0.0	-683000.000	20	19		
	n	91-Pa-233	9137	611	VI	0.0	-715300.000	20	19		
	n	91-Pa-233	9137	612	VI	0.0	-725240.000	20	19		
	n	91-Pa-233	9137	613	VI	0.0	-742400.000	20	19		
	n	91-Pa-233	9137	614	VI	0.0	-760000.000	20	19		
	n	91-Pa-233	9137	615	VI	0.0	-772500.000	20	19		
	n	91-Pa-233	9137	616	VI	0.0	-789000.000	20	19		
	n	91-Pa-233	9137	617	VI	0.0	-798930.000	20	19		
	n	91-Pa-233	9137	618	VI	0.0	-800350.000	20	19		
	n	91-Pa-233	9137	619	VI	0.0	-834170.000	20	19		
	n	91-Pa-233	9137	620	VI	0.0	-851500.000	20	19		
	n	91-Pa-233	9137	621	VI	0.0	-851500.000	20	19		
	n	91-Pa-233	9137	622	VI	0.0	-868800.000	20	19		
	n	91-Pa-233	9137	623	VI	0.0	-873000.000	20	19		
	n	91-Pa-233	9137	649	VI	0.0	-873000.000	53	52		

4.3. Checking ACE libraries

During the processing of ENDF60 [ENDF60] and ENDF66 [LA-UR-03-0954] standard ACE libraries several test were performed using external codes. Some of them have already been added to the internal NJOY testing in RECONR and ACER modules.

The second ACE pass performs ACE consistency, checks and corrects problems that might be detected. In fact, the main questions performed by ACER are [ALEPH-DLG, LA-UR-98-5718]:

1. Do threshold values correspond to Q-values?
 - Checked by RECONR
2. Is the energy grid monotonically increasing?
 - Checked by RECONR (the unionized grid is assumed monotonic). If two points with the same energy are found (i.e.: a jump in the cross section), a consistency problem is signaled but this can be ignored.
3. Check the angular distributions for the correct reference frame (either CM or LAB)
4. Check the angular distributions for unreasonable cosines
5. Is the emission energy less than the incident energy?
6. Do summation cross sections match sums?
 - Checked by RECONR
7. Ensure that probability density functions are non-negative
 - Checked by ACER
8. Are only appropriate interpolation values used?
9. Do threshold reactions start with a zero cross section?
 - Checked by RECONR

Table 23. NJOY output showing several consistency checks

```
ace consistency checks
-----
check reaction thresholds against q values
check that main energy grid is monotonic
check angular distributions for correct reference frame
check angular distributions for unreasonable cosine values
check energy distributions
check photon production sum
check photon distributions
checking particle production sections
deuteron production
checking energy distributions
```

However, ACER does not include the capability to check the proper processing of the unresolved resonance probability tables.

The Probability table (PT) method was implemented in MCNP to account statistically for the average resonance parameters specified in the unresolved resonance range. In this method, the average parameters are used to generate ladders of representative resonances.

Cross sections from these ladders are used to form cross-section probability distribution functions, from which a table of cross sections (total, elastic, fission, and radiative capture) as a function of probability is prepared. MCNP samples the total and reaction cross sections at the energy of the neutron, rather than simply using single average values at this energy.

These PTs are calculated in PURR module. And sigma zero values are not required and could be omitted entirely if the only objective is to generate an ACE library.

Verification of URES library can be performed with a variety of consistency test on the PT data: **[LA-UR-98-5718]**

- Ensure that any competition reaction specified actually exists
- Check the infinitely-dilute total cross section at the energy of the PT against the sum of the infinitely-dilute elastic, fission, capture and competition cross sections.
- Make sure that the cumulative probabilities as given in the PT are in ascending order, and that the distribution is correctly normalized to 1.
- Check negative values of the total, elastic, fission and capture cross sections in each row of the PT. In addition, checks for zero cross sections for the total, elastic and capture.
- Check for zero or negative values of the heating numbers in each row of the PT
- Compare the total cross section from the PT with the sum of the elastic, fission, capture and competition process.
- For each cross section, compare the infinitely dilute value at that neutron energy with the apparent average value from the PT.

The ENDF/B-VI evaluators decided to drop plans to include data for any isotope with a large number of negative cross sections in the PT data. The problems were traced to negative background cross sections in ENDF libraries. (Report **LA-UR-03-594**). So the negative cross section problems in the PT are related with the evaluation and it is not a problem with the purr module of NJOY (the method of calculating the probability table as implemented in NJOY should not lead to negative values by itself **[ALEPH-DLG]**)

In short, there are a number of possible problems or abnormalities with the PTs that can be directly noticed for some isotopes:

- Probability bins with a probability of 0, these bins will not be sampled so it can be accepted
- Zero cross section values (either for the entire bin or for specific reactions)
- Negative cross section values

Zero cross sections can occur either in the lower bins because the cross section becomes very small or when the particular row has a fractional probability of zero (in this case, the row will never be sampled). In these cases, zero cross section can be allowed.

Negative cross sections however cannot be allowed (and the library file has to be recalculated without probability tables), unless they appear in a row with zero fractional probability (in which case they will not be used).

The procedure in this work is to simply omit the PT from ACE file whenever negative values are found.

Table 24. List of materials with PT exception

Cf252	Es253	Na22	Np238
-------	-------	------	-------

4.4. Comparison between JEFF-3.2T3 and other libraries

A Handbook of comparison between JEFF-3.2T3 and other ENDF files (TENDL-2012, JEFF-3.1.2 and ENDF/B-VII.1) has been performed with JANIS4.0. **See ANNEX 6.7.**

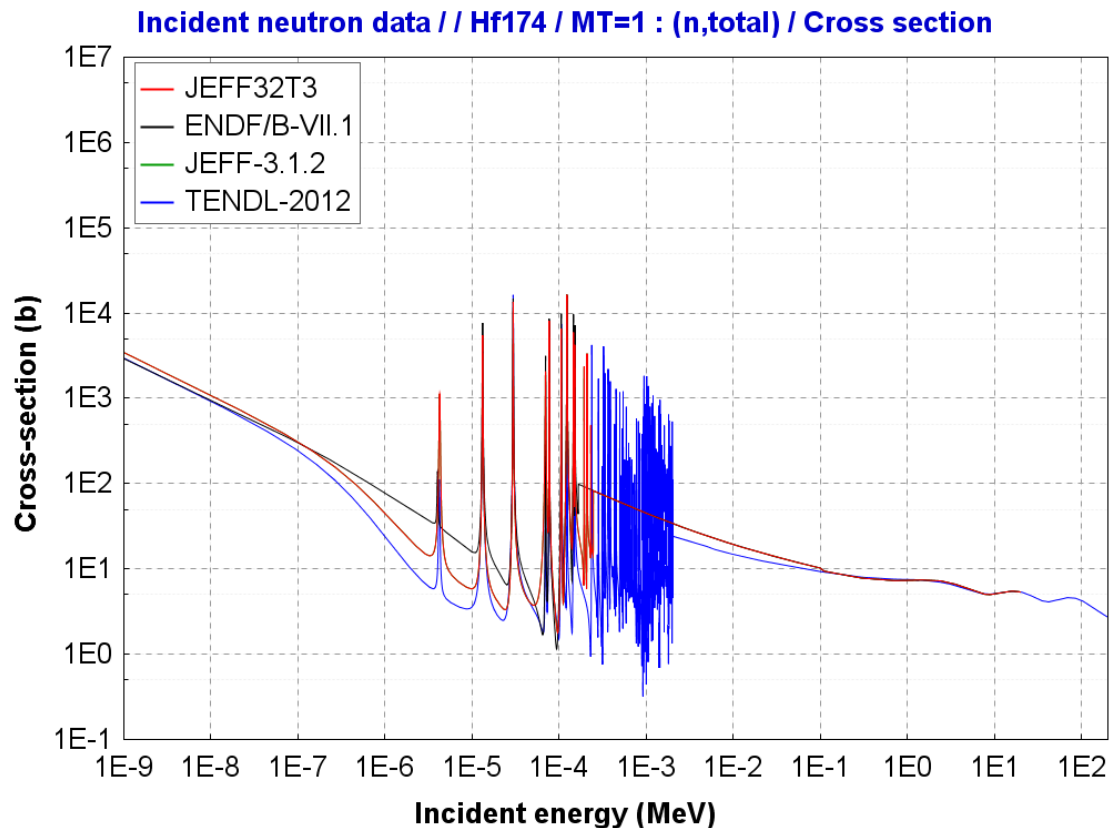
An update of JANIS4.0 version has been developed by NEA Data Bank to perform this Handbook, where a single command-line sentence can be used to perform the entire comparison of the library for any isotope. In this case:

- JEFF-3.2T3 has been update in JANIS4.0 as a new Local Data Based using the WIZARD application. Being the PENDF file processed with NJOY99.393.
- TENDL-2012, JEFF-3.1.2 and ENDF/B-VII.1 have been taken from the NEA Data Base

An example of the command line:

```
java -jar .\janis.jar -o Ac225.png -render Ac225.jns png 1024 768
```

Figure 12. A comparison between different libraries for (n,total) reaction processed with JANIS 4.0



This total cross-section is processed with JANIS4-0 using the following render file.

```
<?xml version="1.0" encoding="UTF-8" ?>
<renderer version="647" timestamp="2013-11-01_09h01m58s656">
  <plot>
    <xvar key="E"/>
    <xscale>LOG_SCALE</xscale>
    <xrange min="1.000 meV" max="200 MeV"/>
    <yscale>LOG_SCALE</yscale>
    <yrange min="0.1 b" max="10000000 b"/>
    <data refs="~N~TENDL-2012~SIG~Hf174~MT1~xs">
      <layer>
        <color>#0000ff</color>
        <stroke>1.0|2|0|10.0|null|0.0</stroke>
      </layer>
    </data>
    <data refs="~N~JEFF-3.1.2~SIG~Hf174~MT1~xs">
      <layer>
        <color>#009900</color>
        <stroke>1.0|2|0|10.0|null|0.0</stroke>
      </layer>
    </data>
    <data refs="~N~ENDF/B-VII.1~SIG~Hf174~MT1~xs">
      <layer>
        <color>#000000</color>
        <stroke>1.0|2|0|10.0|null|0.0</stroke>
      </layer>
    </data>
    <data refs="~N~JEFF32T3~SIG~Hf174~MT1~xs">
      <layer>
        <color>#ff0000</color>
        <stroke>1.0|2|0|10.0|null|0.0</stroke>
      </layer>
    </data>
    <settings name="dpa_averaged_value" key="dpa_averaged_value">
      <strings>
        <title display="true" automatic="true" automaticTemplate="${datatype} / ${dataset} / ${material} /
```

```

${datablock} / ${data}" manualText="" wrapManual="false"/>
    <xAxisLabel display="true" automatic="true" automaticTemplate="${x_name} ${x_unit}" manualText=""
wrapManual="false"/>
    <yAxisLabel display="true" automatic="true" automaticTemplate="${y_name} ${y_unit}" manualText=""
wrapManual="false"/>
    <legend display="true"/>
    <xAxisTicksLabels pattern="0.####E0" displayUnit="1" unitPrefix="3"/>
    <yAxisTicksLabels pattern="0.####E0" displayUnit="1" unitPrefix="4"/>
</strings>
<scheme>
    <pageBox>
        <margins top="10.0" bottom="10.0" left="10.0" right="10.0"/>
        <border stroke="" color="#000000"/>
        <background fill=""/>
    </pageBox>
    <topTextBox visible="true" font="Arial|1|26" textColor="#0000cc" alignment="2" orientation="0">
        <margins top="5.0" bottom="5.0" left="10.0" right="10.0"/>
        <border stroke="" color="#000000"/>
        <background fill=""/>
    </topTextBox>
    <bottomTextBox visible="true" font="Arial|1|26" textColor="#000000" alignment="2" orientation="0">
        <margins top="0.0" bottom="0.0" left="10.0" right="10.0"/>
        <border stroke="" color="#000000"/>
        <background fill=""/>
    </bottomTextBox>
    <leftTextBox visible="true" font="Arial|1|26" textColor="#000000" alignment="2" orientation="2">
        <margins top="10.0" bottom="10.0" left="0.0" right="0.0"/>
        <border stroke="" color="#000000"/>
        <background fill=""/>
    </leftTextBox>
    <rightTextBox visible="true" font="Dialog|0|12" textColor="#000000" alignment="2" orientation="0">
        <margins top="10.0" bottom="10.0" left="10.0" right="10.0"/>
        <border stroke="" color="#000000"/>
        <background fill="#ffffff"/>
    </rightTextBox>
    <centerBox>
        <margins top="10.0" bottom="10.0" left="10.0" right="10.0"/>

```

```

        <border stroke="1.0|2|0|10.0|null|0.0" color="#000000"/>
        <background fill="#ffffff"/>
    </centerBox>
    <plotAreaBox>
        <margins top="10.0" bottom="10.0" left="10.0" right="10.0"/>
        <border stroke="1.0|2|0|10.0|null|0.0" color="#000000"/>
        <background fill="#ffffff"/>
    </plotAreaBox>
    <leftAxis>
        <line stroke="1.0|2|0|10.0|null|0.0" color="#000000"/>
        <majorTics type="1" color="#000000" size="5" twoSides="false" labelsSpacing="10">
            <label visible="true" font="Arial|0|26" textColor="#000000" alignment="2" orientation="0">
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                <border stroke="1.0|2|0|10.0|null|0.0" color="#000000"/>
                <background fill="#ffffff"/>
            </label>
        </majorTics>
        <minorTics type="1" color="#000000" size="4" twoSides="false" labelsSpacing="2">
            <label visible="false" font="Arial Narrow|0|10" textColor="#000000" alignment="2" orientation="0">
                <margins top="10.0" bottom="10.0" left="10.0" right="10.0"/>
                <border stroke="1.0|2|0|10.0|null|0.0" color="#000000"/>
                <background fill="#ffffff"/>
            </label>
        </minorTics>
        <majorGrid stroke="1.0|0|2|10.0|5.0;5.0|0.0" color="#999999"/>
        <minorGrid stroke="1.0|0|2|10.0|2.0;2.0|0.0" color="#f2f2f2"/>
    </leftAxis>
    <rightAxis>
        <line stroke="1.0|2|0|10.0|null|0.0" color="#000000"/>
        <majorTics type="0" color="#000000" size="5" twoSides="false" labelsSpacing="2">
            <label visible="false" font="Arial Narrow|0|10" textColor="#000000" alignment="2" orientation="0">
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                <border stroke="1.0|2|0|10.0|null|0.0" color="#000000"/>
                <background fill="#ffffff"/>
            </label>
        </majorTics>
        <minorTics type="0" color="#000000" size="4" twoSides="false" labelsSpacing="2">

```

```

        <label visible="false" font="Arial Narrow|0|10" textColor="#000000" alignment="2" orientation="0">
            <margins top="10.0" bottom="10.0" left="10.0" right="10.0"/>
            <border stroke="1.0|2|0|10.0|null|0.0" color="#000000"/>
            <background fill="#ffffff"/>
        </label>
    </minorTics>
    <majorGrid stroke="1.0|2|0|10.0|null|0.0" color="#f2f2f2"/>
    <minorGrid stroke="1.0|2|0|10.0|null|0.0" color="#f2f2f2"/>
</rightAxis>
<topAxis>
    <line stroke="1.0|2|0|10.0|null|0.0" color="#000000"/>
    <majorTics type="0" color="#000000" size="5" twoSides="false" labelsSpacing="2">
        <label visible="false" font="Arial Narrow|0|10" textColor="#000000" alignment="2" orientation="0">
            <margins top="10.0" bottom="10.0" left="10.0" right="10.0"/>
            <border stroke="1.0|2|0|10.0|null|0.0" color="#000000"/>
            <background fill="#ffffff"/>
        </label>
    </majorTics>
    <minorTics type="0" color="#000000" size="4" twoSides="false" labelsSpacing="2">
        <label visible="false" font="Arial Narrow|0|10" textColor="#000000" alignment="2" orientation="0">
            <margins top="10.0" bottom="10.0" left="10.0" right="10.0"/>
            <border stroke="1.0|2|0|10.0|null|0.0" color="#000000"/>
            <background fill="#ffffff"/>
        </label>
    </minorTics>
    <majorGrid stroke="1.0|2|0|10.0|null|0.0" color="#f2f2f2"/>
    <minorGrid stroke="1.0|2|0|10.0|null|0.0" color="#f2f2f2"/>
</topAxis>
<bottomAxis>
    <line stroke="1.0|2|0|10.0|null|0.0" color="#000000"/>
    <majorTics type="1" color="#000000" size="5" twoSides="false" labelsSpacing="10">
        <label visible="true" font="Arial|0|26" textColor="#000000" alignment="2" orientation="0">
            <margins top="10.0" bottom="10.0" left="10.0" right="10.0"/>
            <border stroke="1.0|2|0|10.0|null|0.0" color="#000000"/>
            <background fill="#ffffff"/>
        </label>
    </majorTics>

```

```

    <minorTics type="1" color="#000000" size="4" twoSides="false" labelsSpacing="2">
      <label visible="true" font="Arial Narrow|0|10" textColor="#000000" alignment="2" orientation="0">
        <margins top="10.0" bottom="10.0" left="10.0" right="10.0"/>
        <border stroke="1.0|2|0|10.0|null|0.0" color="#000000"/>
        <background fill="#ffffff"/>
      </label>
    </minorTics>
    <majorGrid stroke="1.0|0|2|10.0|5.0;5.0|0.0" color="#999999"/>
    <minorGrid stroke="1.0|0|2|10.0|2.0;2.0|0.0" color="#f2f2f2"/>
  </bottomAxis>
  <legendBox horizontalPosition="3" verticalPosition="1" horizontalSpace="0" verticalSpace="-5"
layerIndentation="20" symbolWidth="30" symbolLabelSpacing="10" visible="true" font="Dialog|0|26" textColor="#000000"
alignment="2" orientation="0">
    <margins top="5.0" bottom="5.0" left="5.0" right="5.0"/>
    <border stroke="1.0|2|0|10.0|null|0.0" color="#666666"/>
    <background fill="#ffffff"/>
  </legendBox>
</scheme>
<plotsPropertiesScheme>
  <colors>
    <color>#ff0000</color>
    <color>#00ff00</color>
    <color>#0000ff</color>
    <color>#00ffff</color>
    <color>#ff00ff</color>
    <color>#999999</color>
  </colors>
  <strokes>
    <stroke>1.0|2|0|10.0|null|0.0</stroke>
  </strokes>
  <marks>
    <mark>Square(0)|3.0</mark>
    <mark>Square(15)|2.0</mark>
    <mark>Triangle(0,false)|3.0</mark>
    <mark>Triangle(0,true)|3.0</mark>
    <mark>Cross()|3.0</mark>
    <mark>Circle(0)|3.0</mark>
  </marks>

```

```
        </marks>
      </plotsPropertiesScheme>
    </settings>
  </plot>
</renderer>
```

Figure 13. A comparison between different libraries for (n,elastic) reaction processed with JANIS 4.0

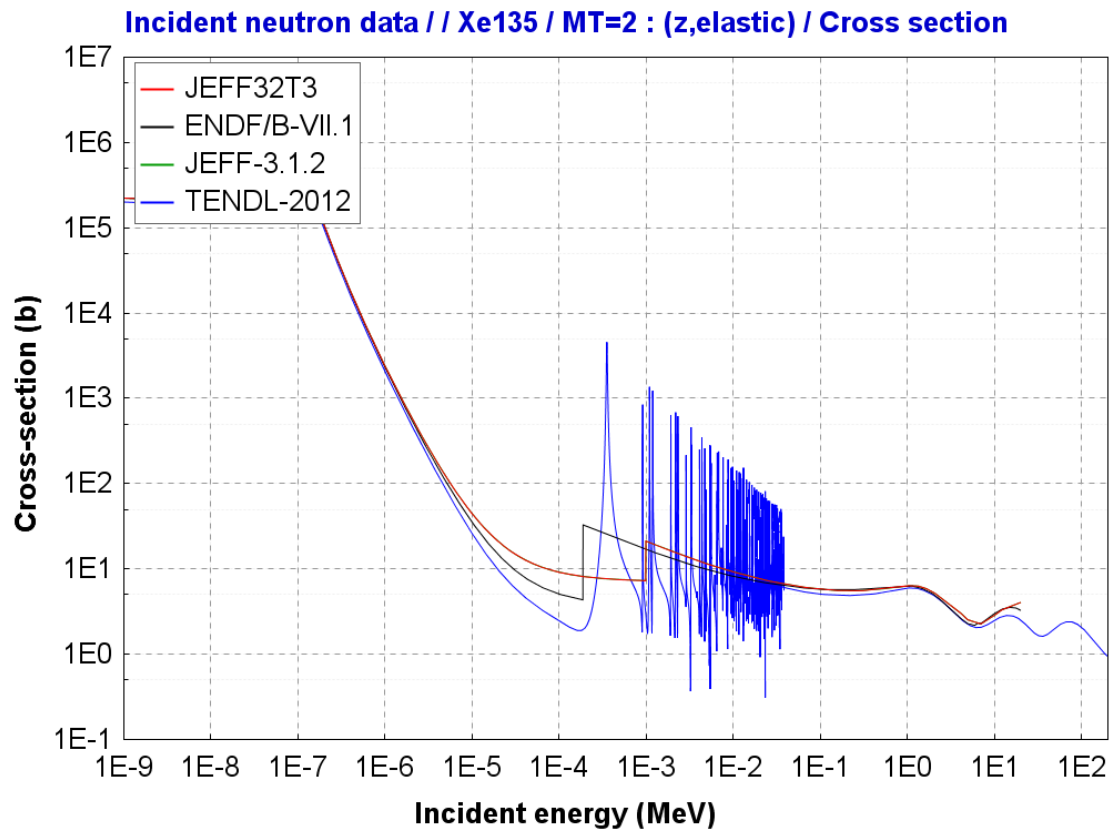


Figure 14. A comparison between different libraries for (n,fission) reaction processed with JANIS 4.0

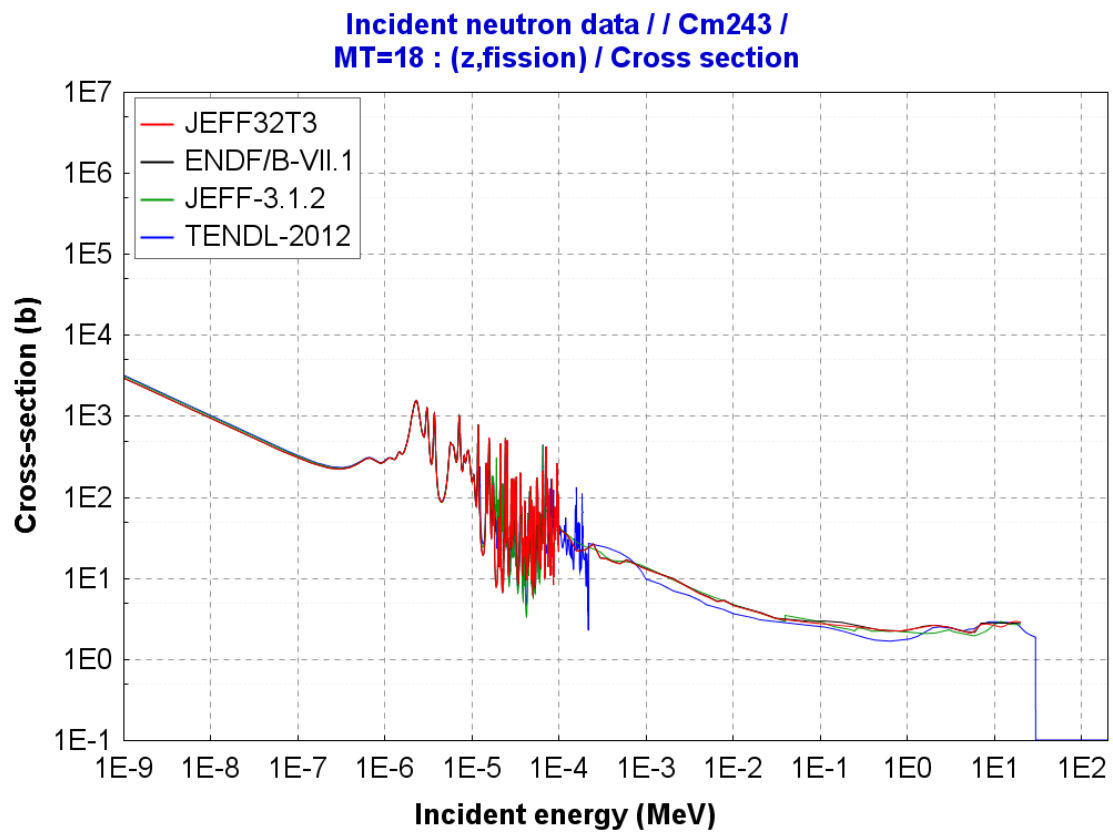
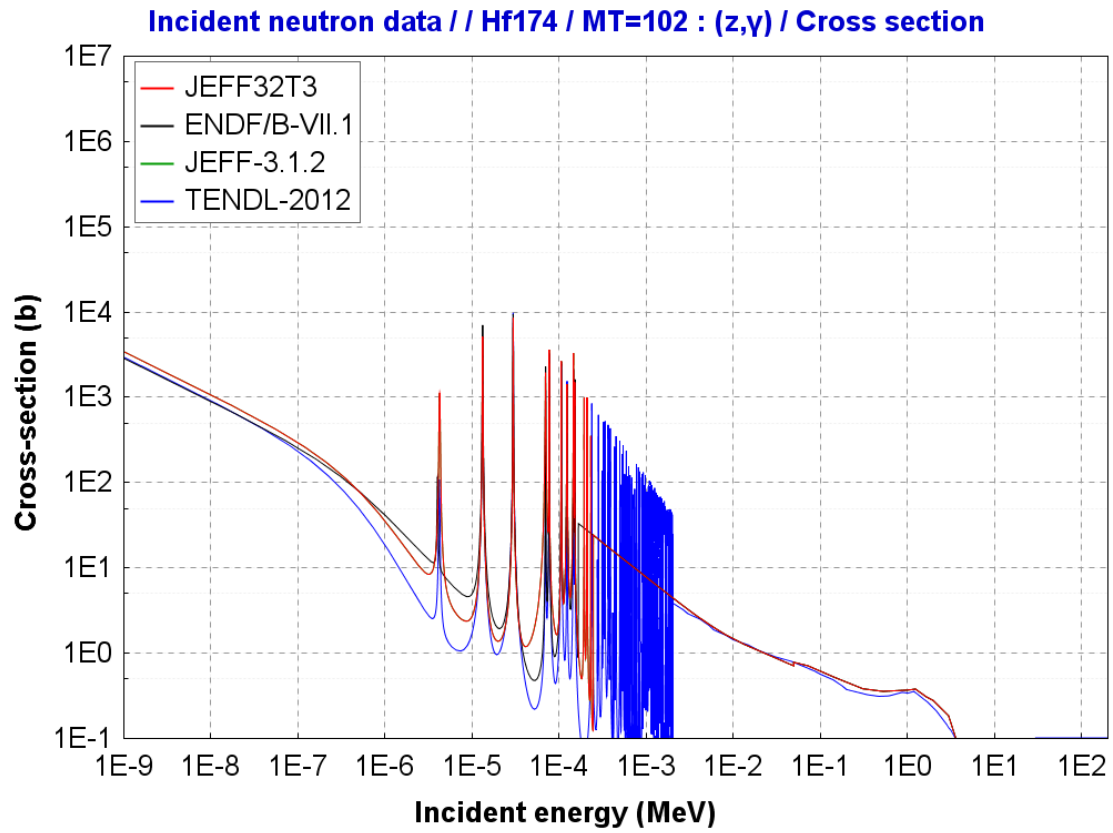


Figure 15. A comparison between different libraries for (n, γ) reaction processed with JANIS 4.0



4.5. QA procedure: comparison & visualization

Our objective in this section is to show the results applied to JEFF-3.2 library using the QA procedure developed by D. López Aldama and A. Trkov in **[ADS-Lib/V1.0]**. Here, *“the human eye will be used as a wonderfully complex tool, able to spot inconsistency and error with amazing precision”* **[LA-UR-02-1235]**:

- Look for unexpected discontinuities in cross sections
- Examine threshold regions
- Examine resonance regions

These ENDF files have been compared with the original evaluation using different procedures:

- Using NJOY code
- Using PREPRO-2004/7/10 code system (LINEAR + RECENT + SIGMA1) **[PREPRO2004]**

We can conclude that the processed data were judged to be acceptable:

- Differences between NJOY and PREPRO2004/7/10 should be investigated
- Differences with other libraries should be considered for later validations.

4.6. Comparison: PREPRO versus NJOY99

The parameters used to run PREPRO in LINEAR, RECENT and SIGMA1:

```
***** Program LINEAR (VERSION 2004-1) *****
For All Data Greater than 1.0000E-10 barns in Absolute Value
Data Linearized to Within an Accuracy of .100000000 per-cent
***** Program RECENT (VERSION 2005-1) *****
for All Data Greater than 1.0000E-10 barns in Absolute Value
Data Linearized to within an Accuracy of .100000000 per-cent
***** Program SIGMA1 (VERSION 2005-1) *****
Data Doppler Broadened to 300.000000 Kelvin
for All Data Greater than 1.0000E-10 barns in Absolute Value
Data Linearized to Within an Accuracy of .100000000 per-cent
```

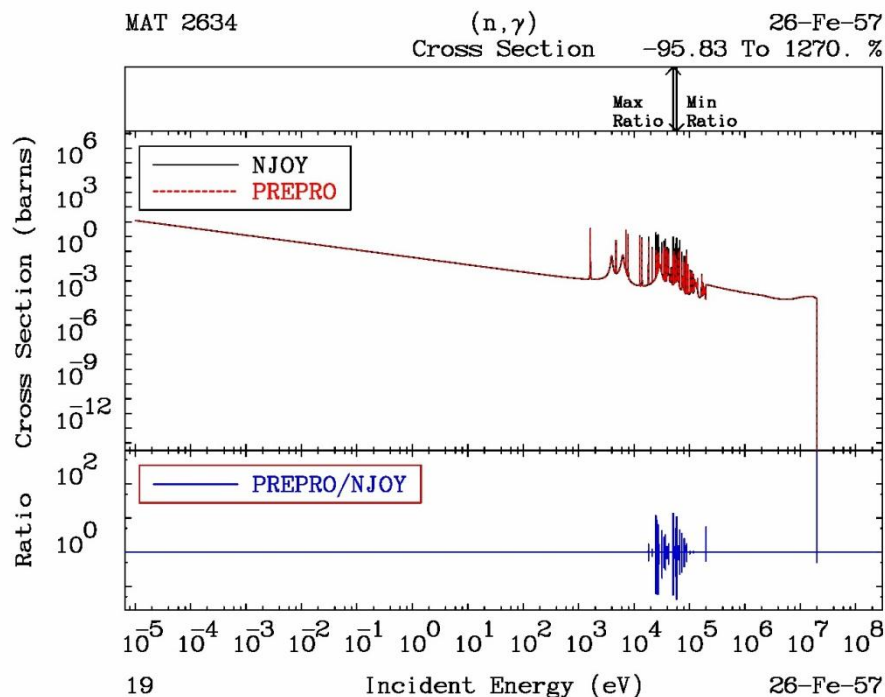
ANNEX 6.8 includes the complete set of this comparison. The main differences are summarized in the following sub-subsections:

4.6.1. Differences in the resonance treatment

List of reactions with a different treatment between PREPRO and NJOY:

Ag-107(n,tot)	Ag-110M (n,tot), (n.elas), (n,gamma)
Fe-56(n,elastic)	Fe-57(n,elastic)(n,gamma)
Gd-157(n,elastic)	I-127(n,tot), (n,elas),(n,gamma)
I-130(n,tot), (n,elas),(n,gamma)	K-41(n,tot), (n,elas),(n,gamma)
Mo-95(n,tot), (n,elas),(n,gamma)	Ni-58(n,tot), (n,elas),(n,gamma)
Ni-60(n,tot), (n,elas)	Pb-205(n,elas)
S-36(n,tot), (n,elas), (n,gamma)	Sc-145(n,tot), (n,elas), (n,gamma)
Sn-113 (n,gamma)	Ti-46(n,tot), (n,elas), (n,gamma)

Figure 16. Total cross section for Fe-57 processed by PREPRO and NJOY99.

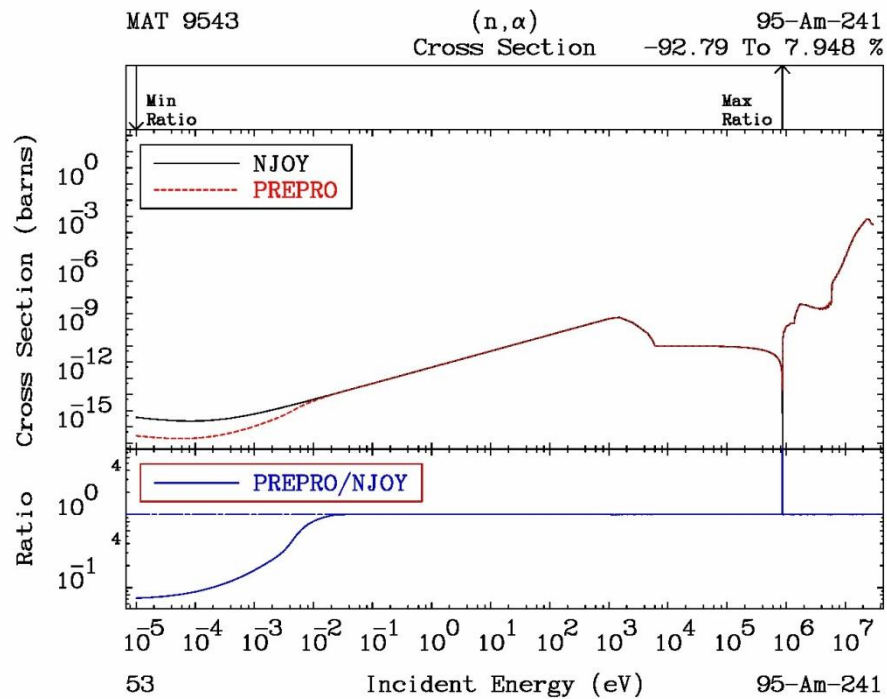


4.6.2. Differences at low energy

List of reactions with a different treatment between PREPRO and NJOY:

Am-241 (n,a)	Cd-106(n,p), (n,a)	Ce-140(n,a)	Ce-141(n,a)
Co-58M(n,tot)	Co-58M(n,p)	Cs-136(n,a)	
Eu-151(n,a)(n,p)	Eu-154(n,a)	Nb-93(n,a)	Nd-142(n,a)
Pm-148M(n,incl), (n,n')		Te-126(n,a)	

Figure 17. Total cross section for Am-241 processed by PREPRO and NJOY99

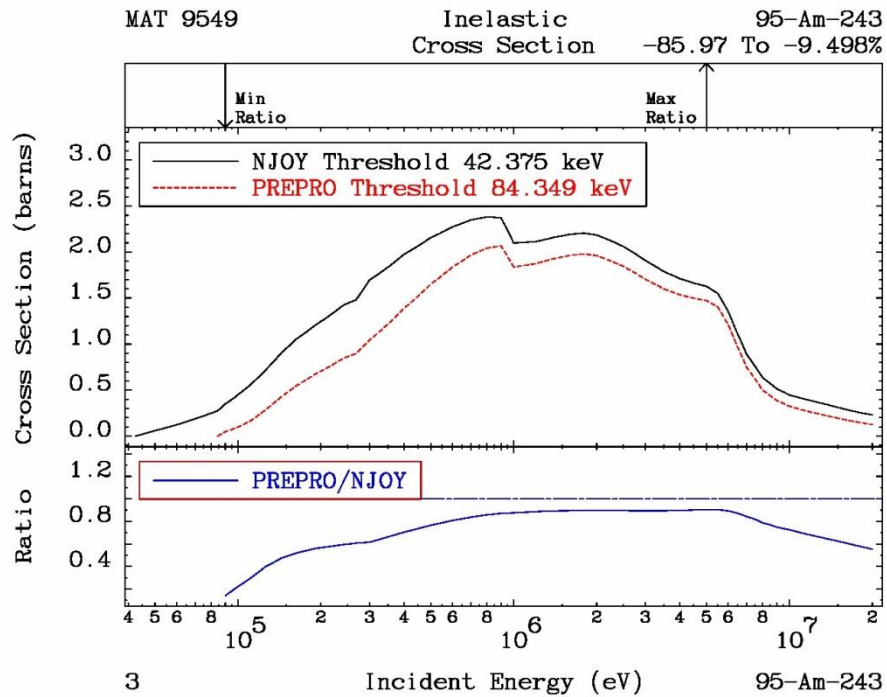


4.6.3. Differences in the inelastic cross-section

List of reactions with a different treatment between PREPRO and NJOY:

Am-243	Bk-247	Cf-249	Cf-250	Cm-242
Cm-243	Cm-244	Cm-245	Cm-246	Cm-247
Cm-248	Cm-250	Pu-236	Pu-238	Y-89

Figure 18. Total cross section for Am-243 processed by PREPRO and NJOY99

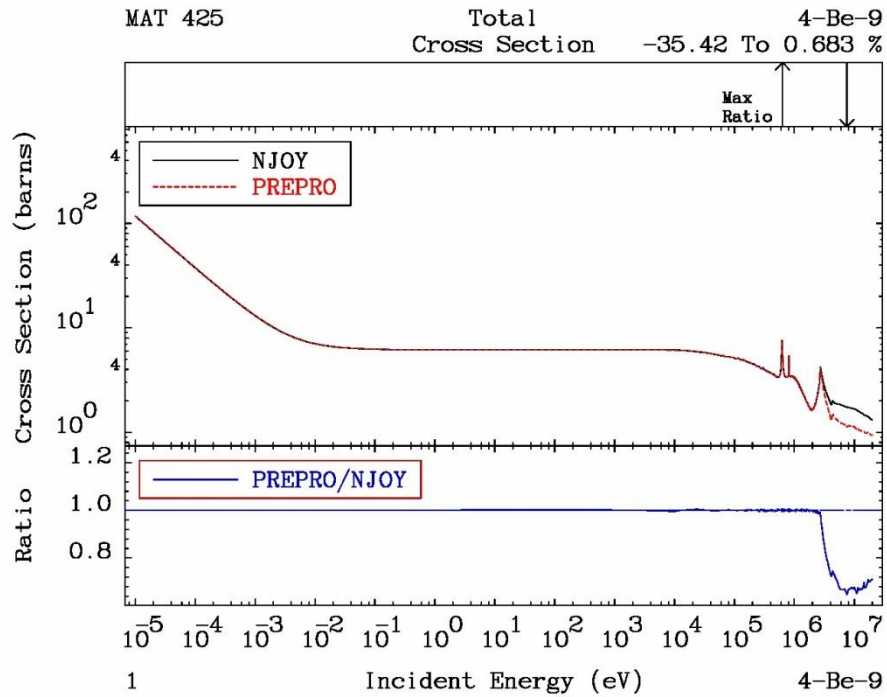


4.6.4.Differences at high energy

List of reactions with a different treatment between PREPRO and NJOY:

Be-9 (n,tot)	Cm-242(n,tot)	Cm-243(n,tot)	Cm-244(n,tot)
Cm-246(n,tot)	Cm-247(n,tot)	Cm-248(n,tot)	Cm-250(n,tot)
Mo-95(n,p)	Pu-236(n,tot)	Pu-238(n,tot)	

Figure 19. Total cross section for Be-9 processed by PREPRO and NJOY99



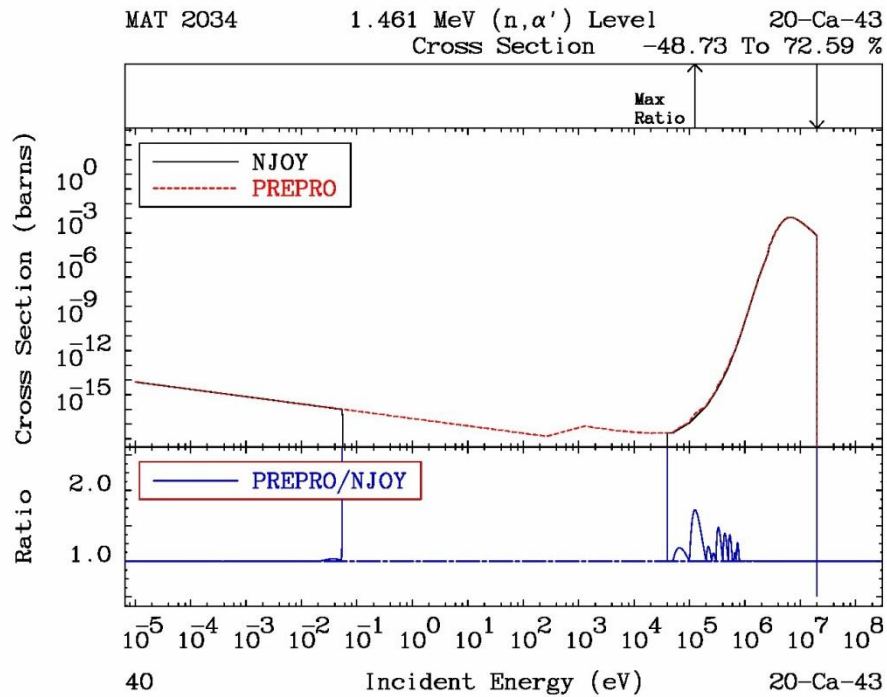
4.6.5. Differences for very low cross-section ($< 1.0E-15$ b)

In BROADR, subroutine "bsigma" uses a "data sigmin/1.d-15/" to return zero broadened values if it is less than "sigmin".

List of reactions with a different treatment between PREPRO and NJOY:

Ca-43 (n,a')	Cd-111(n,a)	Co-60(n,a)	Eu-152(n,2a)
Gd-148(n,2a)	Gd-153(n,2a)	Gd-155(n,a)	Gd-156(n,a)
Ni-58(n,a)	Ni-63(n,a)	Os-192(n,a)	Pb-207(n,a')
Pd-104(n,a')	Pd-108(n,a),(n,a')	Po-209(n,2a)	Pt-198(n,a)
Sb-124(n,a)	Sm-150(n,a)	Tc-99(n,a'), (n,a''),(n,a''')	
Te-128(n,a)	Th-228(n,fission)	Ti-47(n,a')	Tl-205(n,a)
Zn-67(n,p)	Zn-68(n,a)		

Figure 20. Total cross section for Ca-43 processed by PREPRO and NJOY99

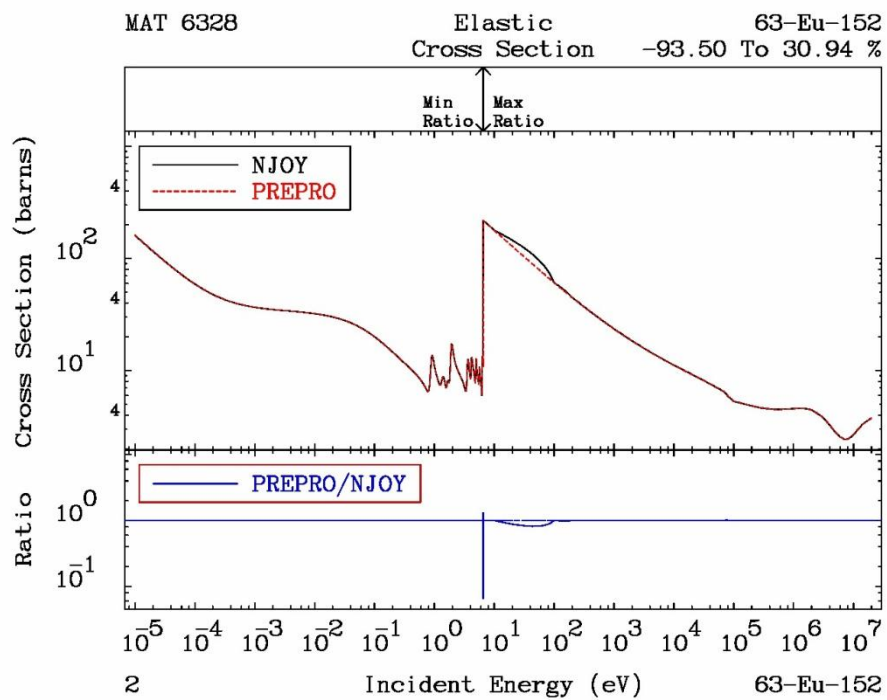


4.6.6. Linearization differences

List of reactions with a different treatment between PREPRO and NJOY:

Eu-152(n,elastic)

Figure 21. Total cross section for Eu-152 processed by PREPRO and NJOY99



5. Analysis of JEFF-3.2T3 Processing with INTER and NJOY codes to obtain integral values

5.1. Introduction

The objective of this work is to process the most recent cross section data libraries (JEFF-3.1.2, ENDF/B-VII.1, TENDL-2012,...) to be compared using the integral values calculated with INTER and NJOY codes.

The PENDF neutron libraries are processed at 293.6 degrees Kelvin.

The analysis of the Kinematic KERMA factors and total damage energy production data are used in this inter-comparison to illustrate failures in JEFF-3.2T3.

See **ANNEX 6.9** to see the information on at 293.6K processed with INTER and BROADR codes.

See **ANNEX 6.7** to see the comparison of JEFF-3.2T3 between different nuclear data libraries.

5.2. INTER calculation at 293.6K

JEFF-3.2T3 PENDF files have been processed with INTER code. INTER is a program that reads a cross section file in ENDF format and calculates the following integral constants:

- Sig(2200): The thermal cross section
- Sig(Ezero): The thermal cross section
- Avg-Sigma: Cross sections averaged over a Maxwellian spectrum
- G-factor: The g-factor
- Res Integ: The resonance integrals
- Sig(Fiss): Cross section averaged over a fission spectrum
- Sig(E14): The 14 MeV cross section

A comparison of the JEFF-3.2T3 with different ENDF files (BROND-2.2, CENDL-2.1, EAF-2007, FENDL-2.1, JEF-2.2, JEFF-3.0, JEFF-3.0A, JENDL-3.3, JENDL-HE, ENDFB-6.8, ENDFB-7.0, ENDFB-7.1, JEFF-3.1, JEFF-3.1.1, JEFF-3.1.2, TENDL-2012) can be seen in **ANNEX 6.9**.

A comparison between JEFF-3.2T3 and ENDF/B-VII.1 based on INTER results is shown in the following Table.

Table 25. Comparison between ENDF/B-VII.1 and JEFF-32T3 for (n,total) reaction after PENDF processing with INTER code.
Value: (ENDF/B-VII.1-JEFF-32T3)/ JEFF-32T3*100.0

Z	A	LISO	Sig(2200) Diff in %	Sig(Ezero) Diff in %	Avg-Sigma Diff in %	G-fact Diff in %	Res Integ Diff in %	Sig(Fiss) Diff in %	Sig(E14) Diff in %
8	17	0	-58.2	-58.2	-58.5	-0.7	-53.7	-40.9	1.5
11	23	0	9.6	9.6	9.5	-0.1	1.6	0	-0.2
15	31	0	29	29	29.1	0.1	50.1	-11.3	-1.1
16	32	0	0.5	0.5	0.5	0	0.4	-4.9	-14.5
16	33	0	-38.7	-38.7	-36	4.4	-7.9	-18.2	-8.2
16	34	0	56.9	56.9	58.3	0.9	66.9	-4.4	-11.5
16	36	0	-99.9	-99.9	-99.9	-0.6	-99.8	-3.7	-6.7
19	39	0	14.1	14.1	15	0.8	20.9	12.4	-1
19	40	0	-26	-26	-28.3	-3.1	-68.4	-14.1	-2
19	41	0	15.1	15.2	15.9	0.6	-2.6	-4.6	-1.5
22	46	0	-68.6	-68.6	-67	5	-71.9	8.3	-2.8
22	47	0	-53.7	-53.7	-52.3	3.1	-36.6	7	-1.8
22	48	0	17	17	15.7	-1	20	-1	-0.7
22	49	0	-77.2	-77.2	-77.7	-2.3	-56.6	9.7	0.3
22	50	0	-62.8	-62.8	-60.3	6.6	-68.6	4.9	1.4
24	53	0	0	0	0	0	0	-3.5	-5.1
24	54	0	0	0	0	0	0	-3.7	-5.8
26	57	0	89.2	89.2	99.9	5.6	20.6	-14.8	-3.7
26	58	0	-51.7	-51.7	-52.4	-1.4	-40.5	-26.2	-4.4
27	58	0	3.5	3.5	3.2	-0.4	8.3	7.2	1.6
28	60	0	-6.7	-6.7	-6.1	0.6	1	0.2	2
28	61	0	8.2	8.2	8.4	0.2	7.1	0	0
28	64	0	14.9	14.9	17.1	1.9	7.9	-4.6	0
30	64	0	26.7	26.7	27.3	0.5	12.7	-1.7	0
30	66	0	27.2	27.2	27.7	0.4	19.3	-5.8	0.9
30	67	0	-31.8	-31.8	-33.9	-3	-17.4	5.1	0.8
30	68	0	25.2	25.2	25.9	0.6	6.9	-3.5	1.4
30	70	0	8.5	8.5	8.5	0	-1	-5	1.9
31	69	0	19.4	19.4	19.9	0.4	7.9	-7.1	-3
31	71	0	16.3	16.3	17.1	0.7	11.7	-6.1	1.6
32	70	0	24.6	24.6	25.3	0.5	17.7	-7.1	-1.4
32	72	0	88.7	88.8	90.5	0.9	30.2	-11.1	-0.2
32	74	0	71.4	71.4	72.3	0.6	18.8	-6.1	1.2
32	76	0	24	24	24.1	0	17.5	-5	1.6
33	75	0	6.4	6.4	6.2	-0.2	4.2	6.8	1
34	74	0	11.8	11.8	13.4	1.5	3.8	9.6	14.5
34	76	0	1	1	1.2	0.2	21.8	9.5	13
34	77	0	0.8	0.8	0.7	-0.1	4.1	10	10.3
34	78	0	11.7	11.7	11.7	0.1	3.1	5.4	10.9

34	79	0	285.7	285.7	275.8	-2.6	122.7	15	8.7
34	80	0	181.6	181.7	186	1.6	20	0.6	7.4
34	82	0	19.8	19.8	19.9	0	19.8	-0.3	7.2
35	79	0	0.4	0.4	-0.1	-0.5	-1.6	13	7.8
35	81	0	25.7	25.7	26.8	0.9	10.5	11	6.5
36	78	0	13.8	13.8	14.7	0.8	22.2	3.2	1.9
36	80	0	3.1	3.1	3.4	0.3	2.4	6.8	7.8
36	82	0	-14.5	-14.5	-15.4	-1	5.8	0.3	5.8
36	83	0	1.6	1.6	1.7	0.1	17.9	7.3	2.2
36	84	0	31.7	31.7	31.8	0.1	4.5	-2.8	4.1
36	85	0	32.4	32.5	33.2	0.5	20.7	-0.8	-0.2
36	86	0	-6.5	-6.5	-6.5	0	-6.1	16.8	2.9
37	85	0	8.1	8.1	8.1	0.1	2.4	-6.1	0.7
37	86	0	-76.9	-76.9	-75.4	6.6	-76.1	0.6	-1.1
37	87	0	-21.1	-21.1	-21.1	-0.1	-8.5	-1.5	1.6
38	84	0	8.1	8.1	8.2	0.1	4.2	8.9	-3.3
38	86	0	32.1	32.1	33.6	1.1	8.9	11.7	14.8
38	87	0	-5.8	-5.8	-5.9	0	1.7	10.5	14.1
38	88	0	26.6	26.6	26.6	0	24	-4	-2.4
38	89	0	31.5	31.5	31.6	0.1	18	10.1	-5.2
38	90	0	22.8	22.8	22.8	0	37.5	9.9	12.3
39	90	0	-30.9	-30.9	-30.1	1.1	-48.6	24	11.3
39	91	0	8.1	8.1	7.2	-0.8	10.3	2.5	11.1
40	90	0	7.8	7.8	7.8	0	4.7	-10.1	-0.4
40	91	0	-6	-6	-6.1	-0.1	-0.2	1	0.6
40	93	0	0	0	0	0	0	5.7	-9.2
40	95	0	0	0	0	0	-0.4	-11.6	-6.5
40	96	0	-6.9	-6.9	-6.9	0	-7.5	-2.7	7.2
42	92	0	9.3	9.3	9.2	-0.1	5.4	0.1	0
42	94	0	2.5	2.5	1.9	-0.6	-5.8	0	0
42	95	0	-2.3	-2.3	-2.4	-0.1	8.1	1.2	-6.9
44	96	0	-14.4	-14.4	-15.7	-1.5	-26.4	-4.7	-33.9
44	98	0	-7.4	-7.4	-12.5	-5.6	-19.5	-5.3	-31.1
44	99	0	-8.8	-8.8	-9.6	-0.9	0.1	3.9	4.9
44	101	0	27.5	27.5	26.3	-1	2.8	-4.4	-4.1
44	106	0	-17.8	-17.8	-17.8	-0.1	0.1	2	1.2
46	102	0	-13.7	-13.7	-12.2	1.7	1.3	-3.4	-38.7
46	110	0	11.7	11.7	11.8	0	11.9	-1.6	-0.7
47	107	0	-0.5	-0.5	-0.5	0	-1.1	-5.6	-0.3
50	112	0	-5.8	-5.7	-5.5	0.2	-2.2	0	0
50	115	0	75.4	75.4	73.4	-1.1	8.4	0	0
50	116	0	-0.2	-0.2	-0.2	0	-6.5	0	0
50	117	0	-12.3	-12.3	-11	1.6	0	0	0
50	118	0	10	10	10.1	0	3.6	0	0
50	120	0	5	5	5	0	4	0	0

50	122	0	2.4	2.4	2.4	0	-1	-5.2	-0.9
50	123	0	53.2	53.2	45.4	-5.1	157.3	-1.1	-0.6
50	125	0	-13.3	-13.3	-12.5	0.8	0.5	1.5	1.8
50	126	0	-16.4	-16.4	-16.1	0.4	6.6	-1.5	-0.7
51	123	0	-6.6	-6.6	-6.5	0.1	-0.2	0.8	-1.2
51	124	0	91.2	91.2	85.4	-3	144.2	-1.4	-0.7
51	125	0	61.3	61.3	54.3	-4.4	24.2	-1.7	-0.7
51	126	0	62	62	57.7	-2.7	115.3	0.6	1.8
52	120	0	-16.5	-16.5	-21.1	-5.5	26.2	-7.7	-33.7
52	122	0	-9.9	-9.9	-9.3	0.6	-13.9	1.7	7.2
52	123	0	2	2	2	0	1.9	5.2	6.6
52	124	0	14.4	14.4	15.4	0.8	10.7	0.7	6.2
52	125	0	-17.6	-17.6	-17.7	-0.1	-7	4.6	6.6
52	126	0	-15.4	-15.4	-14.4	1.2	-4.3	4.4	6.6
52	127	1	9999	9999	9999	-4.1	960.9	4.5	6.6
52	128	0	12.8	12.8	12.9	0.1	4	-0.2	3.2
52	129	1	9999	9999	9999	-9.4	817.8	3.9	6.5
52	130	0	-2.8	-2.8	-2.6	0.2	-9	7.3	2.9
52	132	0	15.1	15.1	14.8	-0.3	22	6	2.9
53	127	0	10.4	10.4	10.7	0.3	10.3	0.2	1.2
53	129	0	10.2	10.2	11.8	1.5	19.8	0.1	4.9
54	124	0	-11	-11	-11.2	-0.3	6.1	-4.2	-3.9
54	126	0	31	31	29.9	-0.8	-22.2	-0.3	2.6
54	131	0	-16.6	-16.7	-18.8	-2.6	-6.5	1.3	-2
54	135	0	0.4	0.4	0.6	0.2	-1.7	1.1	6.5
55	134	0	0.2	0.2	0.2	0	7.7	3.7	5.4
55	136	0	216.7	216.5	196.7	-6.3	33	3.5	6.4
56	130	0	-33	-33	-34	-1.6	-2.3	0	0
56	132	0	39.5	39.5	43.3	2.8	123.7	0	0
56	133	0	-30.7	-30.7	-31.8	-1.5	10.7	5.3	0.8
56	135	0	13.4	13.4	14.6	1	-17.6	0	0
56	136	0	23.9	23.9	23.1	-0.6	-1.5	0	0
56	137	0	9	9	11.8	2.5	10	0	0
56	138	0	-24.4	-24.4	-24.7	-0.3	-22.9	-0.3	-1.4
57	138	0	-3.6	-3.6	-4	-0.3	-12.8	4.9	4.3
57	140	0	-39.7	-39.7	-41.3	-2.7	27.5	-0.7	0.6
58	136	0	-14.5	-14.5	-15.4	-1.1	-13.2	-5.5	1.1
58	138	0	-13.3	-13.3	-13.3	0	-58.8	-2.1	-0.5
58	139	0	-31.2	-31.2	-35.1	-5.8	-98.6	-1.5	-0.4
58	140	0	8.9	8.9	9.1	0.1	0.6	5.2	4.7
58	143	0	56.3	56.3	56.9	0.3	13.3	4.7	0.7
59	142	0	-7.2	-7.2	-8.1	-1	-24.4	1.4	4.6
60	142	0	-1.9	-1.9	-2.1	-0.2	-6.6	6.9	8
60	145	0	-2.5	-2.5	-2.7	-0.2	-1.3	5.4	2.4
60	148	0	120.5	120.6	132.1	5.2	6.2	3.2	-0.2

60	150	0	-4.5	-4.5	-4.3	0.2	-10.8	-3.2	0.9
62	147	0	-34	-34	-36.4	-3.7	-7.2	-0.4	-0.2
62	149	0	-3	-3	-5.3	-2.4	-1	-2.2	-2.9
62	150	0	-1.4	-1.4	-1.2	0.2	3	11.3	9
63	151	0	0.2	0.2	5.2	5	-2.2	-1.6	0.4
63	152	0	0.3	0.3	0.3	0	-6.2	0	0
63	153	0	13.7	13.7	13.4	-0.2	-0.2	-3.3	0.7
63	154	0	-0.2	-0.2	-0.2	0	-5.7	2.2	4.7
64	152	0	-3.4	-3.3	1.7	5.2	58	0	0
64	153	0	4.6	4.6	5.1	0.5	-48.3	-3.1	3.7
64	154	0	-0.6	-0.6	-0.5	0.1	-13.2	0	0
64	155	0	0	0	0	0	-1.1	-3.6	-8.8
64	156	0	-5.8	-5.8	-6.4	-0.6	-0.3	0.3	-3.8
64	157	0	-0.4	-0.4	-0.3	0.2	5.4	1.1	-4.1
64	158	0	30.7	30.7	32.8	1.6	5.1	4.8	9.1
64	160	0	139.9	139.9	141	0.5	-0.1	4.5	9.8
65	160	0	-1.1	-1.1	-1.1	0	-45.7	-11.3	0.9
66	156	0	7.2	7.2	8.2	0.9	-15.6	-5.1	3.2
66	158	0	3.3	3.3	3.8	0.5	-11.1	-5.7	-0.4
67	166	1	0.5	0.5	3.1	2.6	-37.7	-8.9	4.7
68	166	0	7.8	7.8	8.3	0.5	-0.4	-6.5	3.8
68	168	0	14.6	14.6	15.1	0.4	-0.6	-6.3	3.8
68	170	0	6.8	6.8	7.2	0.4	0.6	-6.4	2.5
69	170	0	-79	-79	-78.8	1.2	-80	-5.3	3.2
71	176	0	3.1	3.1	1.6	-1.4	-19.2	-0.7	2.6
72	174	0	-10.3	-10.3	-9.2	1.2	16	0	0
72	176	0	21.6	21.6	21.2	-0.4	7.1	-0.1	0
72	180	0	-8.2	-8.2	-8.6	-0.4	-7.7	0	0
73	181	0	3.6	3.6	3.8	0.2	12.2	2.7	0
74	182	0	12.6	12.6	13.4	0.7	7.7	7.3	2.7
74	183	0	-21.4	-21.4	-22.9	-2	-2	5.9	8.9
74	186	0	-0.5	-0.5	-0.4	0	-8.9	2.2	2.1
75	185	0	1.3	1.3	1.5	0.2	2.7	-6.5	1.5
75	187	0	-2.5	-2.5	-2.9	-0.4	6.8	-3.2	-5.2
77	193	0	-5.4	-5.4	-5.8	-0.4	-3.6	-0.5	0.8
81	205	0	-10.3	-10.3	-10.4	0	-7.5	-2	-0.4
89	225	0	-94.8	-94.8	-94.6	2.9	-23	0.4	-5.5
89	226	0	802.4	802.4	791.1	-1.3	-28.3	-0.8	3.6
89	227	0	-11.1	-11.1	-22	-12.2	-38	0.3	-5.6
90	227	0	-64.6	-64.6	-64.5	0.2	-36.9	-2.1	4.1
90	228	0	16	16	16.9	0.8	-8.8	1.7	3.6
90	229	0	7.4	7.4	6.2	-1.2	-3.6	2.3	-5.6
90	230	0	15.9	15.9	18	1.8	11.2	-8.5	-7.3
90	233	0	-10.9	-10.9	-10.8	0.1	3.7	0.2	3.5
90	234	0	-7.1	-7.1	-7.2	-0.1	-24.5	1.3	3.4

92	237	0	0	0	0	0	-0.2	-6.6	1.5
93	235	0	20.9	20.9	22.2	1.1	19.5	6.8	-0.7
93	236	0	-15.6	-15.6	-13.8	2.2	-2.3	1.5	0.6
93	238	0	19.7	19.7	21	1.2	23.9	1.7	-2.5
93	239	0	-36	-36	-35.4	0.9	80.3	1.8	6.8
94	236	0	-13.9	-13.9	-13.7	0.2	-0.9	1.3	-0.6
94	237	0	-5.5	-5.5	-5.3	0.2	4.8	4.6	-8.1
94	238	0	-0.2	-0.2	-1	-0.8	1.7	-10.9	-14.8
94	242	0	10.5	10.5	10.2	-0.3	-0.5	1	0.3
94	244	0	5.4	5.4	5.7	0.2	-12.1	2.6	10.2
94	246	0	-88.8	-88.8	-88.6	1.7	-60.7	1.9	0.6
95	241	0	-8.5	-8.5	-8.1	0.5	-12.6	-1.7	-3.8
95	243	0	4.8	4.8	4.8	0	15.4	1.1	2.3
96	240	0	0	0	0	0	27	5.8	0.5
96	241	0	0	0	0	0	-0.9	6.9	-0.6
96	249	0	0	0	0	0	9.3	5.9	-2
97	247	0	251.9	251.9	260.7	2.5	-33.2	4.2	-0.5
97	250	0	33.7	33.7	41.8	6	48.6	3.5	2.4
98	250	0	9.3	9.2	6.1	-2.9	39.2	-0.8	2.4
98	251	0	-4.7	-4.7	-5.3	-0.6	-73.9	2.2	3.6
98	254	0	0.6	0.6	0.6	0	135.9	-2.2	2
99	253	0	-8.3	-8.3	-10.8	-2.7	-41.6	-15.1	-38.5
99	254	0	8.1	8.1	8.3	0.2	41.1	-0.2	2.1
99	255	0	-18	-18	-17.4	0.7	183.9	-0.2	2.2
100	255	0	7.2	7.2	7.2	0.1	17.9	-0.3	2.2

Table 26. Comparison between ENDF/B-VII.1 and JEFF-32T3 for (n,fission) reaction after PENDF processing with INTER code.
Value: (ENDF/B-VII.1-JEFF-32T3)/ JEFF-32T3*100.0

Z	A	LISO	Sig(2200)	Sig(Ezero)	Avg-Sigma	G-fact	Res Integ	Sig(Fiss)	Sig(E14)
89	227	0	-65.5	-65.5	-65.6	-0.2	-49.3	-5.2	-49.4
90	227	0	0	0	0	0	59.5	-38.8	-64.8
90	228	0	-50	-50	-50	0	-49.3	251.3	9
90	229	0	0.3	0.3	-2.2	-2.5	-28.8	-28.6	-57.9
90	230	0	0	0	0	0	-4.6	12.1	-13.3
90	233	0	0	0	-0.4	-0.4	9999	-9.4	-2.4
90	234	0	0	0	0	0	0	-6.6	34.8
92	236	0	-23.2	-23.2	-23	0.2	2.8	2.6	3.1
92	237	0	0	0	0	0	-1.5	-29.5	10.1
92	238	0	-36.6	-36.6	-36.6	0	89.5	-2.6	-3.1
93	235	0	165	165	169	1.5	698.8	16.2	0.2
93	236	0	1.3	1.4	3.4	2	13.6	9.6	0.8
93	237	0	13	13	12.1	-0.8	196	1.8	1
93	238	0	8.6	8.6	10.8	2	19.9	-1.9	18.9
93	239	0	0	0	0	0	-69.3	-59.8	-40.7
94	236	0	-15.1	-15.1	-15	0.2	1.1	12.5	1.2
94	237	0	9.3	9.3	9.5	0.2	14	-19	-3.5
94	238	0	-0.7	-0.7	-2.7	-2.1	-27.5	-2.5	0.7
94	240	0	8.3	8.3	7.4	-0.8	-19.3	-2.5	9.9
94	242	0	440.4	440.4	435.9	-0.8	-8.6	-1.4	-4
94	244	0	0	0	0	0	31.4	3.5	5.4
94	246	0	0	0	0	0	242.3	-22.1	-15.4
95	241	0	-3.8	-3.9	-2.8	1.1	7.1	-1.6	9.9
95	242	0	0	0	0	0	0	12.9	11.4
95	242	1	0	0	0	0	0	5	-1.8
95	243	0	0	0	-0.7	-0.7	-9.1	-0.3	-2.2
96	240	0	0	0	0	0	-1.9	-8	-11.1
96	241	0	0	0	0	0	-1.5	-11.2	-5.2
96	244	0	0	0	0	0	18.4	-0.6	4.2
96	245	0	0	0	0	0	0.6	1.1	-5.8
96	246	0	123.9	123.9	123.3	-0.3	47.7	0.3	9.7
96	248	0	0	0	0	0	0	8.2	3.9
96	249	0	0	0	0	0	2.2	-24.6	-20.4
96	250	0	0	0	0	0	0	-16	-33.5
97	247	0	-96	-96	-95.9	3	-99.6	-12.2	8.6
97	249	0	0	0	0	0	-3.7	6.3	-8.1
97	250	0	2.3	2.3	8.5	6.1	22.4	-50.1	12
98	250	0	9999	9999	9999	-6	562.1	-21.8	-9
98	251	0	-7.2	-7.2	-7.9	-0.8	-79	-25.5	7.8
98	252	0	2.7	2.7	3.3	0.7	-9.9	21.6	9.2

98	254	0	0	0	0	0	601.9	-17.4	-14.6
99	254	0	8.3	8.3	8.4	0.2	-7.9	-10.7	6.7
99	255	0	-96.3	-96.3	-96.3	0.4	-99.7	-68.9	-25.7
100	255	0	0	0	0.1	0.1	24.5	-4	5.2

5.3. *BROADR calculation at 293.6K*

JANIS library has been processed at 293.6 K (.0253 eV). BROADR computes:

- fission cross section at thermal
- fission nu-bar at thermal
- capture cross section at thermal
- thermal Maxwellian fission integral (one-group thermal cross sections)
- thermal Maxwellian capture integral
- fission g-factor (deviation from 1/v)
- capture g-factor
- thermal alpha integral
- thermal eta integral
- thermal K1 integral
- fission resonance integral
- capture resonance integral

These integral quantities can be included to perform a data/code analysis:

- Thermal cross section: $\sigma_{0x} = \sigma_x(E_0)$; for $E_0 = 0.0253$ eV
- Maxwellian average at thermal energy:

$$\bar{\sigma}_x = \frac{\int_{E_1}^{E_2} \sigma_x(E) \frac{E}{E_0} \exp\left(-\frac{E}{E_0}\right) dE}{\int_{E_1}^{E_2} \frac{E}{E_0} \exp\left(-\frac{E}{E_0}\right) dE}; \text{ where } E_0 = 1.0E-5 \text{ eV and } E_0 = 3 \text{ eV}$$

If the cross section has a 1/v shape, its integral weighted against a

Maxwellian spectrum for 0.0253 eV is given by: $\bar{\sigma}_x = \frac{\sqrt{\pi}}{2} \sigma_x(E_0)$

- Westcott's g-factor provides a measure of the deviation from a 1/v shape.

$$G_x = \frac{2}{\sqrt{\pi}} \frac{\bar{\sigma}_x}{\sigma_x(E_0)}$$

- Resonance integral: $I_x = \int_{E_3}^{E_4} \sigma_x(E) \frac{dE}{E}$

– Thermal alpha integral:
$$\alpha = \frac{\int_{E_1}^{E_2} \frac{\sigma_c(E)}{\sigma_f(E)} \frac{E}{E_0} \exp\left(-\frac{E}{E_0}\right) dE}{\int_{E_1}^{E_2} \frac{E}{E_0} \exp\left(-\frac{E}{E_0}\right) dE}$$

– Thermal eta integral:
$$\eta = \frac{\int_{E_1}^{E_2} \frac{\nu \sigma_f(E)}{\sigma_a(E)} \frac{E}{E_0} \exp\left(-\frac{E}{E_0}\right) dE}{\int_{E_1}^{E_2} \frac{E}{E_0} \exp\left(-\frac{E}{E_0}\right) dE}$$

- Thermal K1 integral (The quantity K1 is known to be an especially good indicator for k_{eff} .)

$$k1 = \frac{\int_{E_1}^{E_2} [\nu \sigma_f(E) - \sigma_a(E)] \frac{E}{E_0} \exp\left(-\frac{E}{E_0}\right) dE}{\int_{E_1}^{E_2} \frac{E}{E_0} \exp\left(-\frac{E}{E_0}\right) dE} = (\nu \bar{\sigma}_f - \bar{\sigma}_a) \frac{2}{\sqrt{\pi}}$$

5.4. HEATR calculation

The HEATR module generates pointwise heat production cross sections and radiation damage energy production for specified reactions and adds them to an existing PENDF tape.

By default, the code processes the energy-balance total KERMA (MT=301) only. In this work, we have included MT443 and MT444 also.

NJOY computes the $k_{ij}(E)$ factors (KERMA, Kinetic Energy Release in Materials) for material-i and reaction-j at incident energy E. The units are eV-barns.

Using the energy-balance method NJOY computes $k_{ij}(E)$ as follows:

$$k_{ij}(E) = (E + Q_{ij} - \bar{E}_{ijn} - \bar{E}_{ij\gamma}) \sigma_{ij}(E)$$

where:

- Q_{ij} is the mass-difference Q value for material-i and reaction-j
- $\bar{E}_{ijn}$ is the total energy of secondary neutrons including multiplicity
- $\bar{E}_{ij\gamma}$ is the energy of secondary photons including photon yields

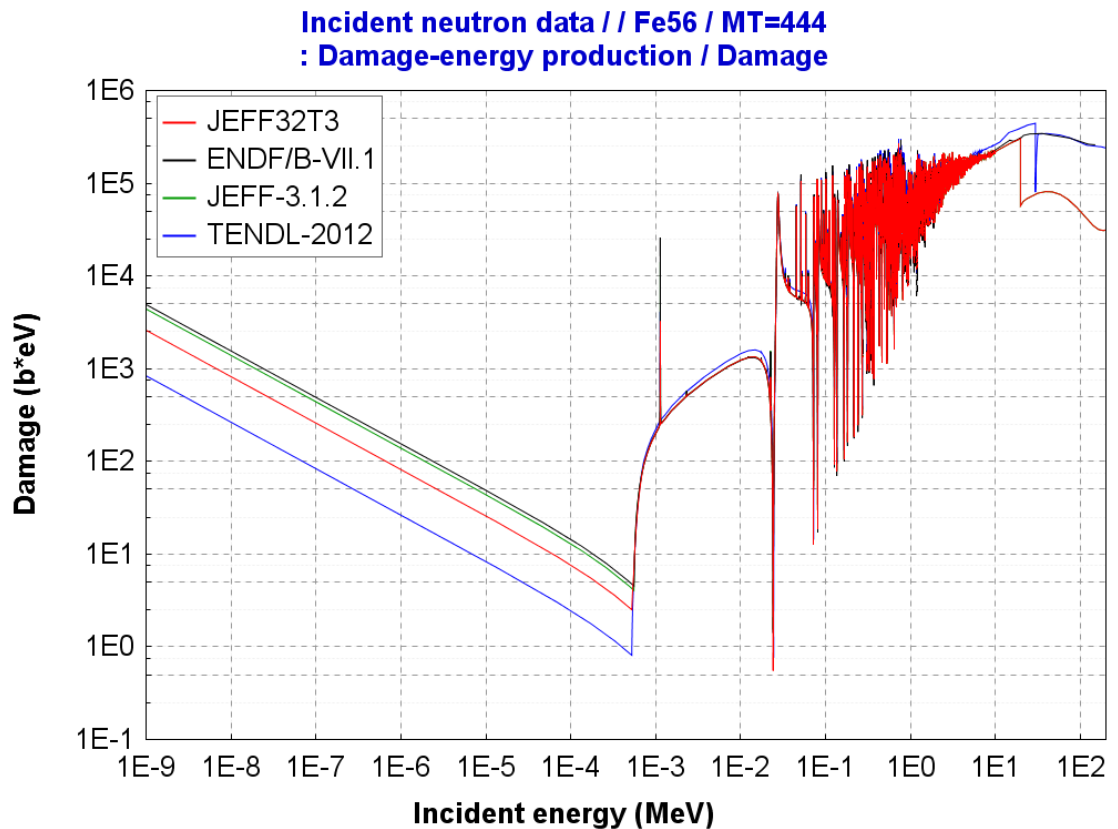
The kinematic KERMA computed when MT443 is requested is very useful for judging the energy-balance consistency of an evaluation. It can also be used instead of the energy-balance value in MT301 when local heating effects are important and the evaluation scores poorly in an energy-balance check.

Damage energy production cross sections (MT444) is interested for important structural materials; this calculation can be omitted for other materials. The Damage output from HEATR is the damage energy production cross section (eV-barns). So, we define as the energy available to cause displacements.

Table 27. Special NJOY's labels are included in JANIS (from Table XV-7, NJOY manual)

Name	MT	Description
HEAT	301	Energy-balance heat production
KERMA	443	Kinematic KERMA factor
DAMAGE	444	Damage-energy production

Figure 22. Comparison of Fe56-MT444 for different evaluated files



In some cases an unphysical jump at 20 MeV is found, or problems in the range from 5 MeV and 20 MeV shows a lack of information in files MF5/MF6 in the ENDF file.

It can be seen:

- Problems in JEFF-3.2T3N
 - 102-Pd
 - 96,98,99-Ru
 - 36-S
 - 120-Te
 - 182,183,184,186,-W (This problem has been reported to KIT evaluators)
- Discontinuity at 30 MeV for all isotopes taken from TENDL2012

Figure 23. Comparison of Pd102-MT444 for different evaluated files

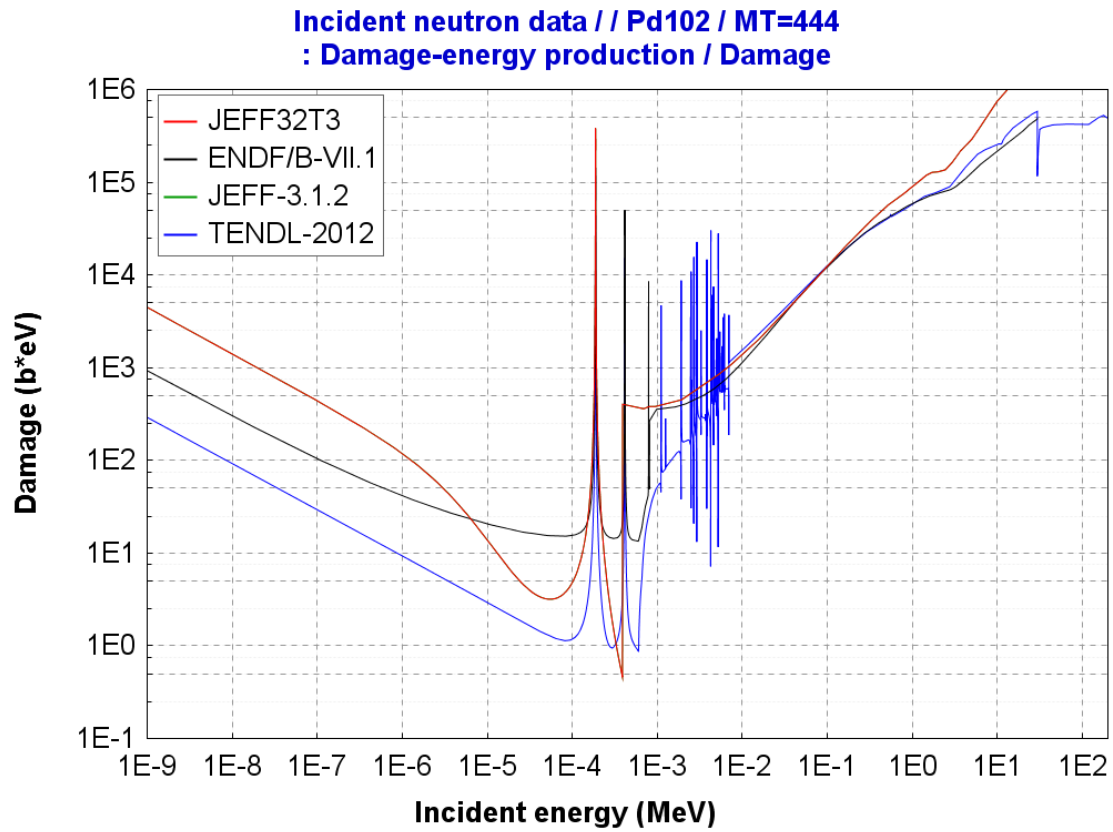


Figure 24. Comparison of Te120-MT444 for different evaluated files

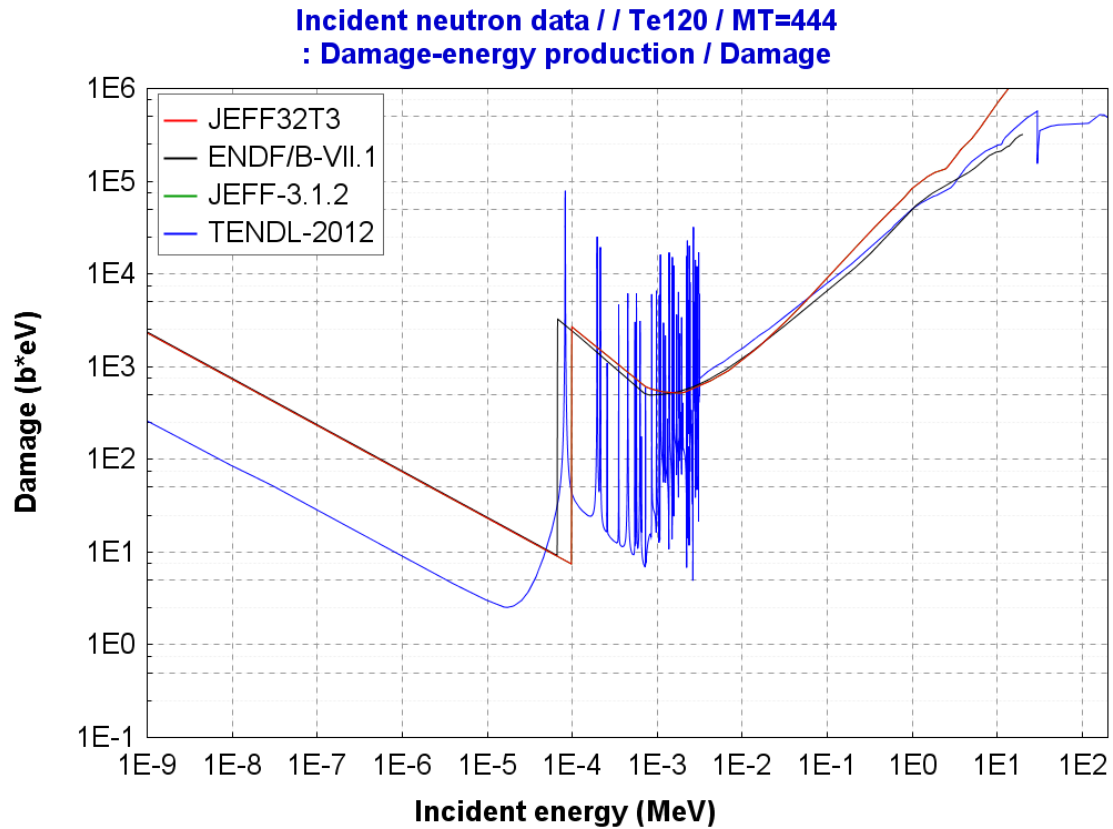


Figure 25. Comparison of Ru96-MT444 for different evaluated files

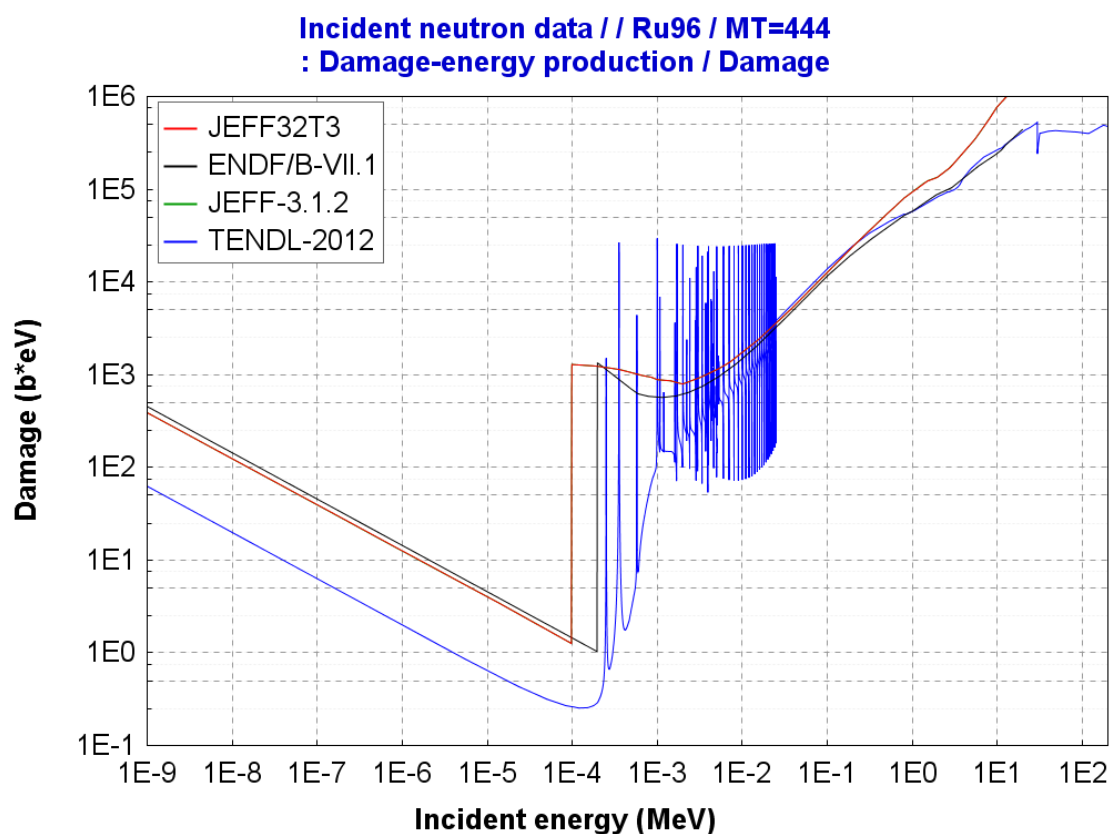


Figure 26. Comparison of S36-MT444 for different evaluated files

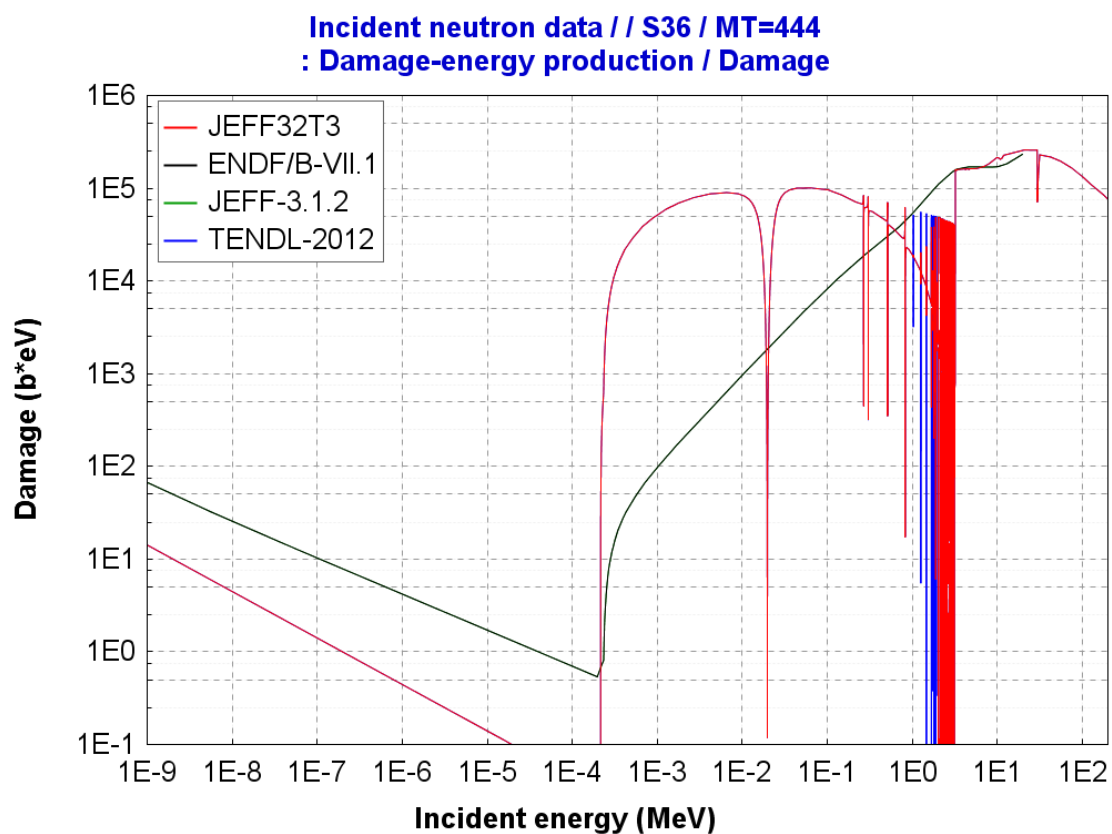
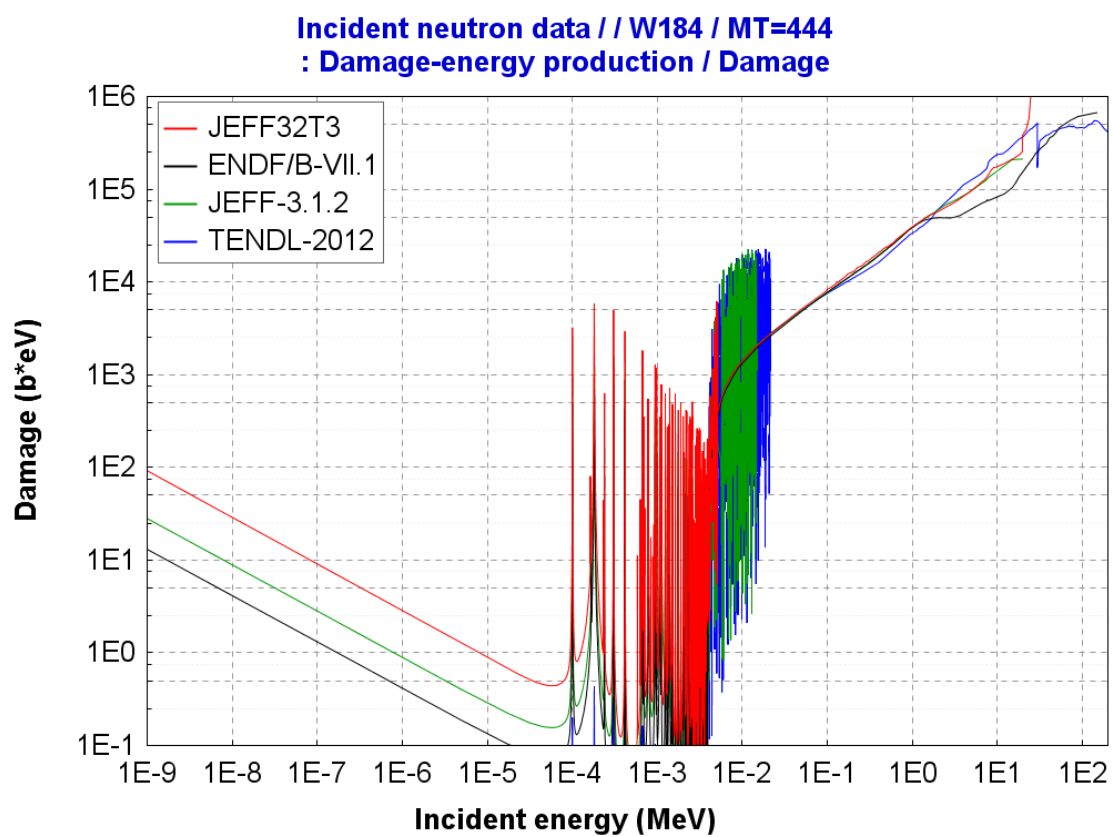


Figure 27. Comparison of W184-MT444 for different evaluated files



6. List of ANNEXES

6.1. *UPDATE Nb-93*

An update of Nb93 is proposed.

6.2. *JEFF-3.2 ACES*

A set of 12 files containing the processed JEFF-3.2T3 at different temperatures. NJOY inputs are also included.

6.3. *JEFF-32 STLs*

A set of 9 materials with STLs have processed at different temperatures.

6.4. *Processing JEFF-3.2T3 covariance data*

A web page “COV_PROCESS_JEFF32T3.htm” has been developed to visualize the present status of the covariance data processing.

A total processing of:

- 34 materials for MF31
- 198 materials for MF32/33
- 156 materials for MF34
- 3 materials for MF35
- 3 materials for MF40

6.5. *MCNP INPUTS*

A set of 123 MCNP inputs used for validation purposes is included.

6.6. *WARNINGS PREPRO*

All the warnings obtained by PREPRO (LINEAR+RECENT+SIGMA1) are summarized in “Warnings_PREPRO.txt”

6.7. COMPARISON BETWEEN DIFFERENT LIBRARIES

A set of figures have been processed with JANIS4.0 :

- 472 figures for MT1 (n, total)
- 472 figures for MT2(n,elastic)
- 72 figures for MT2(n,fission)
- 470 figures for MT102(n,gamma)
- 472 figures for MT444 (damage energy cross-section)

6.8. COMPARISON BETWEEN NJOY AND PREPRO

A set of 3457 figures have been processed using COMPLIT/PREPRO to compare the processing between NJOY and PREPRO.

Most of the figures show small differences.

The most important differences are summarized in Section 4.6

6.9. INTER AND BROADER

Two files "INTER.out" and "BROADR.out" summarize a comparison for the 472 materials using INTER and BROADR/NJOY codes.

The comparison of JEFF-3.2T3 is performed with:

- BROND-2.2
- CENDL-2.1
- EAF-2007
- FENDL-2.1
- JEF-2.2
- JEFF-3.0
- JEFF-3.0A
- JENDL-3.3
- JENDL-HE
- ENDFB-6.8
- ENDFB-7.0
- ENDFB-7.1
- JEFF-3.1
- JEFF-3.1.1
- JEFF-3.1.2
- TENDL-2011
- TENDL-2012

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