^{181}Ta Resonance Region Evaluation Update

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Motivation for a new ^{181}Ta evaluation

- Ta has a high melting point and can be used as a structural material in nuclear applications
- The U.S. Department of Energy (DOE) Nuclear Criticality Safety Program (NCSP) requested that the ENDF-8.0 ^{181}Ta resonance parameter evaluation be extended up to 2.6 keV
- The ENDF-8.0 evaluation of Ta used the Breit-Wigner Multi-level formalism up to 330 eV without any covariance information (evaluated uncertainty and related correlations)
- The new Ta evaluation procedure uses the Reich-Moore approximation of the R-matrix theory implemented in the SAMMY code

RPI C-shaped neutron production target (Ref. 1)

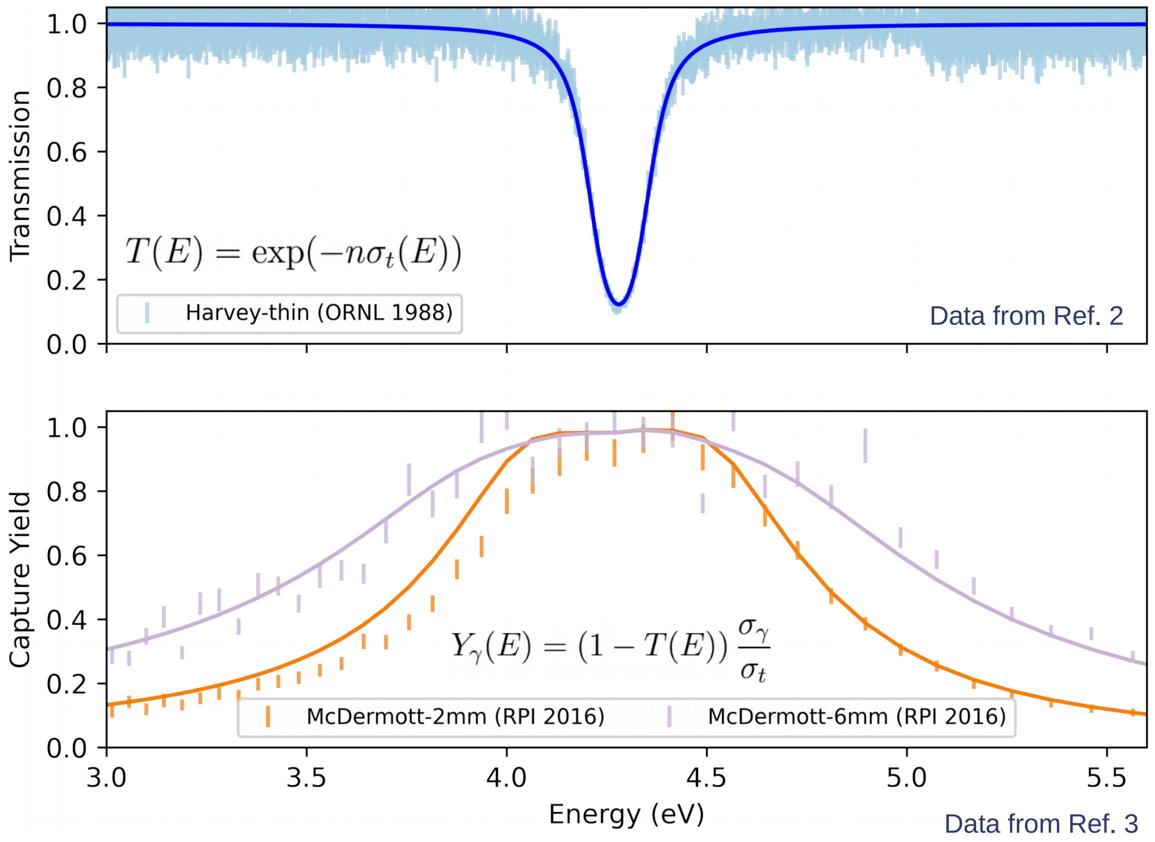
There are several goals for the new ^{181}Ta evaluation

- Modify and extend the current ENDF-8.0 set of resonance parameters in the Resolved Resonance Region (RRR) up to 2.6 keV
- Generate a new set of average resonance parameters in the Unresolved (URR) up to 100 keV (using the RRR parameters)
- Produce “reasonable” covariance information for both the RRR and URR.
- Reproduce accurate coherent and incoherent scattering lengths (derived from the RRR parameters)
- Improve the resonance statistics (derived from the RRR parameters)

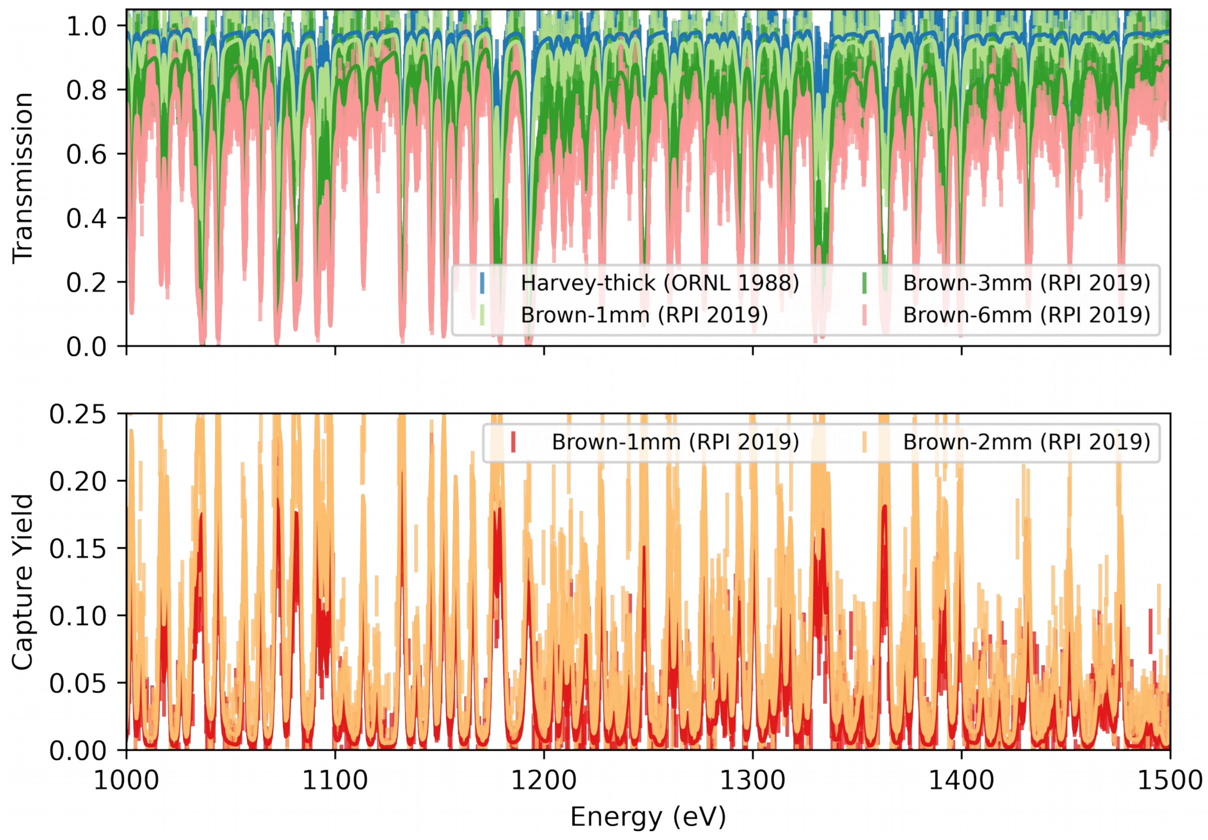
The new ^{181}Ta evaluation used several different experimental data sets in the SAMMY fits

- Transmission (top) and capture yield (bottom) from several experimental data sets are used in a SAMMY Bayesian fitting procedure to obtain a new set of RRR parameters (energies, neutron widths, capture widths) up to 2.6 keV

- The SAMMY fitting procedure includes experimental corrections such as Doppler broadening, resolution broadening, background, normalization, and multiple scattering.



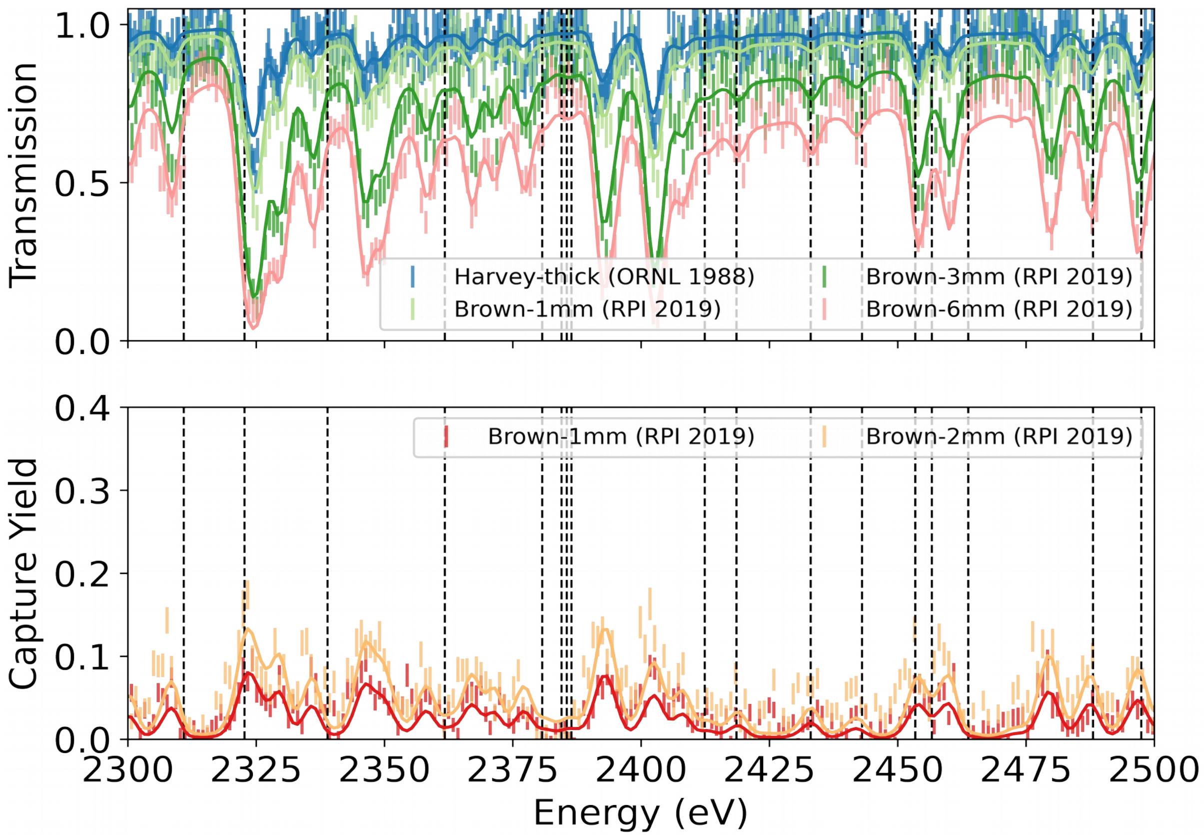
The high level density of ^{181}Ta evaluation can make fitting with SAMMY a challenge



Data from Ref. 2 and Ref. 4

- As energy increases, the width of the resonance increases and the experimental resolution decreases, leading to overlapping resonances
- Fitting overlapping resonances can be challenging if spin assignments are unknown
- A Monte Carlo method was used to randomly assign spins to resonances (if not given in Mughabghab's ATLAS) and add missing levels

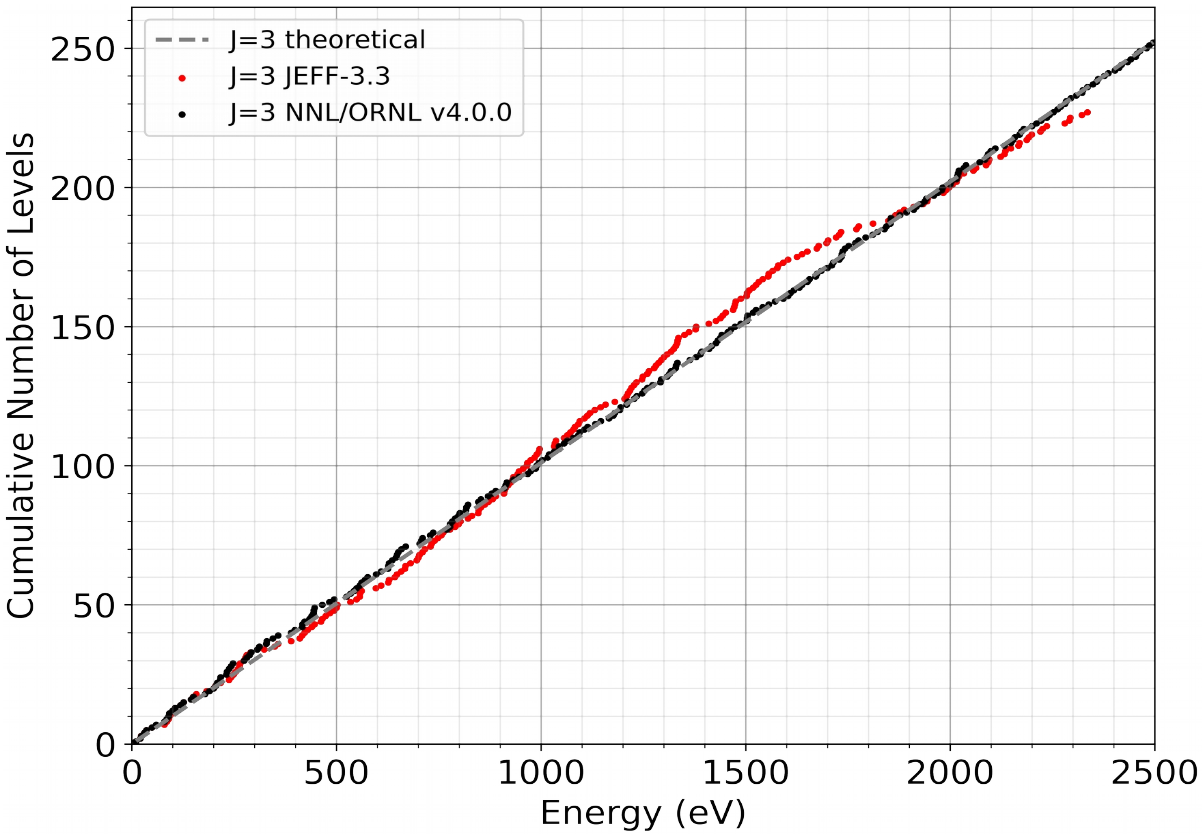
The high level density of ^{181}Ta evaluation can make fitting with SAMMY a challenge

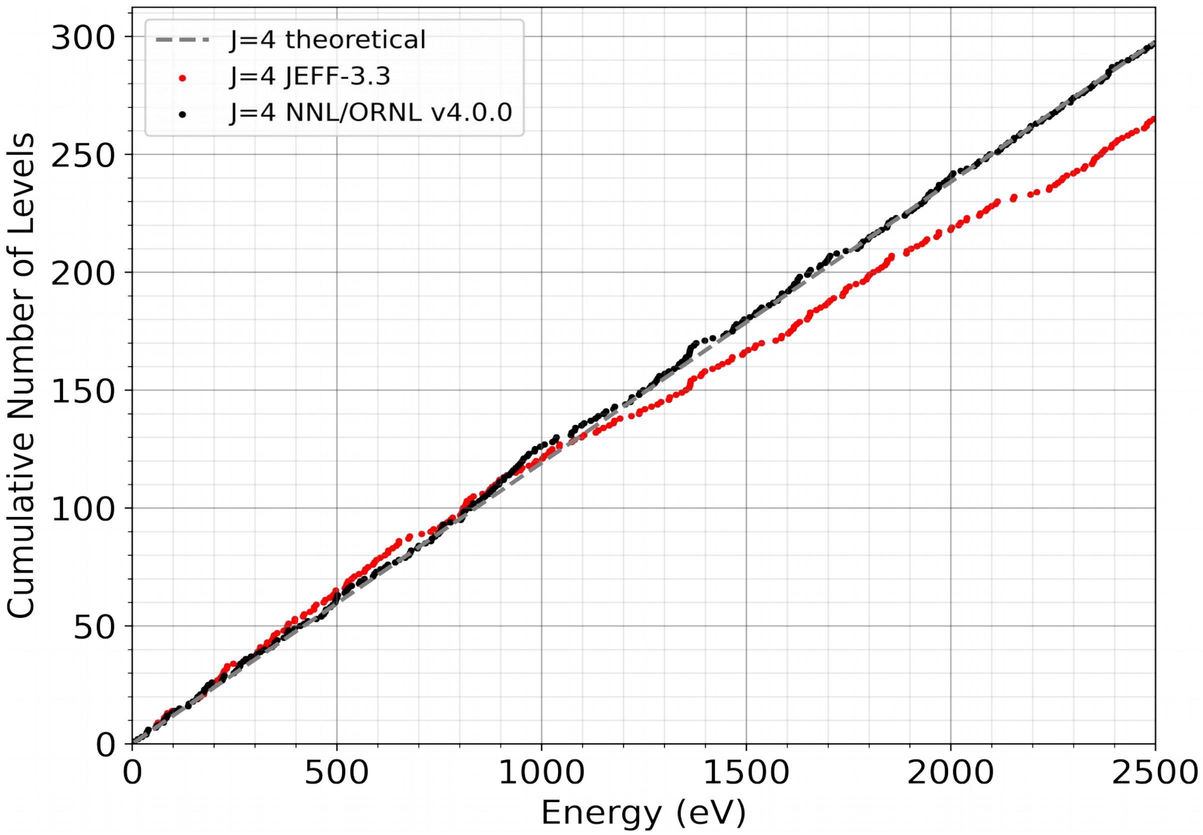


- Vertical lines represent small resonances added by the Monte Carlo method

- A Monte Carlo method was used to randomly assign spins to resonances (if not given in Mughabghab's ATLAS-2018) and add missing levels
- Twenty thousand parameter files were generated to get the initial spin assignments keeping the original JEFF-3.3 resonance energies.
- Twenty thousand more parameter files were then generated to add missing levels and associated neutron and radiation widths
- The theoretical Porter-Thomas, Wigner, and Staircase distributions were used to calculate a chi-squared metric relative to SAMMY results
- The lowest chi-square was selected as the best spin assignments for the resonances

A Monte Carlo method produced better staircase plots relative to previous JEFF-3.3 evaluation

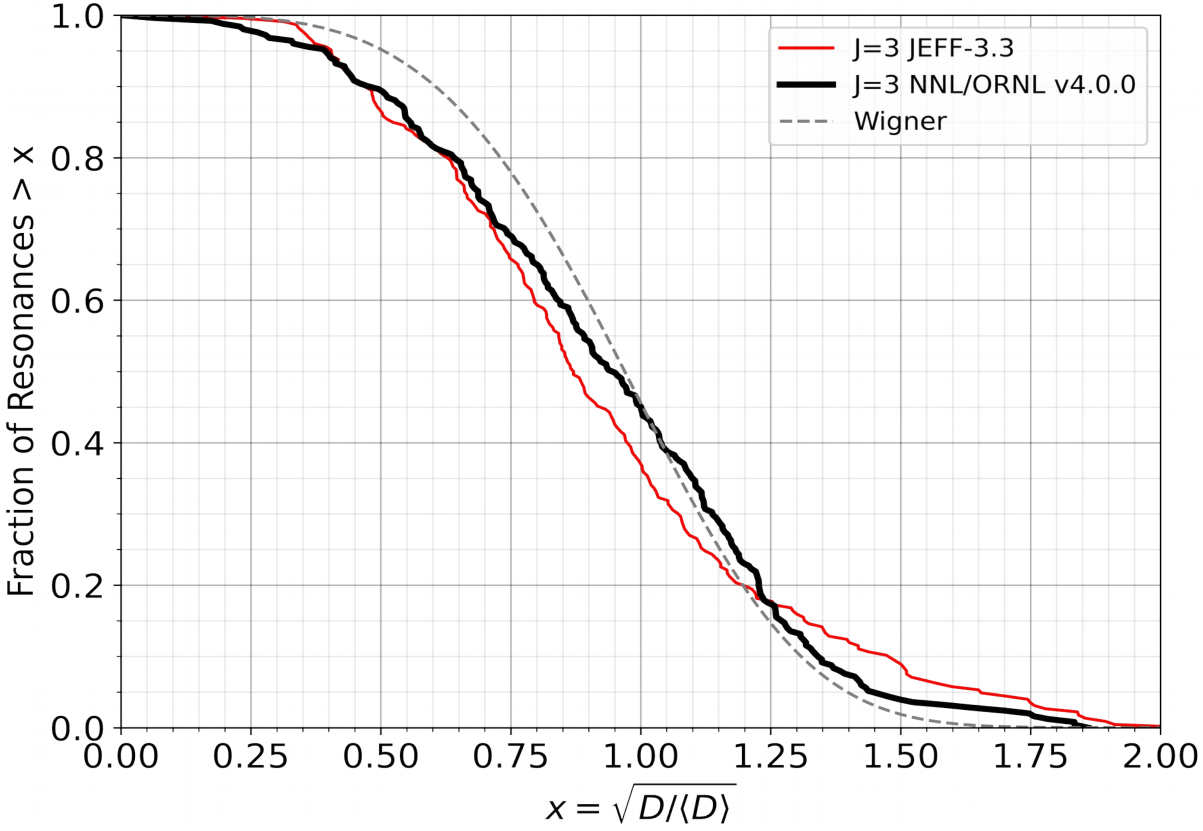


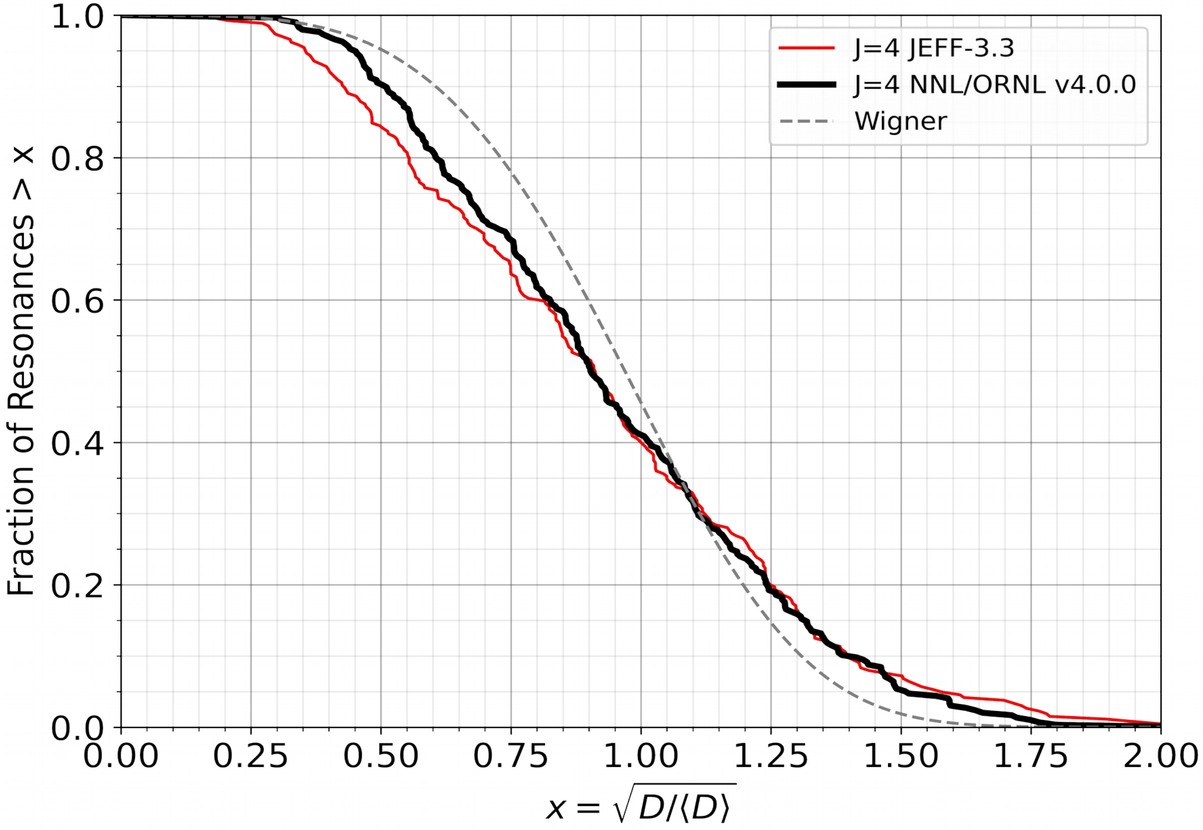


- New Ta evaluation shows improvement relative to JEFF-3.3 and extends ENDF-8.0 to approximately 2.6 keV

- Small resonances (low neutron width) were added during the Monte Carlo process to produce a linear cumulative number of levels.

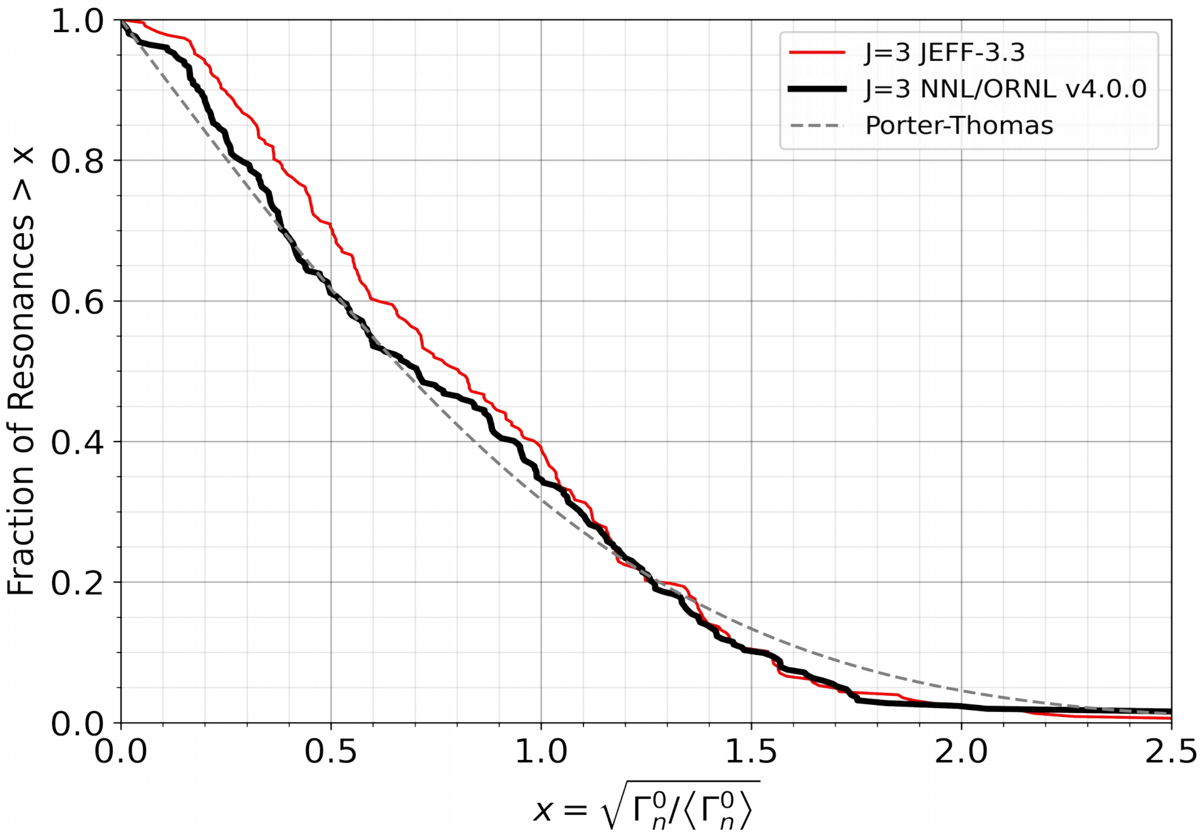
A Monte Carlo method produced better Wigner plots relative to previous JEFF-3.3 evaluation

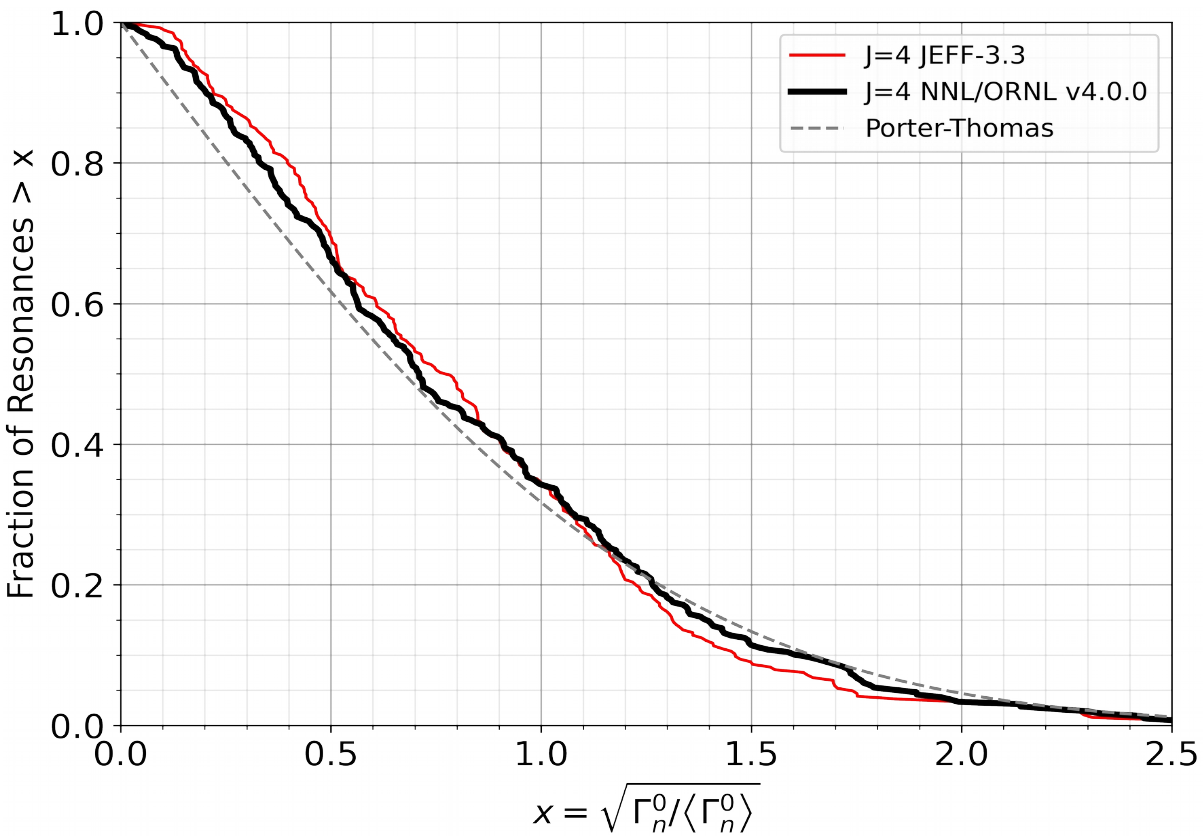




- The new Ta evaluation shows significant improvement when comparing to the Wigner distribution for both J=3 and J=4.

A Monte Carlo method produced better Porter-Thomas plots relative to previous JEFF-3.3 evaluation





- The new Ta evaluation shows significant improvement when comparing Porter-Thomas distribution for both J=3 and J=4.

The scattering lengths can be calculated from the RRR parameters and compared to experiment

Theory

$$a = R' - 2.227 \times 10^3 \left(\frac{A+1}{A}\right) \sum_J \frac{\Gamma^0_{n,J}}{E_{0,J}}$$

Calculate **free** scattering lengths from RRR parameters

$a_+ \rightarrow J = 4$

$a_- \rightarrow J = 3$

$$a_c = g_+ a_+ + g_- a_-$$

coherent

$$a_i = \sqrt{g_+ g_-}(a_+ - a_-)$$

incoherent

Experiment

b_c coherent

b_i incoherent

Measure **bound** scattering lengths (Ref. 5-7)

Convert to **free** Scattering lengths

$$a_c = \left(\frac{A}{A+1}\right) b_c$$

From Koester (Ref. 8)

$$a_c = \left(\frac{A}{A+1}\right) [b_c + Z \times (1.38 \pm 0.03 \times 10^{-3})]$$

From ATLAS (Ref. 7)

ATLAS has larger correction

$$\sigma_c = 4\pi |a_c|^2 \qquad \sigma_i = 4\pi |a_i|^2$$

Calculate **coherent** and **incoherent** scattering cross sections

Theory should be consistent with the measurement(s)

$$\sigma_s = \sigma_c + \sigma_i$$

Calculate **total** scattering cross section

The scattering lengths are used to test RRR parameters

scattering length	NIST	ATLAS-2018	ATLAS-2018 corrected	ENDF-8.0	JEFF-3.3	NNL/ORNL v4.0.0
b_c [fm]	6.91+/-0.07	6.91+/-0.07				
b_i [fm]	-0.29+\-0.03	-0.29+/-0.03*				
a_c [fm]	---	6.97+/-0.07				
a_i [fm]	---	-0.29+/-0.03				
σ_c [b]	---	6.11+/-0.12				
σ_i [b]	---	0.011+/-0.002				

$$a_c = \left(\frac{A}{A+1}\right)\left[b_c + Z \times (1.38 \pm 0.03 \times 10^{-3})\right]$$

* this value was not given in ATLAS-2018, but this is the most likely value

- NIST (Ref. 5,6) and ATLAS (Ref. 7) give bound scattering lengths (from experiment) which need to be converted to free scattering lengths
- When converting bound to free, the ATLAS applies a neutron-electron interaction correction, but this is applied when dealing with neutron transmission experiments (Ref. 8)

The scattering lengths are used to test RRR parameters

scattering length	NIST	ATLAS-2018	ATLAS-2018 corrected	ENDF-8.0	JEFF-3.3	NNL/ORNL v4.0.0
b_c [fm]	6.91+/-0.07	6.91+/-0.07	6.91+/-0.07			
b_i [fm]	-0.29+\-0.03	-0.29+/-0.03	-0.29+/-0.03			
a_c [fm]	---	6.97+/-0.07	6.87+/-0.07			
a_i [fm]	---	-0.29+/-0.03	-0.29+/-0.03			
σ_c [b]	---	6.11+/-0.12	5.93+/-0.12			
σ_i [b]	---	0.011+/-0.002	0.011+/-0.002			

$$a_c = \left(\frac{A}{A+1}\right) b_c$$

The "corrected" values are the target answer that the new evaluation should reproduce

- Koester et al. (Ref. 8, X4#20758001) used a Christiansen filter technique and is not using neutron transmission. Therefore, a smaller conversion factor (from bound to free) may be used.
- This gives a significantly lower value of the free coherent scattering length. It is unclear whether to correct incoherent or not, but makes little difference

The scattering lengths are used to test RRR parameters

scattering length	NIST	ATLAS-2018	ATLAS-2018 corrected	ENDF-8.0	JEFF-3.3	NNL/ORNL v4.0.0
b_c [fm]	6.91+/-0.07	6.91+/-0.07	6.91+/-0.07	---	---	---
b_i [fm]	-0.29+/-0.03	-0.29+/-0.03	-0.29+/-0.03	---	---	---
a_c [fm]	---	6.97+/-0.07	6.87+/-0.07	6.93	6.71	6.91
a_i [fm]	---	-0.29+/-0.03	-0.29+/-0.03	-0.97	-0.25	-0.29
σ_c [b]	---	6.11+/-0.12	5.93+/-0.12	6.03	5.66	6.00
σ_i [b]	---	0.011+/-0.002	0.011+/-0.002	0.118	0.008	0.011

- The free coherent and incoherent values can be calculated from the set of RRR parameters and compared with the target values
- **The preliminary Ta evaluation reproduces the NIST bound scattering lengths but is still within uncertainty of free scattering length target values (in green)**
- Previous evaluations may have values (in red) that are outside of the target value uncertainties (in green)

Conclusions

- The preliminary new ^{181}Ta evaluation extends the RRR up to about 2.6 keV
- The new RRR parameters are used in the URR up to 100 keV
- The new ^{181}Ta evaluation reproduces accurate coherent and incoherent scattering lengths (derived from the RRR parameters)
- The new RRR parameters improve the Wigner, Porter-Thomas, and staircase resonance statistics
- Work continues on generating “reasonable” covariance information for both the RRR and URR.

References

1) Y. Danon, “Experimental Nuclear Data for improvement of evaluated data files”, 2018 Topical Meeting of the Radiation Protection and Shielding Division, August 26-31, 2018, Santa Fe, NM, 2018.

2) Harvey et al., “High-Resolution Neutron Transmission Measurements on U235, Pu239, and U238”, Nuclear Data for Science and Technology, Proceedings of the International Conference, Mito, Japan, 1988.

3) B. McDermott, “Resonance Region Capture Cross Section Measurements In Iron And Tantalum Using A New C6D6 Detector Array”, PhD thesis, RPI, Sep. 2016.

4) J. Brown, “Measurements, Evaluation, and Validation of Ta-181 Resolved and Unresolved Resonance Regions”, PhD thesis, RPI, Aug. 2019.

5) NIST Website, https://www.nist.gov/ncnr/neutron-scattering-lengths-list, Accessed Nov 2018.

6) V. Sears, “Neutron Scattering Lengths and Cross Sections”, Newtron News, Vol. 3, No. 3, 1992.

7) Mughabghab, “Atlas of Neutron Resonances”, Sixth Ed., 2018.

8) L. Koester et al., “Neutron Scattering Lengths: A Survey of Experimental Data and Methods”, Atomic Data and Nuclear Data Tables, Vol. 49, No. 1, 65-120, 1991.