Calculation of Integral Quantities with ENDF/B-VII.1 Evaluated Neutron Library

Boris Pritychenko

National Nuclear Data Center

Brookhaven National Laboratory

Upton, NY 11973-5000, USA

BROOKHAVEN NATIONAL LABORATORY

a passion for discovery

U.S. DEPARTMENT OF ENERGY | Office of Science

Status of Previous Work

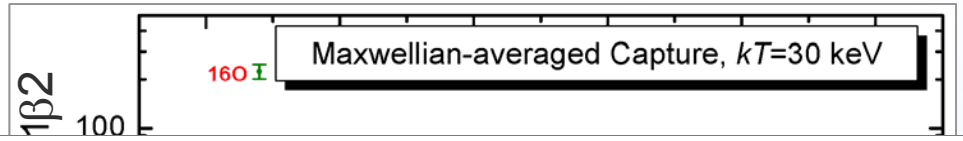
- ENDF/B-VII.0, JEFF-3.1, JENDL-3.3 & ENDF/B-VI.8 MACS and reaction rates have been calculated, providing a complimentary source of $\sigma(n,\gamma)$ for *s*-process, ADNDT **96**, 645 (2010)

$$\sigma^{Maxw}(kT) = \frac{2}{\sqrt{\pi}} \frac{a^2}{(kT)^2} \int_0^\infty \sigma(E_n^L) E_n^L e^{-\frac{a E_n^L}{kT}} dE_n^L$$

- Atlas of Neutron Resonances & KADONIS were used to identify ENDF library deficiencies
- No Maxwellian-averaged Cross Section (MACS) Uncertainties

ENDF/B-VII.1 Maxwellian-averaged Cross Sections

- ENDF/B-VII.1 $\sigma \oplus \delta\sigma(n,\gamma)$ were calculated
- KADONIS was used by CSEWG collaboration to improve ENDF
- Improvements for: ^{3}He, ^{9}Be,C-0/^{12}C, ^{16}O, ^{58}Co, . Nd region
- Theoretical values were adopted for ^{38}Ar, ^{82}Se, ^{115m}Cd, ^{141}Ce, ^{143}Pr and ^{148m,149}Pm
- MACS & Uncertainties would be published in ENDF/B-VII.1 paper



gadolinium isotopes," PhD dissertation, North Carolina State University (2010).

[286] R. Bahran, Y. Danon, M. Rapp, D. Williams, D. Barry, G. Leinweber, R. Block, J. Hoole, "A New High Resolution Neutron Transmission Detector at the RPI Gaerttner LINAC Laboratory", Submitted Proceedings of the Tenth International Topical Meeting on Nuclear Applications of Accelerators (AccApp 2011), Knoxville, TN, (2011).

[287] M. Herman, "Summary Document (Minutes) Presentations & Reports, CSEWG 2010". Available online http://www.nndc.bnl.gov/meetings/csewg2010.

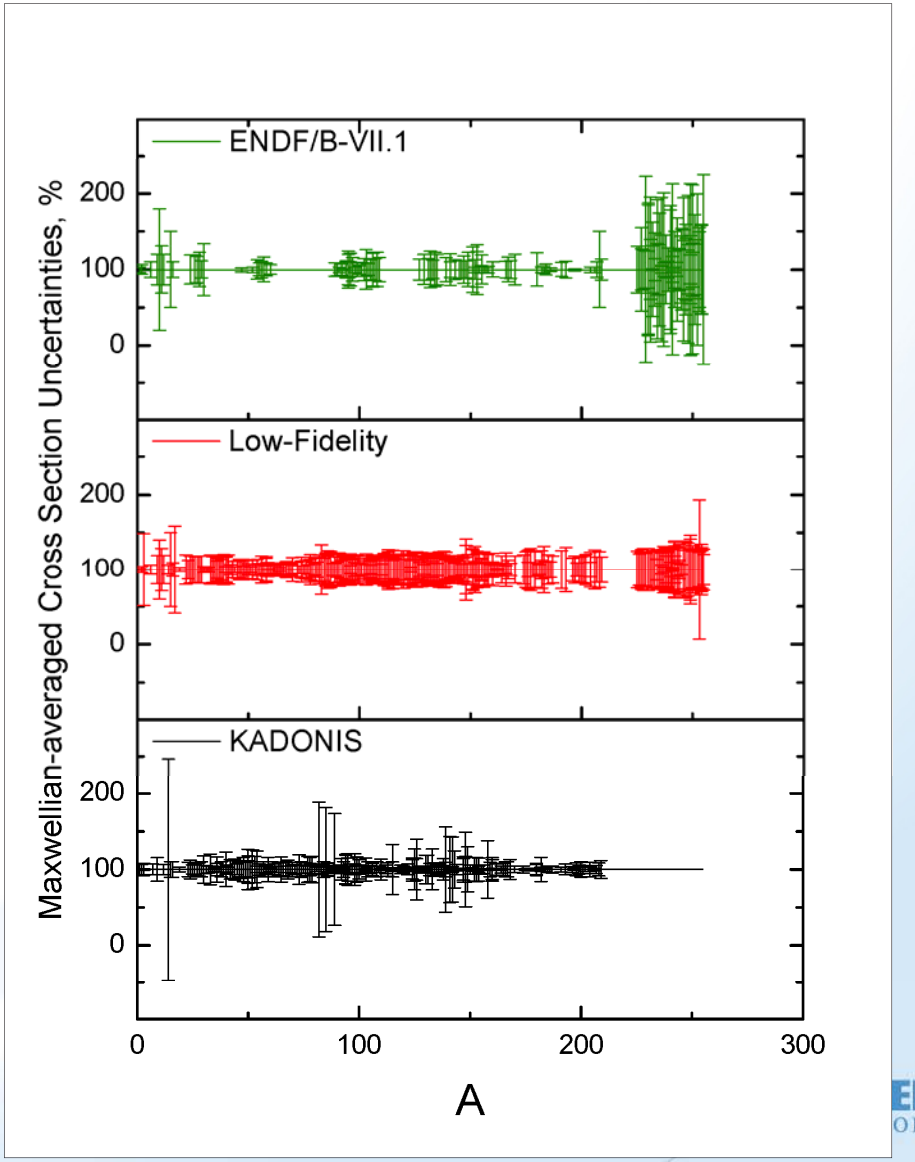
APPENDIX A: MAXWELLIAN-AVERAGED 30-KEV CAPTURE

TABLE XLI: Maxwellian-averaged cross sections from ENDF/B-VII.0 [1], ENDF/B-VII.1, KADoNiS [36] and their ratios at kT=30 keV (C-calculated from BNL-325 data [133], T-theoretical data in KADoNiS).

Material	VII.0 (barns)	VII.1 (barns)	KADoNiS (barns)	VII.0/VII.1	KADoNiS/VII.1
1-H - 1	1.525E-4	1.525E-4±5.853E-6	2.540E-4±2.000E-5	1.000E+0	1.666E+0±1.311E-1
1-H - 2	1.998E-6	1.998E-6±1.265E-7	3.000E-6±2.000E-7	1.000E+0	1.502E+0±1.001E-1
1-H - 3					
2-He- 3	2.455E-8	2.126E-5	7.600E-6±6.000E-7	1.155E-3	3.575E-1±2.822E-2
2-He- 4					
3-Li- 6	3.275E-5	3.276E-5±3.181E-6		9.997E-1	
3-Li- 7	4.645E-5	4.645E-5±2.103E-5	4.200E-5±3.000E-6	1.000E+0	9.042E-1±6.459E-2
4-Be- 7					
4-Be- 9	1.128E-4	9.298E-6±1.860E-6	1.040E-5±1.600E-6	1.213E+1	1.119E+0±1.721E-1
5-B - 10	4.299E-4	4.299E-4±1.720E-4		1.000E+0	
5-B - 11	6.575E-5	6.575E-5±2.026E-5		1.000E+0	
6-C-0/6-C-12	1.344E-6	1.623E-5±3.243E-6	1.540E-5±1.000E-6	8.281E-2	9.489E-1±6.161E-2
7-N - 14	6.682E-5	6.683E-5	4.100E-5±6.000E-5[C]	9.999E-1	6.135E-1±8.978E-1
7-N - 15	9.191E-6	9.190E-6±4.595E-6	5.800E-6±6.000E-7	1.000E+0	6.311E-1±6.529E-2
8-O - 16	1.692E-7	3.154E-5±3.154E-6	3.800E-5±4.000E-6	5.365E-3	1.205E+0±1.268E-1
8-O - 17	4.707E-6	4.708E-6		9.998E-1	
9-F - 19	4.362E-3	4.511E-3	3.200E-3±1.000E-4	9.670E-1	7.094E-1±2.217E-2
11-Na- 22	8.011E-3	8.011E-3		1.000E+0	
11-Na- 23	1.829E-3	1.829E-3	2.100E-3±2.000E-4	1.000E+0	1.148E+0±1.093E-1
12-Mg- 24	3.793E-3	3.793E-3±7.168E-4	3.300E-3±4.000E-4	1.000E+0	8.700E-1±1.055E-1
12-Mg- 25	5.279E-3	5.279E-3±1.732E-3	6.400E-3±4.000E-4	1.000E+0	1.212E+0±7.577E-2
12-Mg- 26	8.645E-5	8.645E-5±1.625E-5	1.260E-4±9.000E-6	1.000E+0	1.457E+0±1.041E-1
13-Al- 27	3.303E-3	3.303E-3±5.615E-4	3.740E-3±3.000E-4	1.000E+0	1.132E+0±9.083E-2
14-Si- 28	3.608E-3	3.608E-3±7.998E-4	1.420E-3±1.300E-4	1.000E+0	3.936E-1±3.603E-2
14-Si- 29	7.755E-3	7.755E-3±8.328E-4	6.580E-3±6.600E-4	1.000E+0	8.485E-1±8.511E-2
14-Si- 30	4.432E-3	4.432E-3±1.514E-3	1.820E-3±3.300E-4	1.000E+0	4.106E-1±7.446E-2
15-P - 31	7.237E-3	7.238E-3	1.740E-3±0.000E-5	9.999E-1	2.404E-1±1.243E-2
16-S - 32	5.658E-3	5.658E-3	4.100E-3±2.000E-4	1.000E+0	7.246E-1±3.535E-2
16-S - 33	2.274E-3	2.274E-3	7.400E-3±1.500E-3	1.000E+0	3.254E+0±6.596E-1
16-S - 34	2.330E-4	2.330E-4	2.260E-4±1.000E-5	1.000E+0	9.700E-1±4.292E-2
16-S - 36	6.326E-4	6.327E-4	1.710E-4±1.400E-5	9.998E-1	2.703E-1±2.213E-2
17-Cl- 35	7.534E-3	7.529E-3	9.680E-3±2.100E-4	1.001E+0	1.286E+0±2.789E-2
17-Cl- 37	2.057E-3	2.041E-3	2.120E-3±7.000E-5	1.008E+0	1.039E+0±3.430E-2
18-Ar- 36	8.838E-3	8.838E-3	9.000E-3±1.500E-3[T]	1.000E+0	1.018E+0±1.697E-1
18-Ar- 38	1.369E-4	1.369E-4	3.000E-3±3.000E-4[T]	1.000E+0	2.191E+1±2.191E+0
18-Ar- 40	2.249E-3	2.249E-3	2.540E-3±1.000E-4	1.000E+0	1.129E+0±4.446E-2
19-K - 39	1.848E-2	1.056E-2	1.180E-2±4.000E-4	1.750E+0	1.117E+0±3.788E-2
19-K - 40	1.939E-2	1.939E-2	3.100E-2±7.000E-3[T]	1.000E+0	1.599E+0±3.610E-1
19-K - 41	3.136E-2	2.029E-2	2.200E-2±7.000E-4	1.546E+0	1.084E+0±3.450E-2
20-Ca- 40	5.142E-3	5.142E-3	5.730E-3±3.400E-4	1.000E+0	1.114E+0±6.612E-2

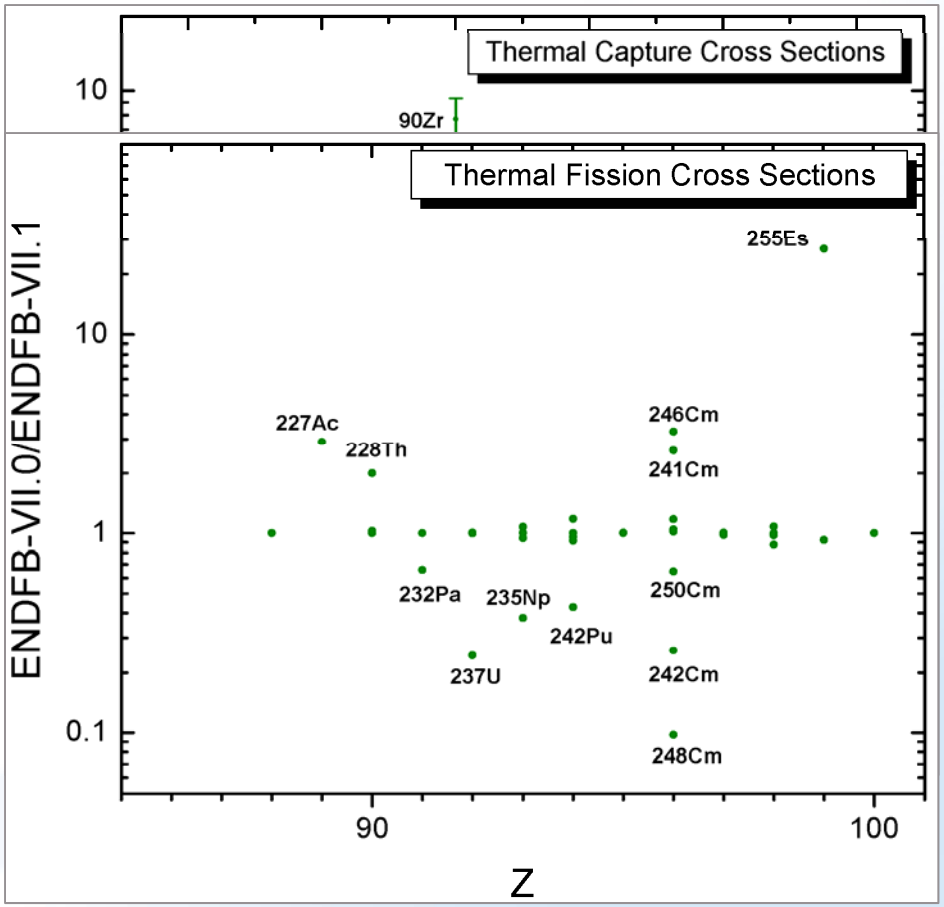
MACS Uncertainties, *kT*=30 keV

- Uncertainties constrain nucleosynthesis models
- ENDF/B-VII.1, priority materials for nuclear industry, minor actinides lack data
- Low-fidelity (2008), complete ENDF/B-VII.0
- KADoNiS, experimental, *s*-process



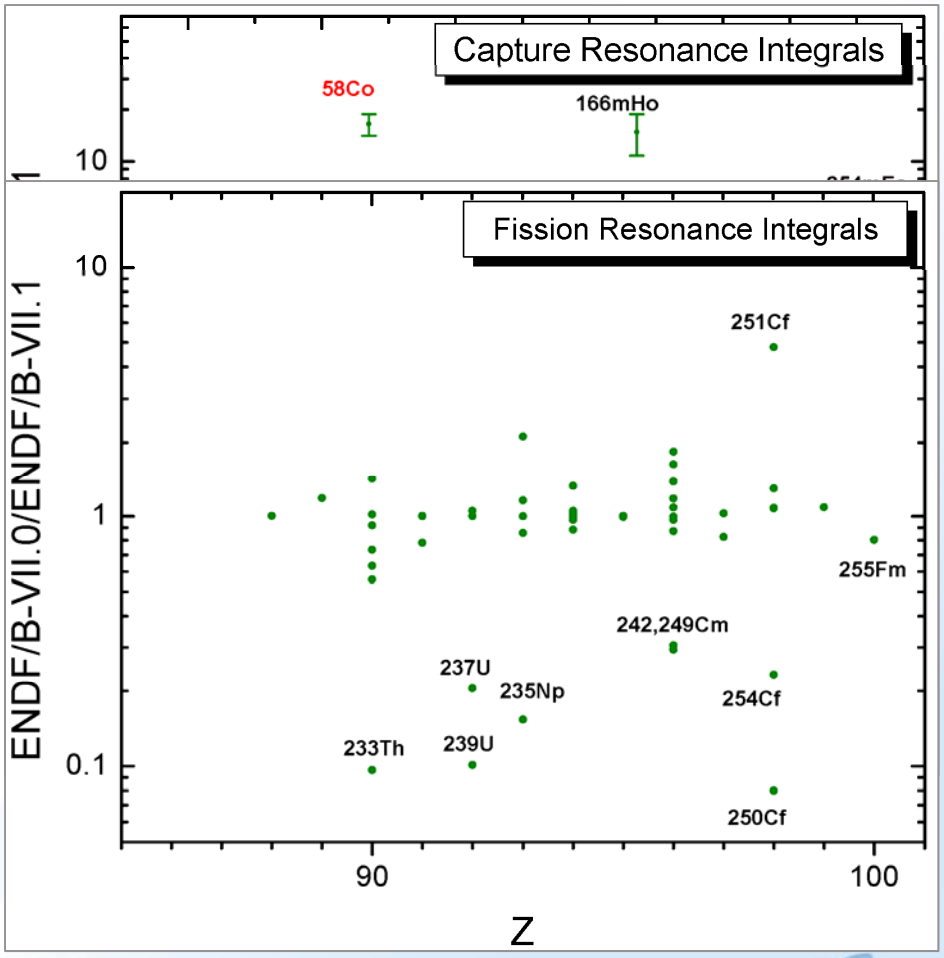
Thermal Cross Sections

- ENDF/B-VII.1 β3 MT=102 (n,γ),18 (n,F)
- Several data outliers in this case could be traced to the lack of measurements and incomplete overlap of experimental and theoretical data for ^{17}O,^{103}Ru,^{166m}Ho and ^{46}Ca, ^{58}Co,^{135}Cs, ^{204}Hg, respectively
- Outliers often indicate updates due to new data
- Zr-95 in beta5



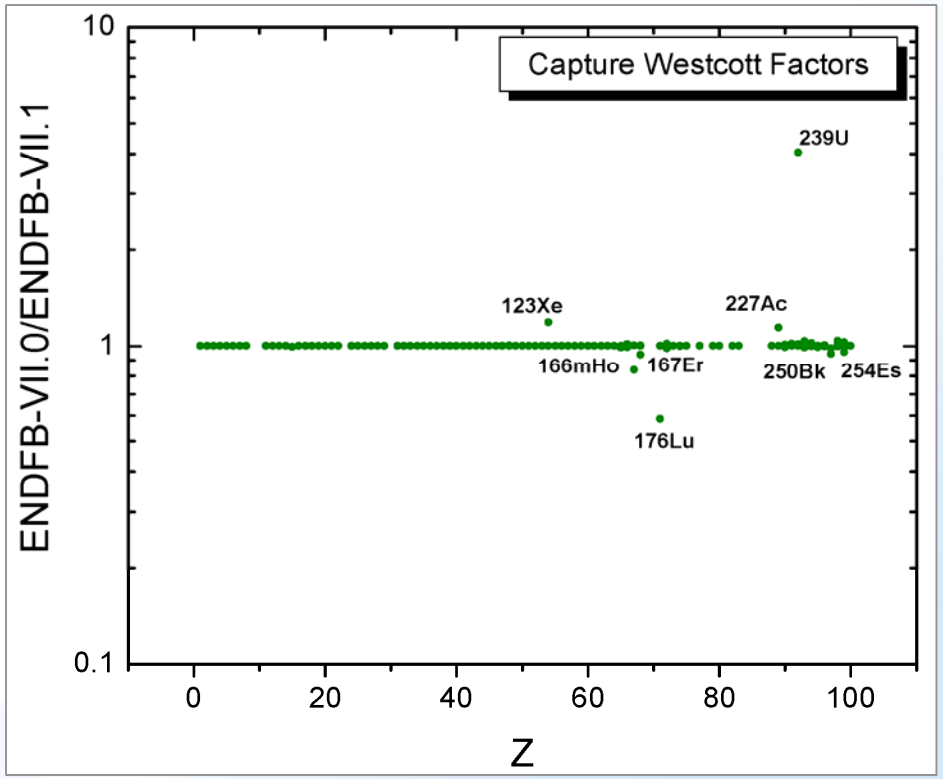
Resonance Integrals

- RI = $\int\sigma(E)/E\ dE$
- ENDF/B-VII.1 β3 MT=102 (n,γ),18 (n,F)
- ^{16}O,^{58}Co are fixed in β4
- Resonance integrals for neutron capture and fission were calculated for 0.5 eV - 20 MeV incident neutron energy range
- Fission or Actinide region differences are due to adoption of Actinoid file from JENDL-4



Westcott g-Factors

- WF = $\sigma_{Maxw}/\sigma_{Therm}$
- WF==1 if $\sigma \sim 1/v$
- ENDF/B-VII.1 β3 MT=102 (n,γ)
- In ENDF/B-VII.1 library Westcott factors evolved from 3.997 to 0.989 and from 1.002 to 1.711 for ^{239}U and ^{176}Lu, respectively. ^{176}Lu agrees with the recommended value of 1.75.



Conclusion & Outlook

- Thermal & Maxwellian Cross sections, Resonance Integrals and Westcott factors are produced for ENDF/B-VII.1 release
- Several ENDF deficiencies were identified and fixes are implemented
- ENDF/B-VII.1 MACS and their uncertainties are calculated and will be publicly released in December 2011
- Exchange of ideas between CSEWG and nuclear astrophysics communities
- Many thanks to M.W. Herman, M.B. Chadwick,

  S.F. Mughabghab and the CSEWG collaboration for help and support

s-proces Nucleosynthesis

- *s*-process path agrees well with ENDF neutron evaluations
- Equilibrium conditions can be observed along valley of stability:

$$\sigma_A N_A = \sigma_{A-1} N_{A-1} =$$

- ENDF/B-VII.1+Low-Fidelity= Independent proof for *s*-process nucleosynthesis (ENDF evaluators are often unaware of astro-physical models)