Status of astrophysical abundances and rates calculation using ENDF/B libraries

Boris Pritychenko[1]

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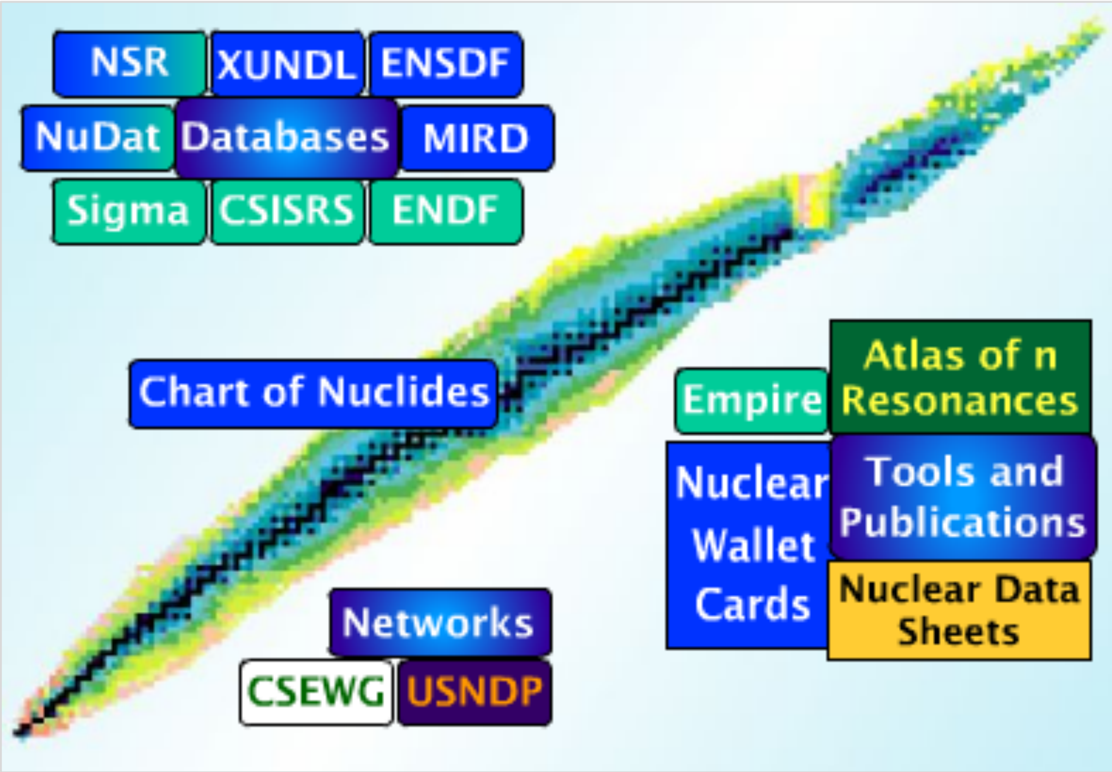
BROOKHAVEN NATIONAL LABORATORY

U.S. DEPARTMENT OF ENERGY

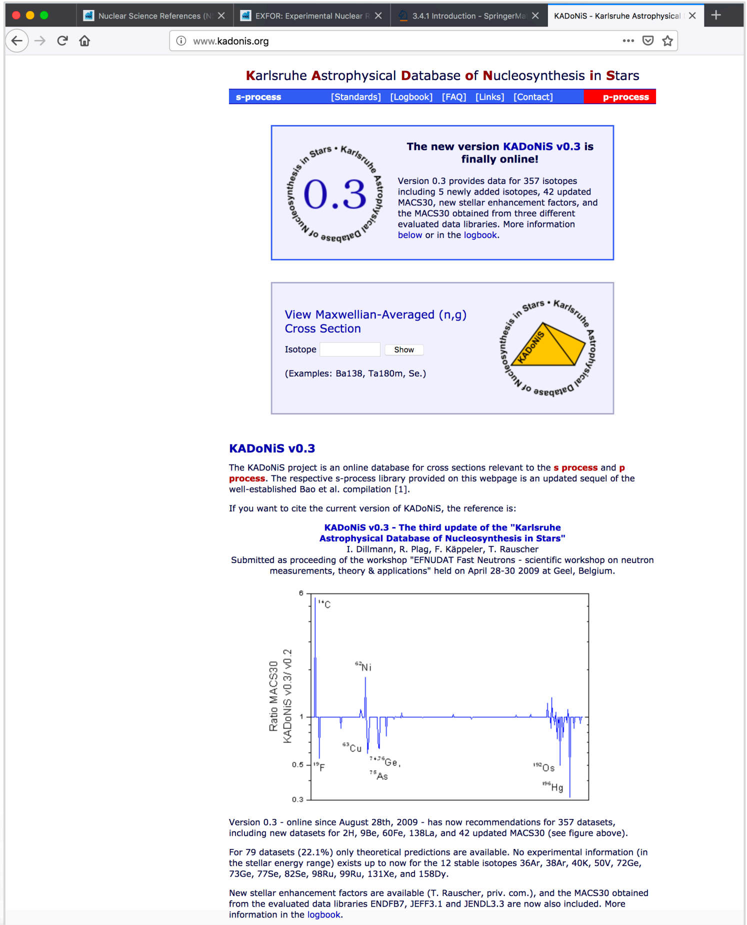
National Nuclear Data Center

- The National Nuclear Data Center (NNDC) collects, evaluates, and disseminates nuclear physics data for basic nuclear research and for applied nuclear technologies. The NNDC is a worldwide resource for nuclear data.
- Major Databases
  - ENDF: Evaluated Nuclear (reaction) Data File
  - EXFOR: Experimental Nuclear Reaction Data
  - ENSDF: Evaluated Nuclear Structure Data File
  - XUNDL: eXperimental Unevaluated Nuclear Data List
  - NSR: Nuclear Science References
- Web Services: *www.nndc.bnl.gov*
- Nuclear model development and research projects



Recent Re-analysis of KADoNiS Library

- KADoNiS (Karlsruhe Astrophysical Database of Nucleosynthesis in Stars) has been extensively used in stellar nucleosynthesis calculations, and its cross sections are normalized (biased) to a ^{197}Au(n,γ) activation measurement of W. Ratynski, F. Kaeppeler, Phys. Rev. C 37, 595 (1988).
- The activation Maxwellian-averaged cross section (MACS) 30 keV value of 582±9 mb disagrees with the International Evaluation of Neutron Cross Section Standards value of 620±11 mb.
- The standards are extensively used in ENDF/B-VIII.0 library.
- Re-analysis of gold neutron capture cross sections by R. Reifarth et *al*. showed an impact of neutron backing material scattering; ENDF libraries are essentially based on the TOF-measurements and not affected by this issue.
- The revised ^{197}Au(n,γ) activation MACS value of 612±6 mb is consistent with the ENDF value, and the KADoNiS cross sections have been updated for 63 target nuclides from ^{103}Rh to ^{197}Au.
- Only corrected cross section plots are available publicly while we need data for GW170817 modeling.



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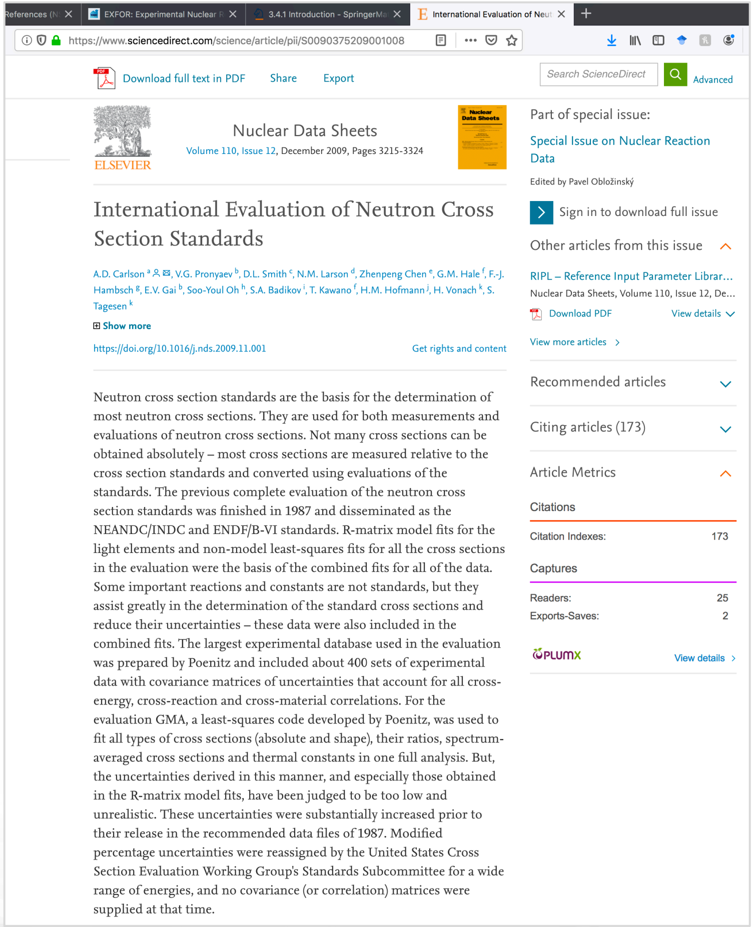

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DOI 10.1140/epjp/i2018-12295-3

THE EUROPEAN PHYSICAL JOURNAL PLUS

Review

Neutron-induced cross sections*

From raw data to astrophysical rates

René Reifarth[1,a], Philipp Erbacher[1], Stefan Fiebiger[1], Kathrin Göbel[1], Tanja Heftrich[1], Michael Heil[2], Franz Käppeler[3], Nadine Klapper[1], Deniz Kurtulgil[1], Christoph Langer[1], Claudia Lederer-Woods[4], Alberto Mengoni[5,6], Benedikt Thomas[1], Stefan Schmidt[7], Mario Weigand[1], and Michael Wiescher[8]

[1] Goethe University Frankfurt am Main, Frankfurt, Germany
[2] GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, Germany
[3] Karlsruhe Institute of Technology, Karlsruhe, Germany
[4] School of Physics and Astronomy, University of Edinburgh, Edinburgh, UK
[5] ENEA, Bologna, Italy
[6] INFN, Sezione di Bologna, Bologna, Italy
[7] Frankfurt Institute for Advanced Studies, Frankfurt, Germany
[8] University of Notre Dame, Notre Dame, IN, USA

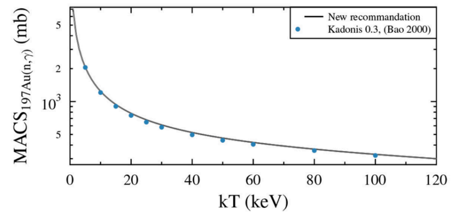


Fig. 13. New (based on [59,60,63])and old [21,22,71] recommendation for the *MACS* of ^{197}Au.

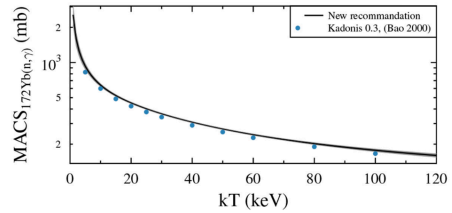
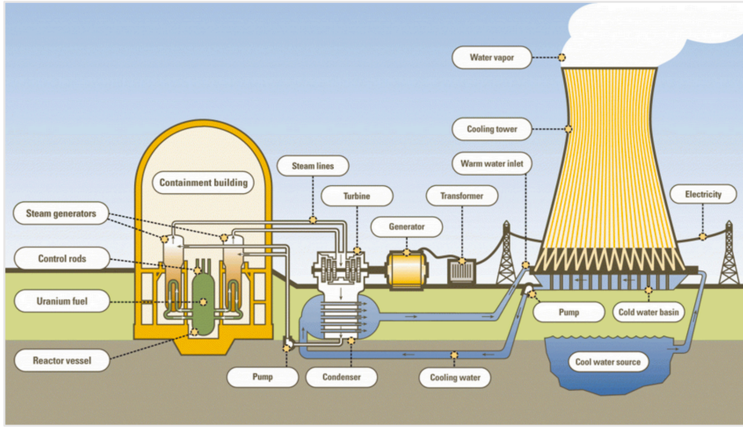


Fig. 14. New and old [21,71,72] recommendation for the *MACS* of ^{172}Yb.

ENDF/B (Evaluated Nuclear Data File) Library

- In the light of the previous disclosure, it is absolutely essential to develop fully traceable, documented and unbiased nuclear data sets for stellar nucleosynthesis calculations.
- ENDF/B is a primary nuclear reaction data library for applications, and it is focused on target nuclei near the valley of stability.
- The ENDF/B library was originally produced by the Cross Section Evaluation Working Group (CSEWG) collaboration in 1968 for nuclear power plant design, criticality safety, shielding, and national security applications.
- It gained a worldwide popularity, many nations forged their own evaluated nuclear data libraries using the ENDF-6 format, and its user community has broadened into applied and fundamental sciences since introduction of evaluated neutron cross sections in MCNP, and GEANT computer codes simulations.
- The recently released ENDF/B-VIII.0 library by the CSEWG collaboration represents the state of the art in nuclear reaction data evaluations.



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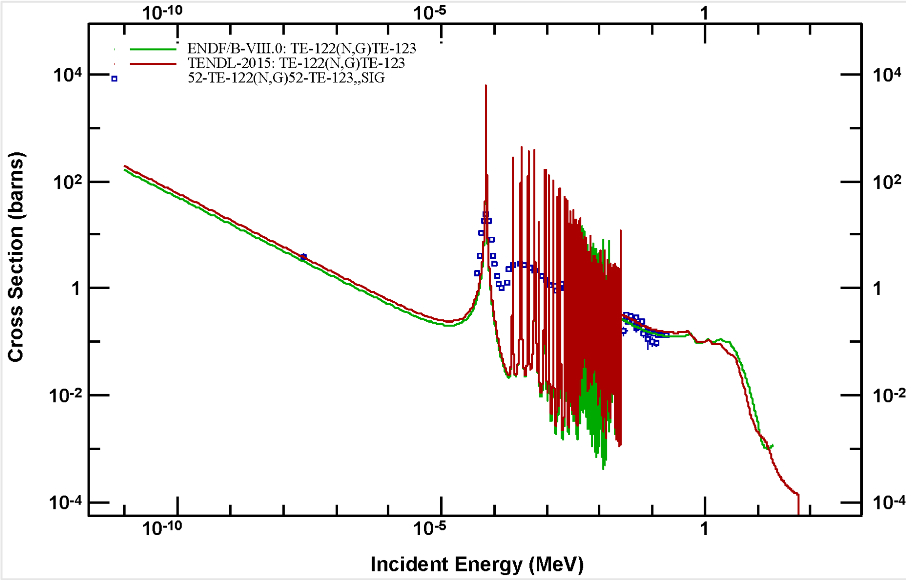
ENDF & Slow Neutron Capture

- ENDF neutron targets list matches well with an *s*-process path.
- Slow neutron capture Maxwellian-averaged cross sections (MACS) can be expressed as

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

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^L_n is a neutron energy in the laboratory system and m_1 and m_2 are masses of a neutron and target nucleus.

- Calculation of MACS and astrophysical reaction rates by Doppler broadening cross sections and numerical integration.



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ELSEVIER
Atomic Data and Nuclear Data Tables
Volume 96, Issue 6, November 2010, Pages 645-748

Calculations of Maxwellian-averaged cross sections and astrophysical reaction rates using the ENDF/B-VII.0, JEFF-3.1, JENDL-3.3, and ENDF/B-VI.8 evaluated nuclear reaction data libraries

B. Pritychenko, S.F. Mughaghab, A.A. Sonzogni

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https://doi.org/10.1016/j.adt.2010.05.002

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Abstract

We have calculated the Maxwellian-averaged cross sections and astrophysical reaction rates of the stellar nucleosynthesis reactions (n, γ), (n, fission), (n, p), (n, α), and (n, 2n) using the ENDF/B-VII.0, JEFF-3.1, JENDL-3.3, and ENDF/B-VI.8 evaluated nuclear reaction data libraries. These four major nuclear reaction libraries were processed under the same conditions for Maxwellian temperatures (*kT*) ranging from 1 keV to 1 MeV. We compare our current calculations of the *s*-process nucleosynthesis nuclei with previous data sets and discuss the differences between them and the implications for nuclear astrophysics.

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ELSEVIER
Nuclear Data Sheets
Volume 113, Issue 12, December 2012, Pages 3120-3144

Neutron Thermal Cross Sections, Westcott Factors, Resonance Integrals, Maxwellian Averaged Cross Sections and Astrophysical Reaction Rates Calculated from the ENDF/B-VII.1, JEFF-3.1.2, JENDL-4.0, ROSFOND-2010, CENDL-3.1 and EAF-2010 Evaluated Data Libraries

B. Pritychenko [a], S.F. Mughabghab [a]
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https://doi.org/10.1016/j.nds.2012.11.007

Abstract

We present calculations of neutron thermal cross sections, Westcott factors, resonance integrals, Maxwellian-averaged cross sections and astrophysical reaction rates for 843 ENDF materials using data from the major evaluated nuclear libraries and European activation file. Extensive analysis of newly-evaluated neutron reaction cross sections, neutron covariances, and improvements in data processing techniques motivated us to calculate nuclear industry and neutron physics quantities, produce *s*-process Maxwellian-averaged cross sections and astrophysical reaction rates, systematically calculate uncertainties, and provide additional insights on currently available neutron-induced reaction data. Nuclear reaction calculations are discussed and new results are presented. Due to space limitations, the present paper contains only calculated Maxwellian-averaged cross sections and their uncertainties. The complete data sets for all results are published in the Brookhaven National Laboratory report.

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ELSEVIER

Nuclear Data Sheets

Volume 148, February 2018, Pages 1-142

Nuclear Data Sheets

ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data

D.A. Brown [a], M.B. Chadwick [b], R. Capote [c], A.C. Kahler [b], A. Trkov [c], M.W. Herman [a], A.A. Sonzogni [a], Y. Danon [d], A.D. Carlson [e], M. Dunn [f], D.L. Smith [g], G.M. Hale [b], G. Arbanas [h], R. Arcilla [a], C.R. Bates [b], B. Beck [i], B. Becker [j], F. Brown [b], R.J. Casperson [i], J. Conlin [b], D.E. Cullen [i], M.-A. Descalle [i], R. Firestone [k], T. Gaines [l], K.H. Guber [h], A.I. Hawari [m], J. Holmes [n], T.D. Johnson [a], T. Kawano [b], B.C. Kiedrowski [o], A.J. Koning [c], S. Kopecky [p], L. Leal [q], J.P. Lestone [b], C. Lubitz [r], J.I. Márquez Damián [s], C.M. Mattoon [i], E.A. McCutchan [a], S. Mughabghab [a], P. Navratil [t], D. Neudecker [b], G.P.A. Nobre [a], G. Noguere [u], M. Paris [b], M.T. Pigni [h], A.J. Plompen [p], B. Pritychenko [a], V.G. Pronyaev [v], D. Roubtsov [w], D. Rochman [x], P. Romano [g], P. Schillebeeckx [p], S. Simakov [y], M. Sin [z], I. Sirakov [aa], B. Sleaford [i], V. Sobes [h], E.S. Soukhovitskii [ab], I. Stetcu [b], P. Talou [b], I. Thompson [i], S. van der Marck [ac], L. Welser-Sherrill [b], D. Wiarda [h], M. White [b], J.L. Wormald [m], R.Q. Wright [h], M. Zerkle [n], G. Žerovnik [p], Y. Zhu [m]

ENDF Validation: *s*-process Modeling

- The *s*-process abundance of an isotope $N_{(A)}$ depends on its precursor $N_{(A-1)}$ quantity as

$$\frac{dN_{(A)}}{dt} = \sigma_{(A-1)} N_{(A-1)} + \sigma_{(A)} N_{(A)}$$

- This equation was analytically solved (classical model)

$$\sigma_{(A)} N_{(A)} = \frac{f N_{56}}{\tau_0} \prod_{i=56}^{A} \left[1 + \frac{1}{\sigma(i)\tau_0}\right]^{-1}$$

- Select *s*-process only nuclides along the process path and fit MACS abundance product values using least squares.
- Use fitting parameters to calculate *s*-process contributions and compare with the presently-observed product values.
- The observed surplus is commonly attributed to an *r*-process (rapid neutron capture) contribution.

TABLE I: *s*-process strong component neutron fluence parameters for ENDF/B-VIII.0 and TENDL-2015 libraries [15, 16].

Parameters	ENDF/B-VIII.0	TENDL-2015
f	0.00434±0.00123	0.00355±0.00059
τ_0	0.31256±0.02947	0.37488±0.03013

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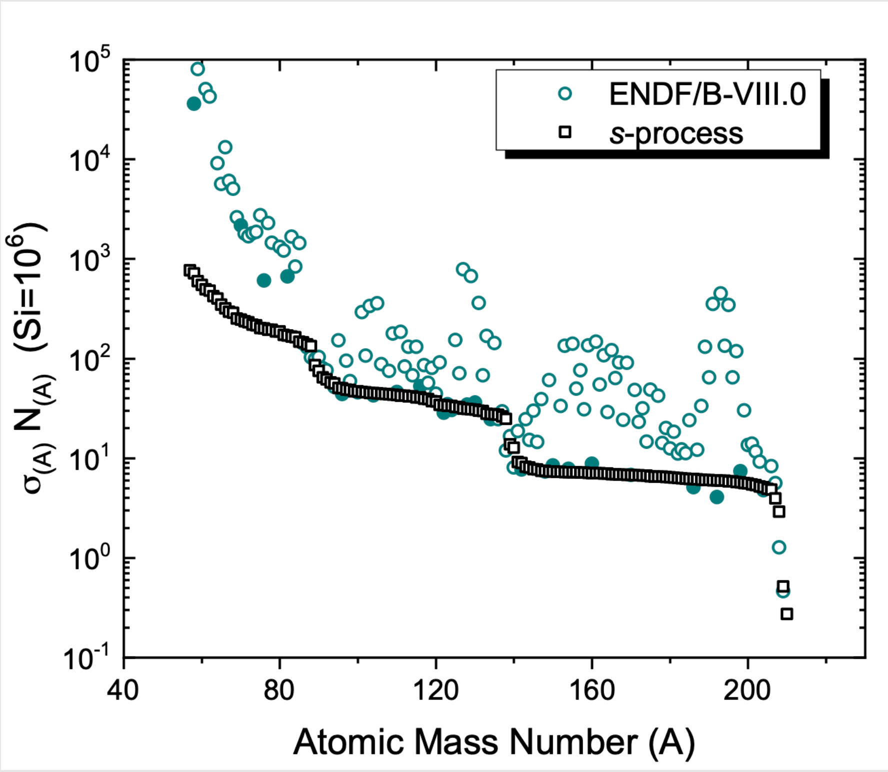

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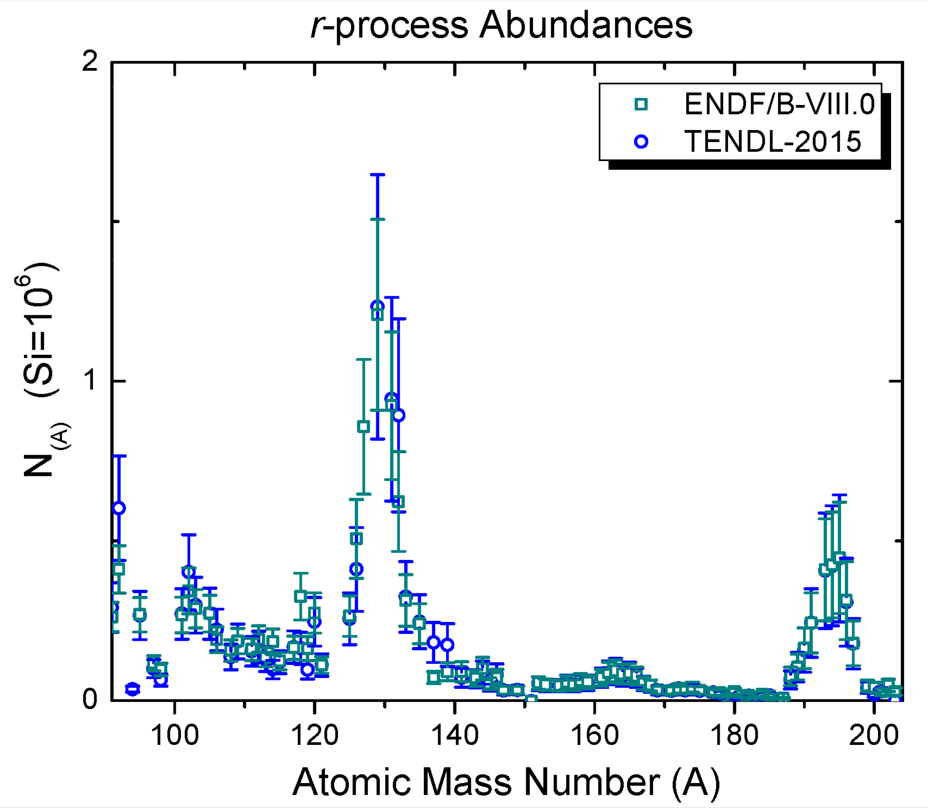
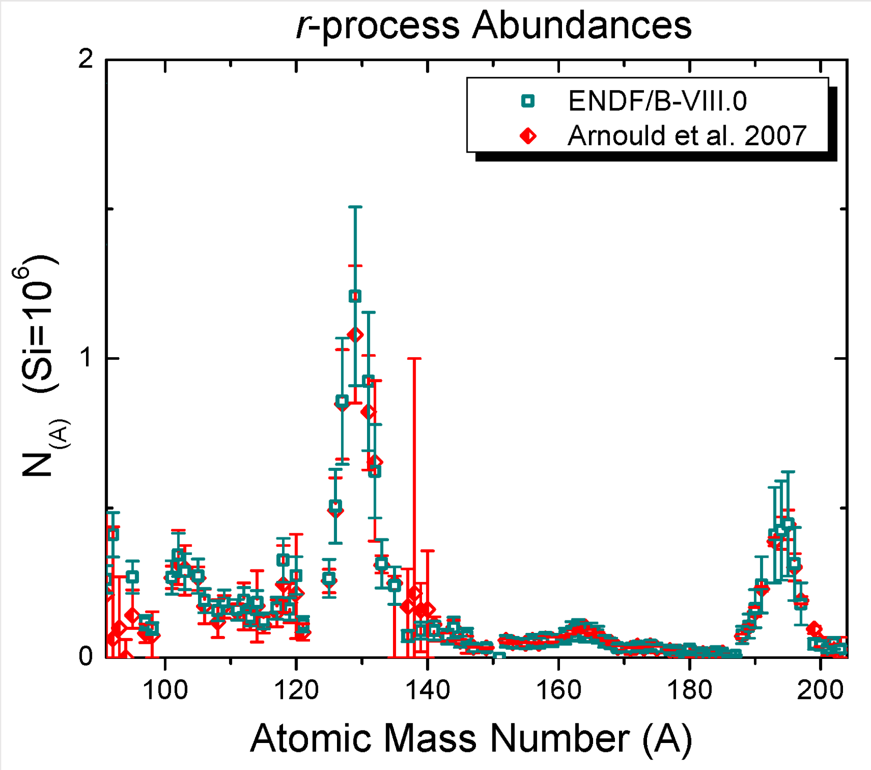


Analysis of *r*-process Abundances

- *M. Arnould et al., Phys. Rep. 450, 97 (2007)* is based on H. Palme, H. Beer, Abundances of the Elements in the Solar System, in Landolt Bornstein, New Series, Group VI, Astron. & Astrophys., Vol. 3, Subvol. a, (Berlin: Springer), p. 196 (1993).
- ENDF/B-VIII.0 *r*-process abundances agree well with M. Arnould et al. except (N=82): ^{138}Ba and ^{140}Ce (n,γ).
- *s*-process overproduction in ^{138}Ba was observed by Palme & Beer, its abundance was interpreted by Arnould et al. as $0.214^{+0.786}_{-0.214}$ (Si=10^6), ^{140}Ce (n,γ) cross sections will be further investigated in the next release of ENDF/B library.
- ENDF library clearly contains high quality data and can be used in astrophysical modeling.
- Classic model precision for non-branching heavy nuclei ~3%, and it is reliable for heavy nuclei.



REACLIB: Astrophysical Reaction Rates

- Next, calculate ENDF/B-VIII.0 & TENDL-2015 reaction rates for (n,γ), (n,F), (n,p) and (n,α) within 0.01-10 GK range, fit the data into REACLIB data format. Start testing with codes like MESA….
- KADoNiS has rates for kT=1-100 keV based on (n,γ) *kT*=30 keV cross sections.
- The complementary theoretical calculations of T. Rauscher, F.K. Thielemann extend the range to 0.1-10 GK (*kT* =8-800 keV) using the statistical model NON-SMOKER code derived from the SMOKER.
- *S*-process range of *kT*=8-90 keV.
- No SEF correction in rates.

$$
\begin{aligned}
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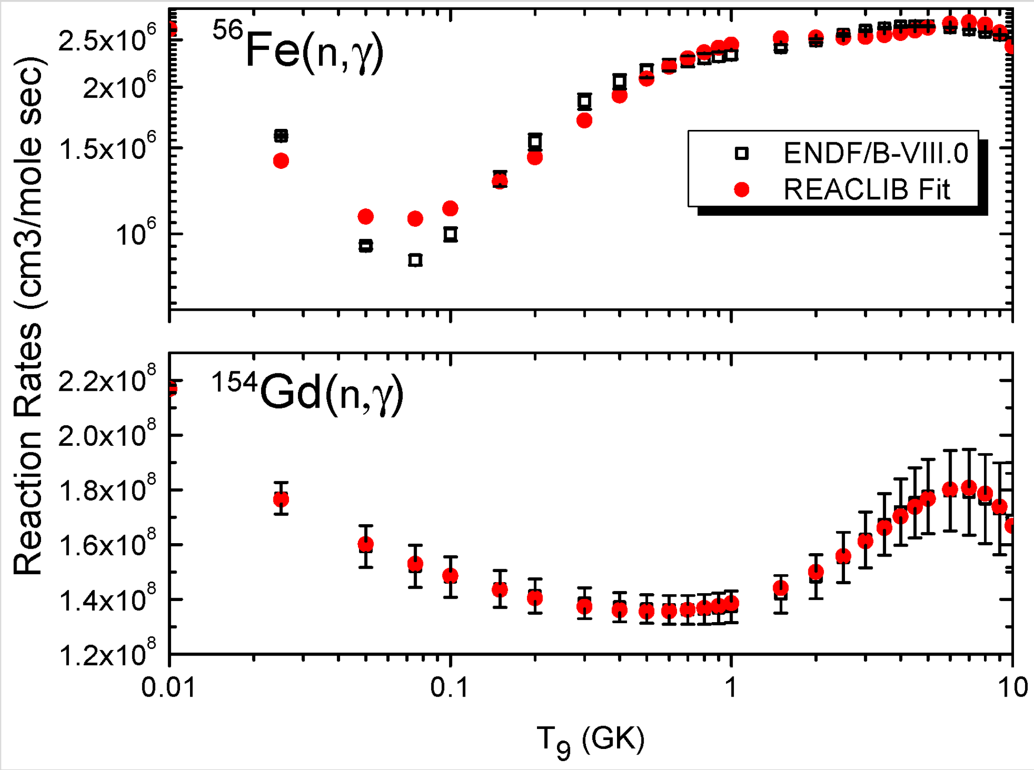

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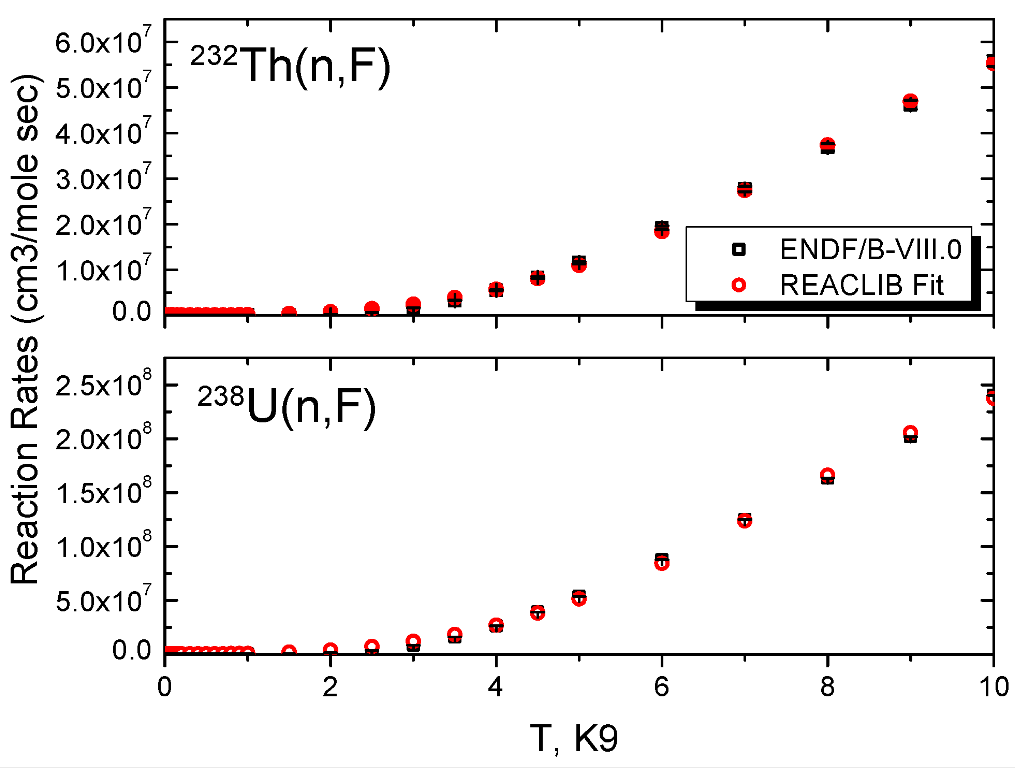
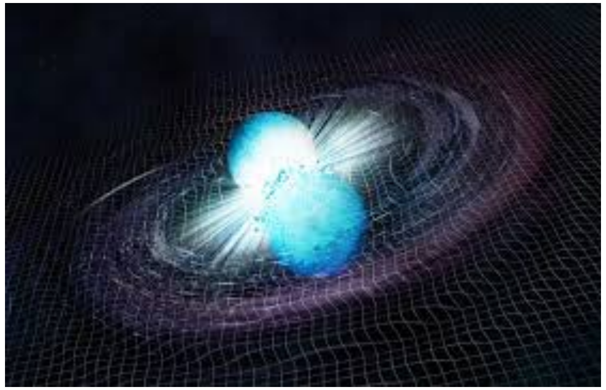


Takeaways

- GW170817 neutron star merger renewed interest in stellar nucleosynthesis calculations.
- *r*-process abundances have been calculated using ENDF/B-VIII.0 and TENDL-2015 evaluated neutron cross sections and Lodders, Palme and Gail solar system abundances.
- Current work: (n,γ), (n,F), (n,p) and (n,α) ENDF reaction rates fitting, production of REACLIB files and future computations with nuclear astrophysics codes.
- Rates are ready for public release.



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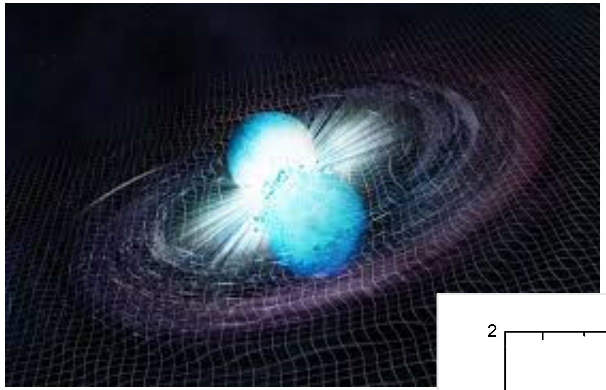

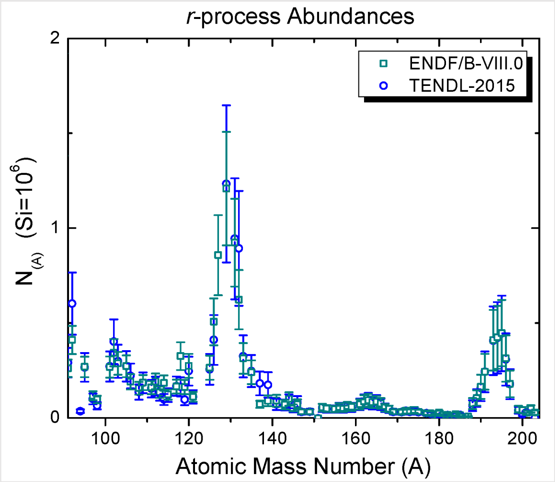

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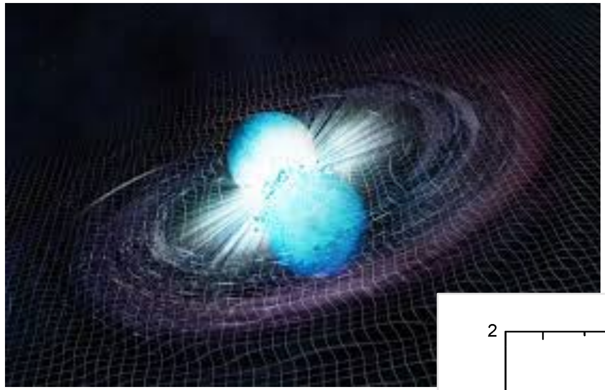

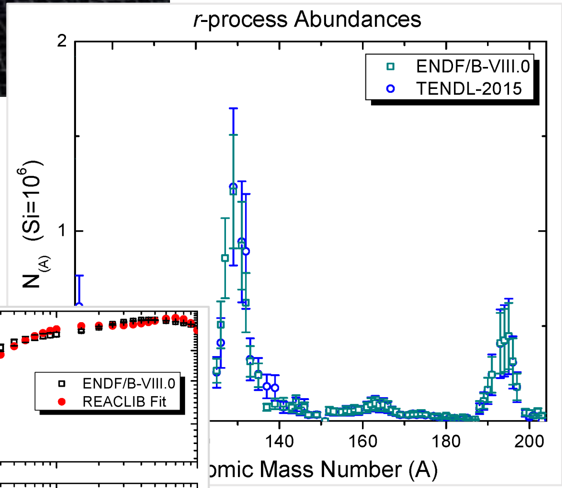

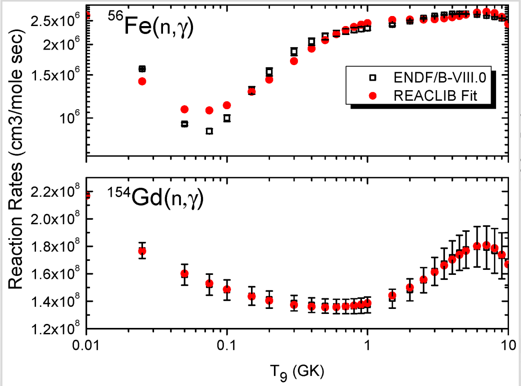

Stellar Enhancement Factors (SEF)

- SEF calculations rely on nuclear structure data
- Multiple calculations produce different results
- No experimental verifications
- It is better to apply then separately

The presently-discussed astrophysical reaction rates are based on the ground state (g.s.) cross sections. Stellar Enhancement Factors (SEF) could affect astrophysical reaction rate values in plasma environment. The factor f is defined as the ratio of the stellar rate R^* relative to the ground state rate $R_{g.s.}$ measured in laboratory [45]

$$f = \frac{R^*}{R_{g.s.}} = \frac{R^*}{R_{lab}}. \tag{5}$$

These factors originate from stellar reaction cross sections σ^* that could be estimated as a sum of the cross sections σ_x for the excited states x with excitation energy E_x and spin J_x, weighted with the Boltzmann excitation probability [41]

$$\sigma^* = \frac{\Sigma_x (2J_x + 1)\sigma^x e^{\frac{-E_x}{kT}}}{\Sigma_x (2J_x + 1) e^{\frac{-E_x}{kT}}}. \tag{6}$$