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SOURCE

Free atom scattering cross sections and normalization of thermal scattering data

CSEWG Meeting - November 2021

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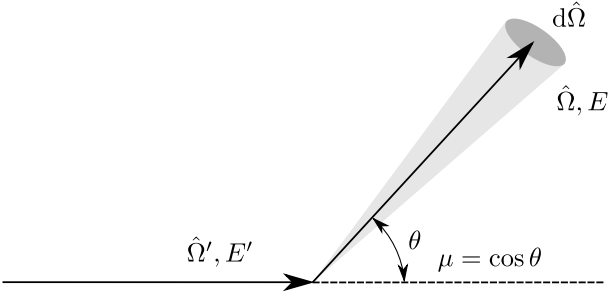
Acknowledgments

- To Danila Roubtsov, with whom we started discussing this for the normalization of the thermal scattering evaluations in JEFF 3.3 and ENDF/B-VIII.0
- To my colleagues at the European Spallation Source, particularly Thomas Kittelman, who brought back this discussion for the normalization of data in NCrystal[1].

[1] Cai, X-X., and Thomas Kittelmann. "NCrystal: A library for thermal neutron transport." Computer Physics Communications, 246, 106851 (2020).

Neutron and thermal scattering sublibraries

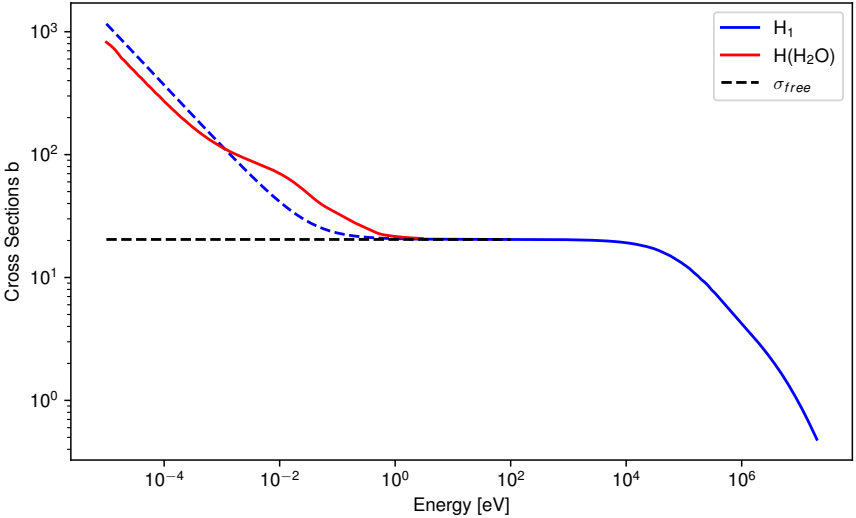
Neutron sublibrary	Thermal scattering sublibrary
Information is given per nuclide	Information is given per compound.
Nuclear interaction is complex	Nuclear interaction is simple (constant scattering lengths or cross sections)
Condensed matter physics is simple	Condensed matter physics is complex
Angular momentum is important	Neutron spin and coherence is important



$$\sigma_s(E', \hat{\Omega}' \to E, \hat{\Omega}) = \frac{\sigma_b}{4\pi k_B T}\sqrt{\frac{E}{E'}}S(\alpha, \beta)$$

$$\alpha = \frac{E + E' - 2\sqrt{E'E}\mu}{Ak_B T}, \ \beta = \frac{E - E'}{k_B T}, \ A = m/m_n;$$

$$\sigma_b = \sigma_{\text{free}}\,(1 + 1/A)^2$$

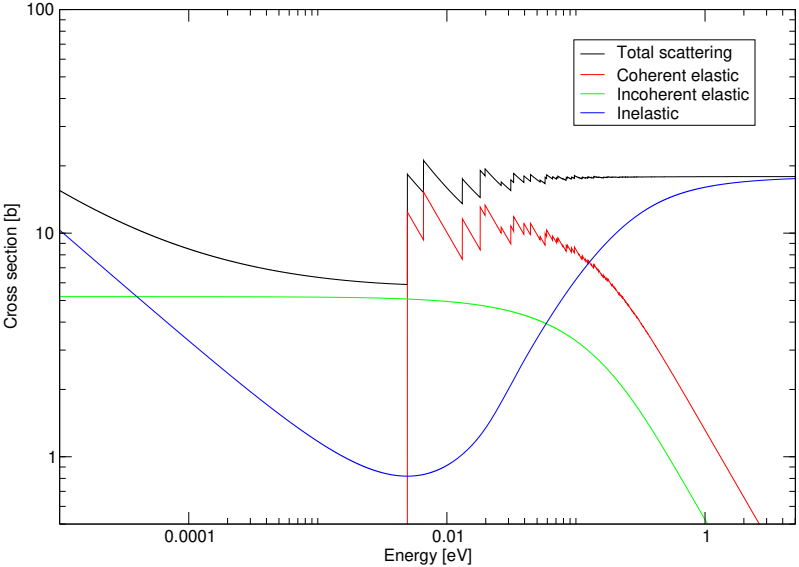

H_1
$H(H_2O)$
σ_{free}
Cross Sections b
10^3
10^2
10^1
10^0
10^{-4}
10^{-2}
10^0
10^2
10^4
10^6
Energy [eV]

More complexity

- In thermal scattering, neutron wavelengths are similar to the interactomic distances, producing interference effects.
- These interference elastic and inelastic effects are proportional to $\sigma_{\text{coh}} = 4\pi \left(\bar{b}\right)^2$, the bound coherent cross section.
- The remainder, $\sigma_{\text{inc}} = \sigma_b - \sigma_{\text{coh}} = 4\pi \left[\bar{b^2} - \left(\bar{b}\right)^2\right]$, is the bound incoherent cross section.

$\Rightarrow$ For each nuclide we need to know either b^-, b^+, or σ_{coh}, σ_{inc}, but also make sure that:

$$\sigma_{\text{free}} = \frac{\sigma_{\text{coh}} + \sigma_{inc}}{(1 + 1/A)^2}$$



Thermal scattering cross section for nickel at room temperature.

Compilations and sources

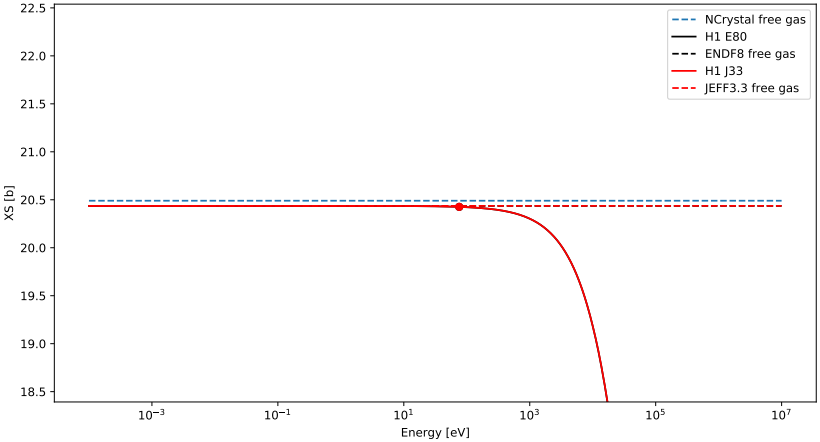
- Sears, V. F. "Neutron scattering lengths and cross sections." Neutron news 3, no. 3 (1992): 26-37. Available online: `https://www.ncnr.nist.gov/resources/n-lengths/list.html`
- Koester, L., H. Rauch, and E. Seymann. "Neutron scattering lengths: a survey of experimental data and methods." Atomic data and nuclear data tables 49, no. 1 (1991): 65-120.
- Dawidowski, J. et al. "Neutron scattering lengths and cross sections." In Experimental Methods in the Physical Sciences, vol. 44, pp. 471-528. Academic Press, 2013.
- Experimental data is also available in EXFOR (`BA,AMP`; `BA,SIG`; `FA/INC,SIG`; `FA/COH,SIG`).

(but these sources are not necessarily consistent with evaluated nuclear data libraries)

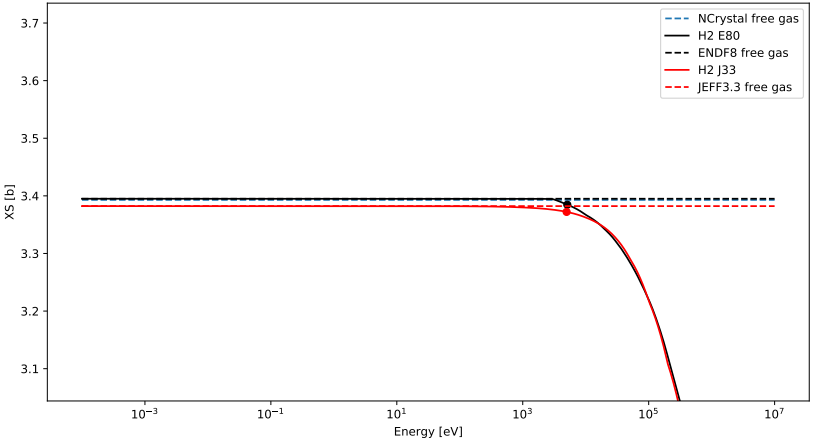
Some examples

- NCrystal (based on the data from Koester):
  `https://github.com/mctools/ncrystal/blob/master/ncrystal_core/src/NCAtomDB.cc`
- JEFF 3.3, reconstructed at T=0K with NJOY into ACE and plotted with OpenMC.
- ENDF/B-VIII.0, reconstructed at T=0K with NJOY into ACE and plotted with OpenMC.

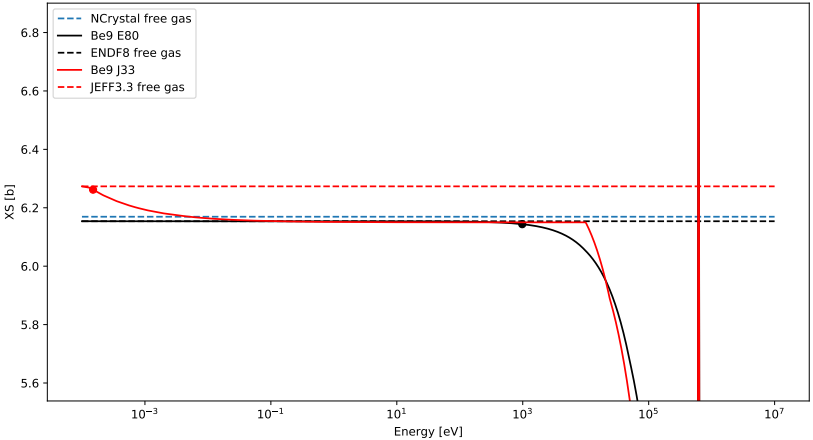
Processing nuclide: H1, abundance: 99.98%
ENDF-6 evaluation: n-001_H_001.endf
NCrystal free atom cross section: 20.4900 b
ENDF-6 0K, 0 eV XS: 20.4361 b
Relative difference between NCrystal and ENDF8: 0.26%
Energy of 1% departure: 7.58e+01 eV



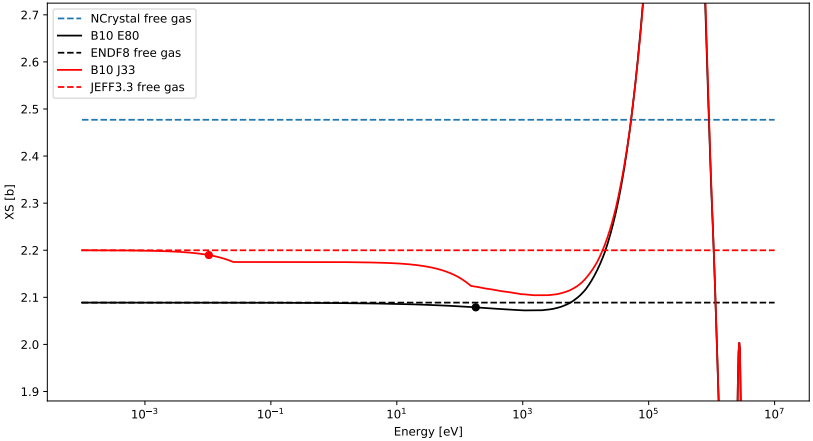
Processing nuclide: H2, abundance: 0.02%
ENDF-6 evaluation: n-001_H_002.endf
NCrystal free atom cross section: 3.3930 b
ENDF-6 0K, 0 eV XS: 3.3950 b
Relative difference between NCrystal and ENDF8: -0.06%
Energy of 1% departure: 5.10e+03 eV



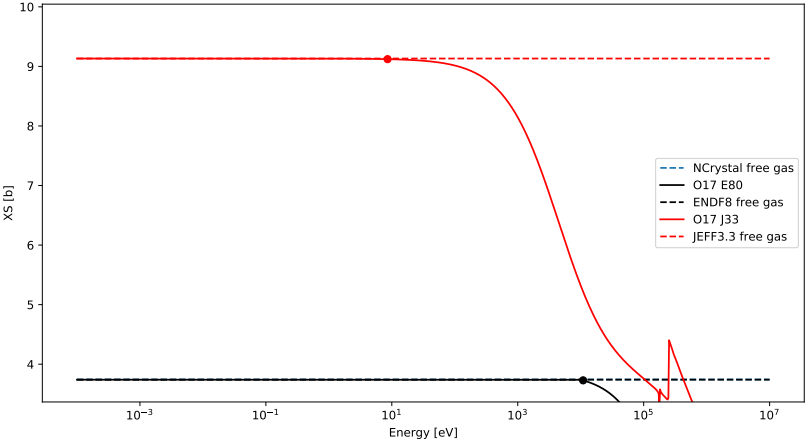
Processing nuclide: Be9, abundance: 100.00%
ENDF-6 evaluation: n-004_Be_009.endf
NCrystal free atom cross section: 6.1693 b
ENDF-6 0K, 0 eV XS: 6.1539 b
Relative difference between NCrystal and ENDF8: 0.25%
Energy of 1% departure: 9.82e+02 eV



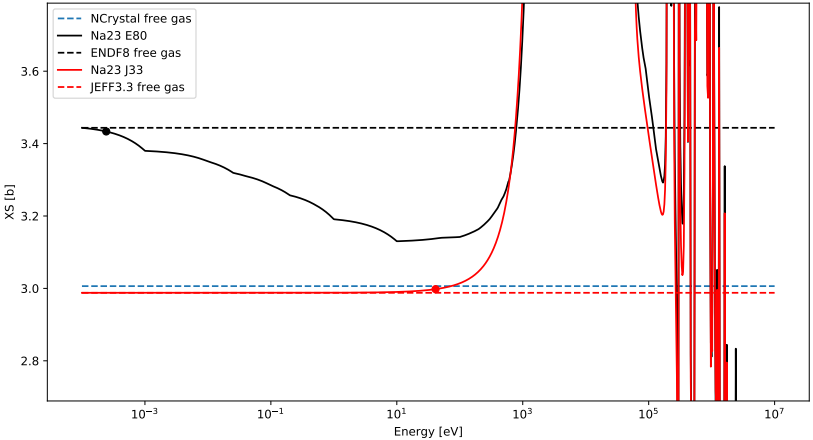
Processing nuclide: B10, abundance: 19.82%
ENDF-6 evaluation: n-005_B_010.endf
NCrystal free atom cross section: 2.4771 b
ENDF-6 0K, 0 eV XS: 2.0888 b
Relative difference between NCrystal and ENDF8: 18.59%
Energy of 1% departure: 1.80e+02 eV



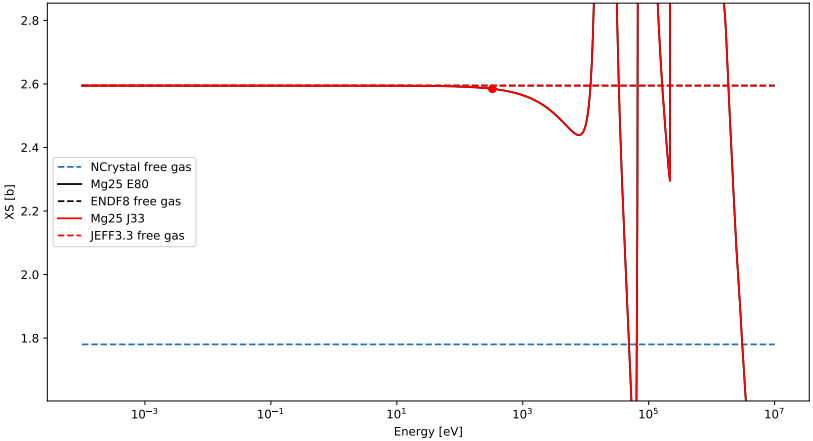
Processing nuclide: O17, abundance: 0.04%
ENDF-6 evaluation: n-008_O_017.endf
NCrystal free atom cross section: 3.7447 b
ENDF-6 0K, 0 eV XS: 3.7400 b
Relative difference between NCrystal and ENDF8: 0.12%
Energy of 1% departure: 1.09e+04 eV



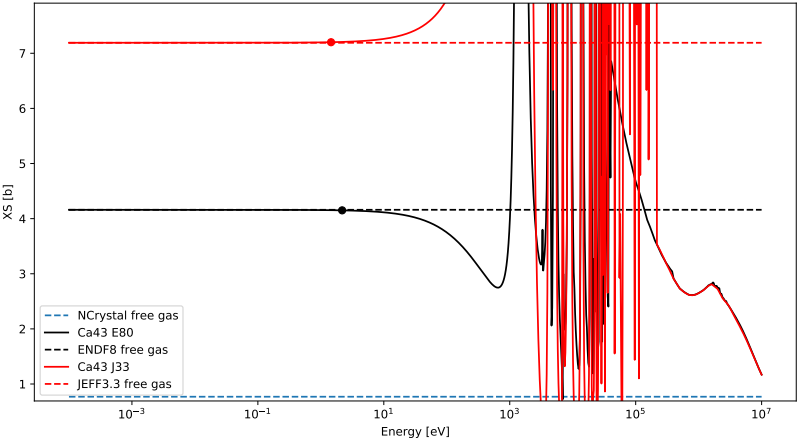
Processing nuclide: Na23, abundance: 100.00%
ENDF-6 evaluation: n-011_Na_023.endf
NCrystal free atom cross section: 3.0063 b
ENDF-6 0K, 0 eV XS: 3.4436 b
Relative difference between NCrystal and ENDF8: -12.70%
Energy of 1% departure: 2.43e-04 eV



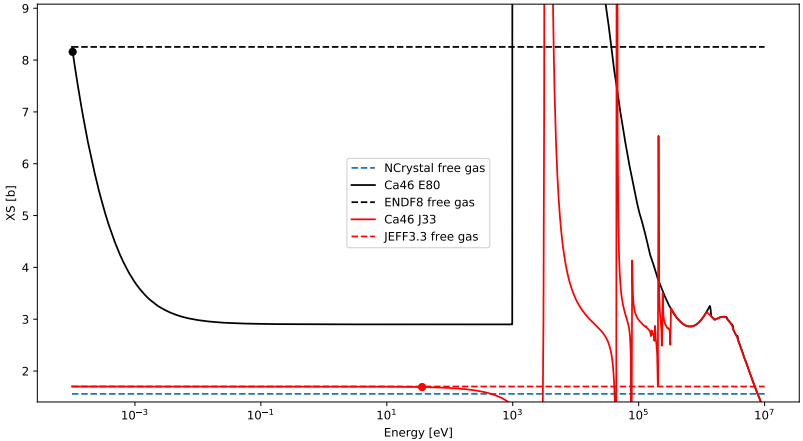
Processing nuclide: Mg25, abundance: 10.02%
ENDF-6 evaluation: n-012_Mg_025.endf
NCrystal free atom cross section: 1.7801 b
ENDF-6 0K, 0 eV XS: 2.5947 b
Relative difference between NCrystal and ENDF8: -31.39%
Energy of 1% departure: 3.30e+02 eV



Processing nuclide: Ca43, abundance: 0.14%
ENDF-6 evaluation: n-020_Ca_043.endf
NCrystal free atom cross section: 0.7693 b
ENDF-6 0K, 0 eV XS: 4.1605 b
Relative difference between NCrystal and ENDF8: -81.51%
Energy of 1% departure: 2.18e+00 eV



Processing nuclide: Ca46, abundance: 0.00%
ENDF-6 evaluation: n-020_Ca_046.endf
NCrystal free atom cross section: 1.5594 b
ENDF-6 0K, 0 eV XS: 8.2535 b
Relative difference between NCrystal and ENDF8: -81.11%
Energy of 1% departure: 1.03e-04 eV



Conclusions

- Thermal scattering evaluations require values for normalization, which should be compatible with evaluations in the neutron sublibrary.
- One normalization, σ_{free}, can be extracted from the asymptotic value of $\sigma_{\text{el}}(E, T = 0K)$, but we need also to separate it into $\sigma_{\text{inc}}, \sigma_{\text{coh}}$.
- Reconstruction at $T = 0K$ is a simple test that can be automated and incorporated into V & V pipelines.
- Artifacts and inconsistencies are easy to spot.

Questions / challenges

- Can we obtain b^-, b^+ from the nuclear evaluation codes and store them in `MF=1 / MT=451`?
- Scattering lengths and cross sections can be measured with great precision using thermal scattering techniques. Is this feedback useful for nuclear evaluations?
- These questions were always there, but latent, because thermal scattering libraries were limited to a few materials. But new tools, like NCrystal, are changing the scenario:
  `https://github.com/mctools/ncrystal/wiki/Data-library`

TSL Issue # 13

Inconsistent use of the characteristic bound cross section for incoherent elastic scattering:
`https://git.nndc.bnl.gov/endf/library/thermal_scatt/-/issues/13`

- The normalization value for the incoherent inelastic reaction (`MF=7/MF=4`) is stored as $M_0 f0$, the product of the numbers of atoms times the free atom cross section.
- The normalization value for the incoherent elastic reaction (`MF=7/MF=2`) is stored as σ_b^{inc}, without multiplying by the numbers of atoms.
- THERMR divides both by M_0, but AMPX does not.
- The evaluation for H(CH_2) historically follows the NJOY convention.

TSL Issue # 13

Possible solutions:

- Change the field in the ENDF-6 format to be $M_n * \sigma_b^{inc}$, or
- Change NJOY to divide the free atom cross section by M_n, but not the bound elastic cross section. Also, fix polyethylene, lucite and revert the change in solid methane.

Thanks for your time.
Questions?