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Complete calculation of evaluated Maxwellian-averaged cross sections and their uncertainties for s-process nucleosynthesis

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Present contribution represents a significant improvement of our previous calculation of Maxwellian-averaged cross sections and astrophysical reaction rates. Addition of newly-evaluated neutron reaction libraries, such as ROSFOND and Low-Fidelity Covariance Project, and improvements in data processing techniques allowed us to extend it for entire range of s-process nuclei, calculate Maxwellian-averaged cross section uncertainties for the first time, and provide additional insights on all currently available neutron-induced reaction data. Nuclear reaction calculations using ENDF libraries and current Java technologies will be discussed and new results will be presented.

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1. Introduction

Nuclear reactions play an important role in stellar nucleosynthesis and are responsible for producing heavy chemical elements from light elements that were generated in the Big Bang. Present-day calculations of s-process nucleosynthesis are often based on dedicated nuclear astrophysics data tables, such as work of Bao et *al.* [1], or its successor KADONIS [2], however it is essential to produce complementary neutron-induced reaction data sets. ENDF-6 formatted evaluated neutron libraries contain various data for all known nuclei, including neutron capture cross sections for more than 680 individual nuclei from ^{1}H to ^{257}Fm in the range of neutron energy from 10^{-5} eV to 20 MeV. Nuclear-reactor and national-security application communities used these data extensively in the eV and MeV energy ranges, while keV data were less utilized. This creates a unique opportunity to utilize evaluated neutron data for non-traditional intermediate-energy applications, such as s-process nucleosynthesis, and create a new set of ENDF benchmarks. This work represents a significant upgrade of our previous calculation of Maxwellian-averaged cross sections and astrophysical reaction rates [3]. In addition of newly-evaluated neutron reaction libraries, such as JENDL-4, CENDL-3.1, ROSFOND 2010 and Low-Fidelity Covariance Project [4, 5], improvements in data processing techniques allowed us to extend calculations for the entire range of s-process nuclei and produce Maxwellian-averaged cross section uncertainties for the first time. Nuclear reaction calculations using evaluated neutron libraries and current Java technologies will be discussed and new results will be presented.

2. Calculation of Maxwellian-averaged Cross Sections and Uncertainties

ENDF libraries are based on theoretical calculations that are often adjusted to fit experimental data [6]. There are two kinds of ENDF cross section data representations: groupwise (averaged over energy interval) and pointwise. The first kind is often used in reactor physics calculations, while the second one is better suited for nuclear physics applications. Generic ENDF library cross sections (MF=3) do not contain information on neutron resonances. To resolve this problem for neutron physics calculations the codes PREPRO [7] and NJOY [8] are often used to produce a pointwise version of the libraries that include the resonance region data and provide cross section information within ENDF range of energies from 10^{-5} eV to 20 MeV. Here, we used the code PREPRO to reconstruct the resonance region with a precision of 0.1%.

Maxwellian-averaged cross sections can be expressed as [3]

$$\sigma^{Maxw}(kT) = \frac{2}{\sqrt{\pi}} \frac{(m_2/(m_1+m_2))^2}{(kT)^2} \int_0^\infty \sigma(E_n^L) E_n^L e^{-\frac{E_n^L m_2}{kT(m_1+m_2)}} dE_n^L \tag{2.1}$$

where k and T are the Boltzmann constant and temperature of the system, respectively and E is an energy of relative motion of the neutron with respect to the target. Here E_n^L is a neutron energy in the laboratory system and m_1 and m_2 are masses of a neutron and target nucleus, respectively.

Previously [3], Maxwellian-averaged cross sections and astrophysical reaction rates were produced using the Simpson method on linearized ENDF cross sections (MF=3). This simple method allowed quick calculated integral values with good precision. However the degree of precision was within $\sim$1% [3, 9]. This general limitation can be overcome in the linearized ENDF files because

Table 1: Evaluated nuclear libraries and KADONIS Maxwellian-averaged neutron capture cross sections in mb at *kT*=30 keV for *s*-process nuclei.

Isotope	JENDL-4.0	ROSFOND 2010	ENDF/B-VII.0	KADONIS [2]
36-Kr- 82	9.582E+1	9.483E+1	1.027E+2±2.097E+1	9.000E+1±6.000E+0
42-Mo- 96	1.052E+2	1.035E+2	1.036E+2±1.690E+1	1.120E+2±8.000E+0
44-Ru-100	2.065E+2	2.062E+2	2.035E+2±3.949E+1	2.060E+2±1.300E+1
46-Pd-104	2.700E+2	2.809E+2	2.809E+2±4.488E+1	2.890E+2±2.900E+1
48-Cd-110	2.260E+2	2.346E+2	2.346E+2±4.219E+1	2.370E+2±2.000E+0
50-Sn-116	9.115E+1	1.002E+2	1.002E+2±1.875E+1	9.160E+1±6.000E-1
52-Te-122	2.644E+2	2.639E+2	2.349E+2±4.883E+1	2.950E+2±3.000E+0
52-Te-123	8.138E+2	8.128E+2	8.063E+2±1.063E+2	8.320E+2±8.000E+0
52-Te-124	1.474E+2	1.473E+2	1.351E+2±2.682E+1	1.550E+2±2.000E+0
54-Xe-128	2.582E+2	2.826E+2	2.826E+2±6.823E+1	2.625E+2±3.700E+0
54-Xe-130	1.333E+2	1.518E+2	1.518E+2±2.993E+1	1.320E+2±2.100E+0
56-Ba-134	2.301E+2	2.270E+2	2.270E+2±4.038E+1	1.760E+2±5.600E+0
56-Ba-136	7.071E+1	7.001E+1	7.001E+1±1.087E+1	6.120E+1±2.000E+0
60-Nd-142	3.557E+1	3.701E+1	3.341E+1±4.252E+1	3.500E+1±7.000E-1
62-Sm-148	2.361E+2	2.444E+2	2.449E+2±4.416E+1	2.410E+2±2.000E+0
62-Sm-150	4.217E+2	4.079E+2	4.227E+2±3.601E+2	4.220E+2±4.000E+0
64-Gd-154	9.926E+2	1.010E+3	9.511E+2±1.070E+2	1.028E+3±1.200E+1
66-Dy-160	8.702E+2	8.293E+2	8.328E+2±6.769E+1	8.900E+2±1.200E+1
72-Hf-176	5.930E+2	4.529E+2	4.571E+2±4.811E+1	6.260E+2±1.100E+1
80-Hg-198	1.612E+2	1.612E+2	1.612E+2±1.621E+1	1.730E+2±1.500E+1
82-Pb-204	8.355E+1	7.242E+1	7.242E+1±7.699E+0	8.100E+1±2.300E+0

the cross section value is linearly-dependent on energy within a particular bin [10]

$$\sigma(E) = \sigma_1 + (E - E_1)\frac{\sigma(E_2) - \sigma(E_1)}{E_2 - E_1} \tag{2.2}$$

where $\sigma(E_1), E_1$ and $\sigma(E_2), E_2$ are pointwise cross section and energy values for the corresponding energy bin. Last equation is a good approximation of neutron cross section values for a sufficiently dense grid. This allowed us to calculate definite integrals using Wolfram Mathematica online integrator [11]. Summing integrals for all energy bins will produce an exact integral value for Maxwellian-averaged cross section. Low-Fidelity cross section covariances were used to calculate uncertainties for ENDF/B-VII.0 data [5, 12]. Final results for JENDL-4.0, ROSFOND 2010 and ENDF/B-VII.0 libraries [13, 4, 12] are shown in Table 1. Due to space limitations only selected data are shown and CENDL-3.1, JEFF-3.1 cross sections are omitted.

In *s*-process nucleosynthesis, we assume that product of neutron-capture cross section (at 30 keV in mb) times solar system abundances (relative to Si = 10^6) as a function of atomic mass should be constant for equilibrium nuclei [14]:

$$\sigma_A N_A = \sigma_{A-1} N_{A-1} = constant \tag{2.3}$$

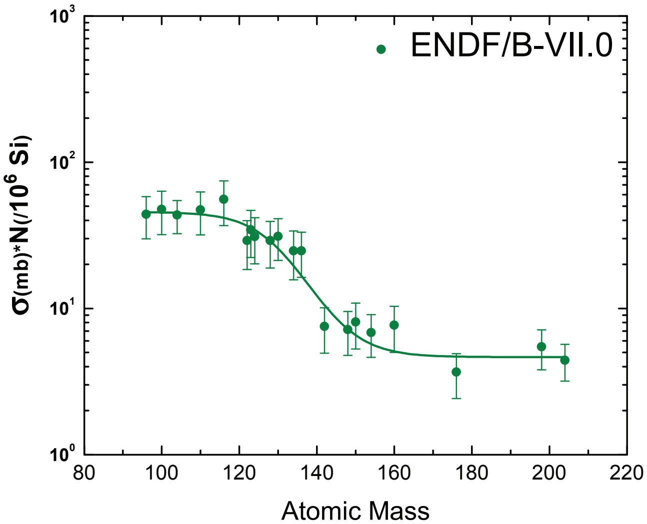

Figure 1: ENDF/B-VII.0 product of neutron-capture cross section (at 30 keV in mb) times solar system abundances (relative to Si = 10^6) as a function of atomic mass for nuclei produced only in the *s*-process.

To verify this phenomenon, the calculated $\langle\sigma_\gamma^{Maxw}(30keV)\rangle$ from the ENDF/B-VII.0 library [12] were multiplied by solar abundances taken from Anders and Grevesse [15], and plotted in Figure 1. Visual inspection of the Figure indicates two local equilibrium and ledge-precipice break at $A \sim 138$ for the ENDF/B-VII.0 fit. Relatively high product value for ^{116}Sn is due to the fact that ^{116}Sn has *r*-process contribution [15].

In FY 2011, present contribution results will be used to upgrade 'Maxwellian-averaged Cross Sections and Astrophysical Reaction Rates' Web application *http://www.nndc.bnl.gov/astro*. The Web application frontpage is shown in Figure 2.

3. Conclusion & Outlook

Maxwellian-averaged cross sections for neutron capture have been calculated using JENDL-4, CENDL-3.1, ROSFOND 2010, ENDF/B-VII.0 and JEFF-3.1 libraries using Low-Fidelity covariance project data. ROSFOND 2010 library (686 materials) [4] provides the most complete coverage along the s-process path. In fact, it contains information on 347 out of 354 isotopes (98% coverage). The only *s*-process isotopes that are missing in ROSFOND are: ^{12}C, ^{110}Ag, ^{132,133,135,137}Ce and ^{142}Pr. Carbon and Praseodymium cross sections can be found in the CENDL-3.1 and ENDF/B-VII.0 or JEFF-3.1 libraries, respectively. Typical neutron library, such as ENDF/B-VII.0 (393 materials), provides 80% coverage of the *s*-process path.

The comparison of Maxwellian-averaged cross section values from Table 1 indicates a good agreement between KADONIS and evaluated nuclear libraries. Future work on ENDF libraries will provide additional improvements and benefits for nuclear astrophysics and applications communities.

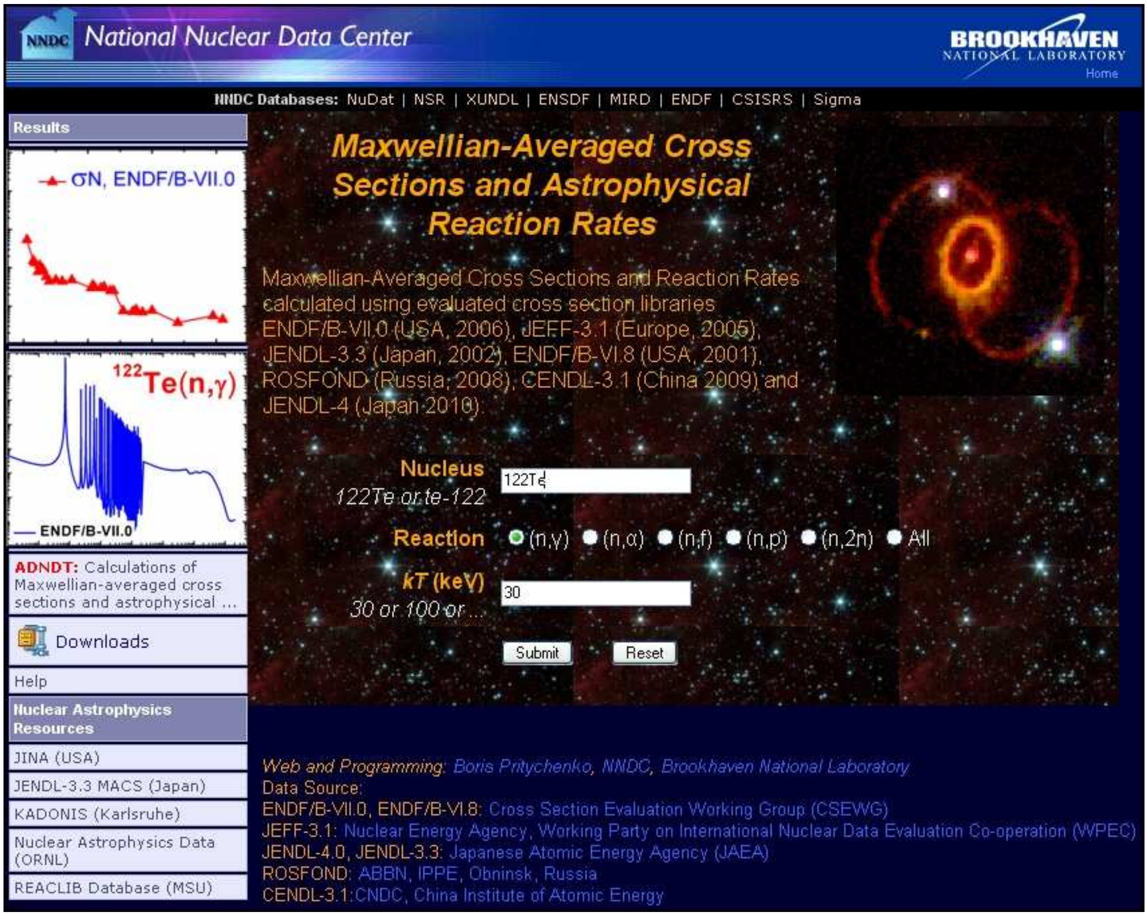

Figure 2: 'Maxwellian-averaged Cross Sections and Astrophysical Reaction Rates' Web application, *http://www.nndc.bnl.gov/astro*.

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