NNL Testing of ENDF/B-VIII.0(β4) H-H_2O at Elevated Temperatures

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Outline

- H-H_2O Evaluation
  - Fundamental physical model
  - Observations and implications for reactor applications
  - Testing at elevated temperatures
  - Recommendations
- NJOY Patch
  - Need to restore S(α,β) floor in LEAPR

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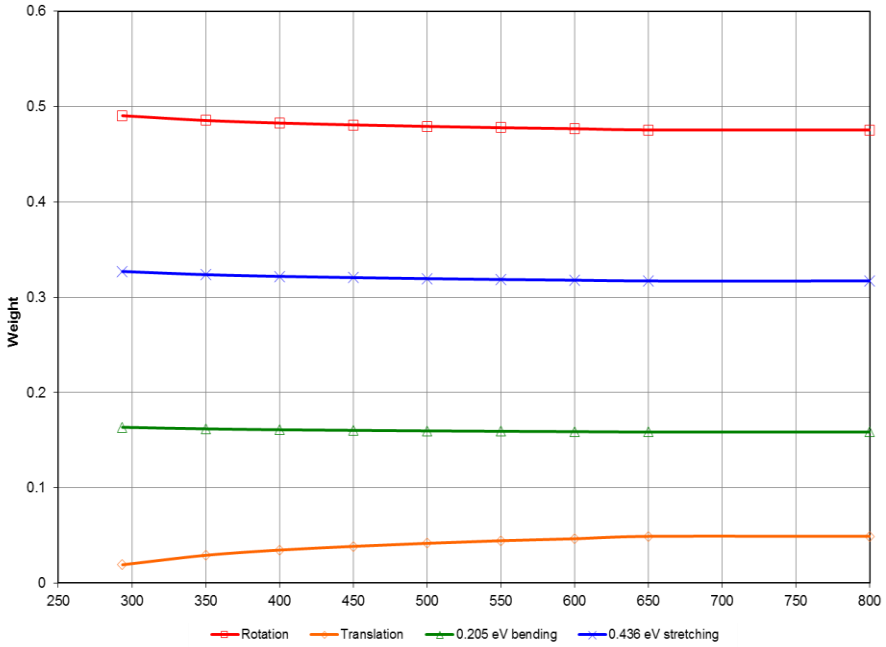
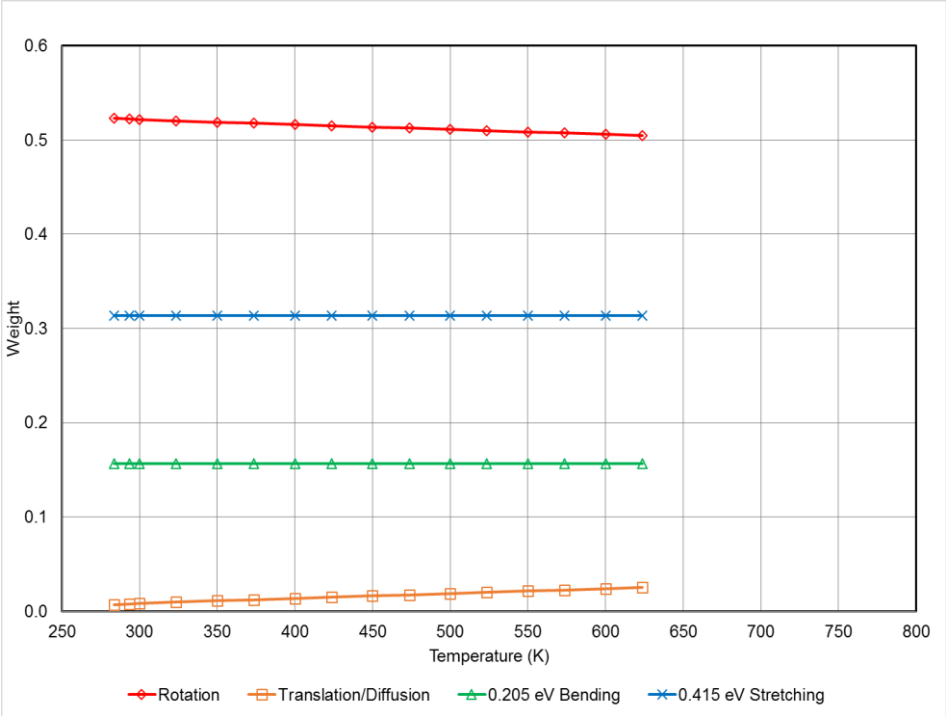
Fundamental Physical Models Similar

ENDF/B-VII.1



ENDF/B-VIII.0(β4)



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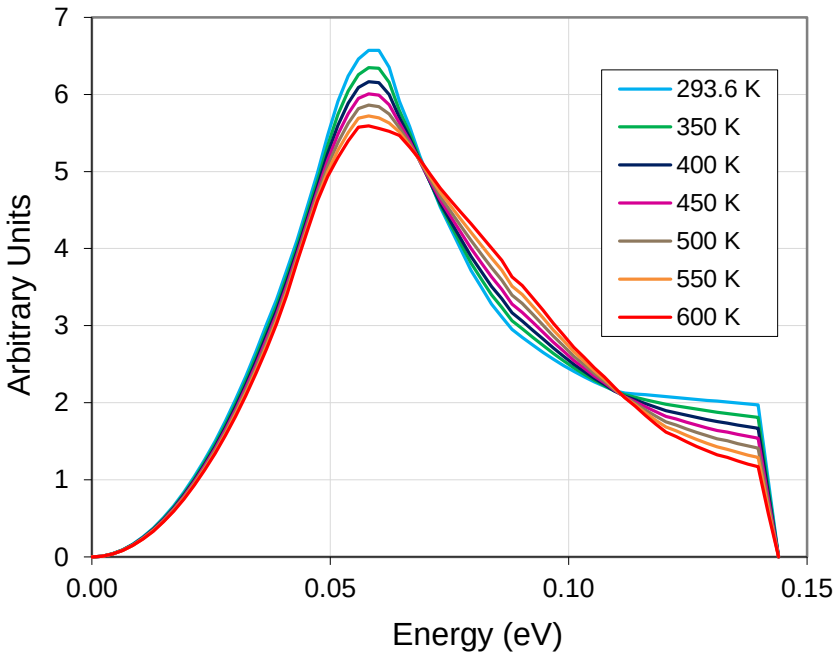
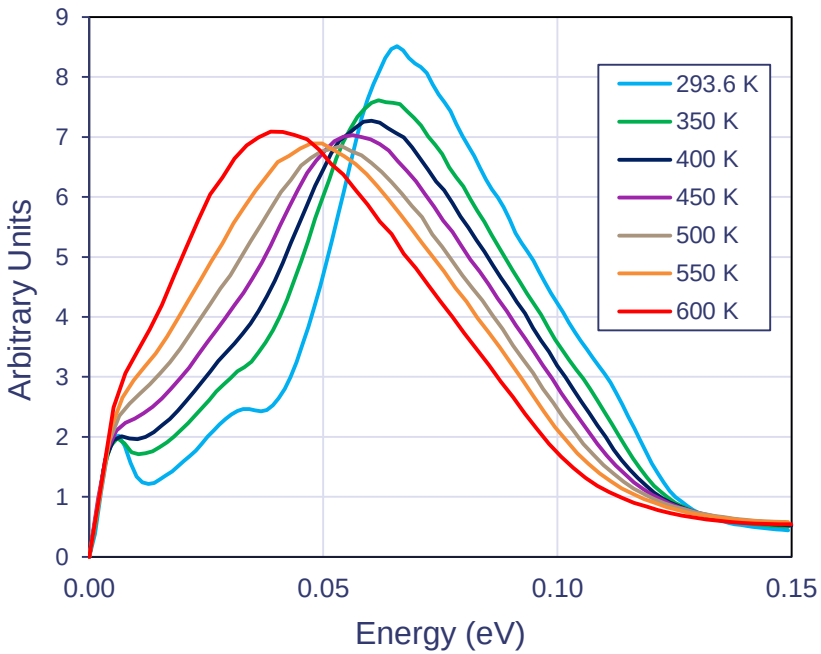
Major Differences in Hindered Rotation Mode Phonon DOS

ENDF/B-VII.1



ENDF/B-VIII.0(β4)



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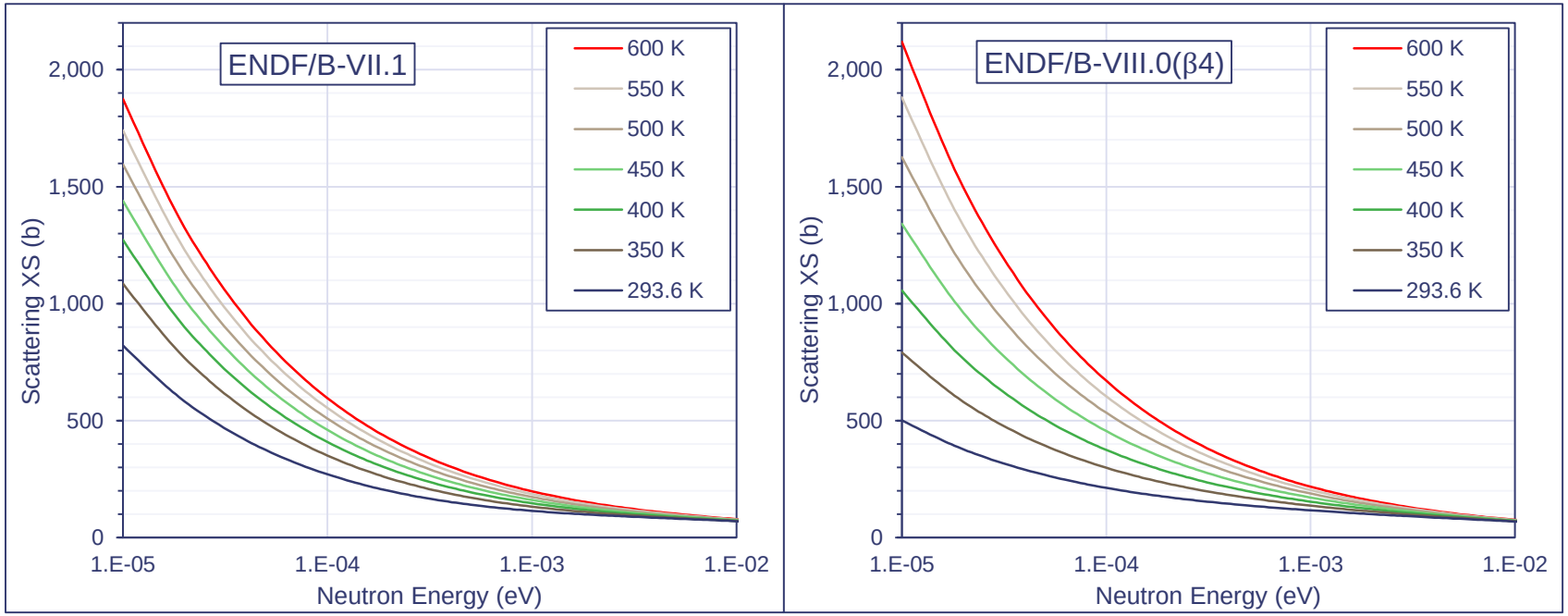
H-H_2O ENDF/B-VII.1 and ENDF/B-VIII.0(β4) Low-Energy Thermal Scattering Cross Section Comparison



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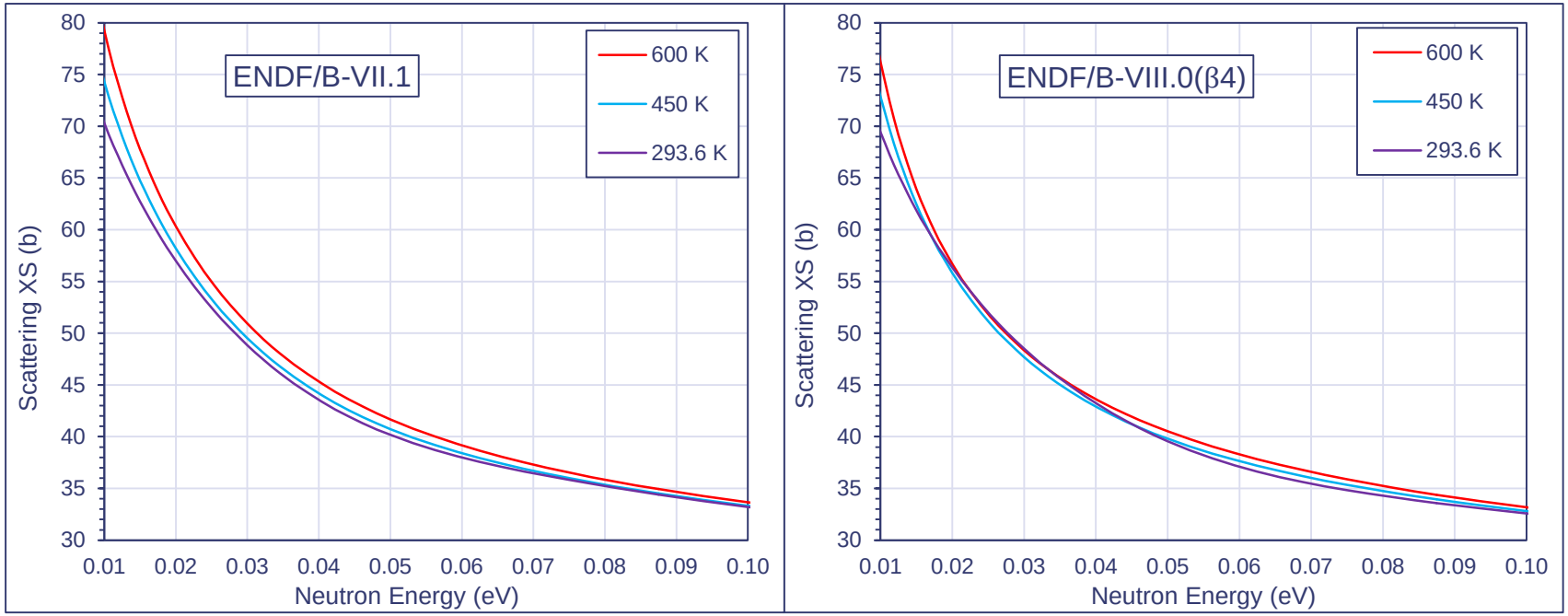
H-H_2O ENDF/B-VII.1 and ENDF/B-VIII.0(β4) Intermediate-Energy Thermal Scattering Cross Section Comparison



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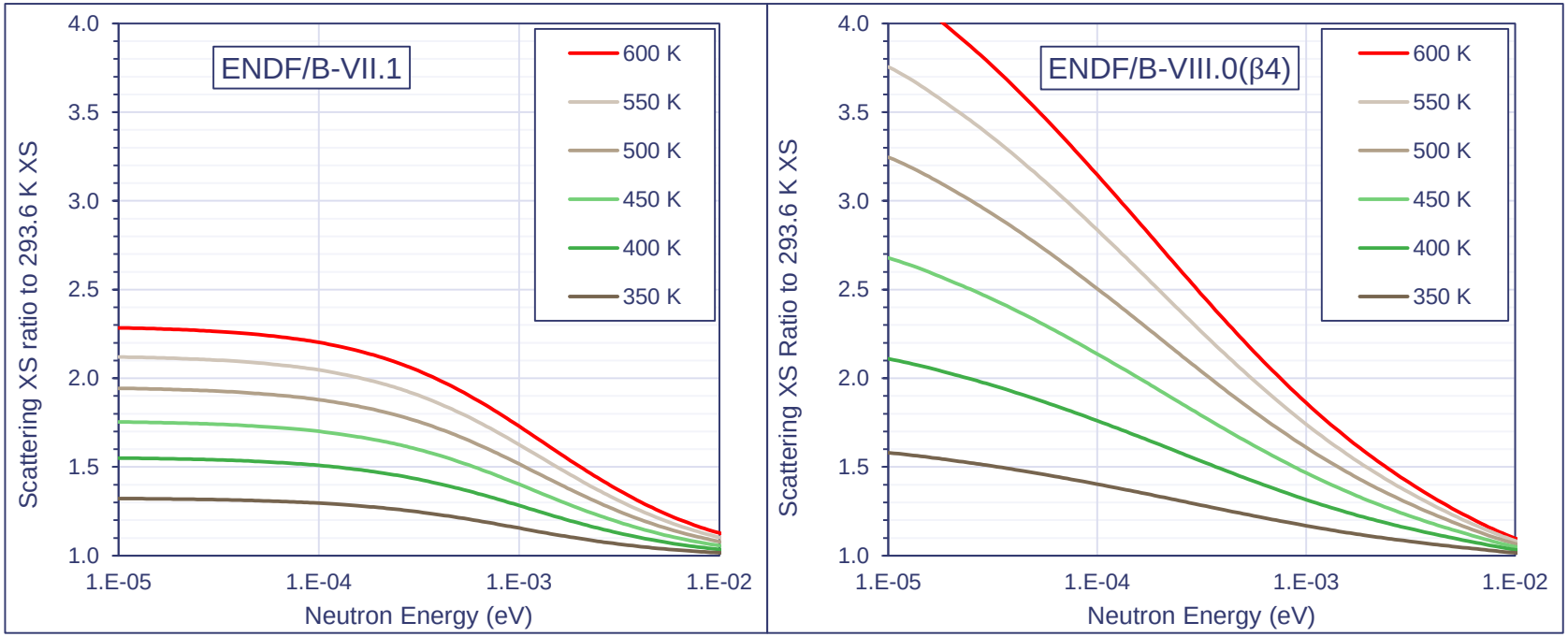
H-H_2O ENDF/B-VII.1 and ENDF/B-VIII.0(β4) Temperature-Dependence of Low-Energy Thermal Scattering Cross Section Ratios to 293.6 K Cross Sections



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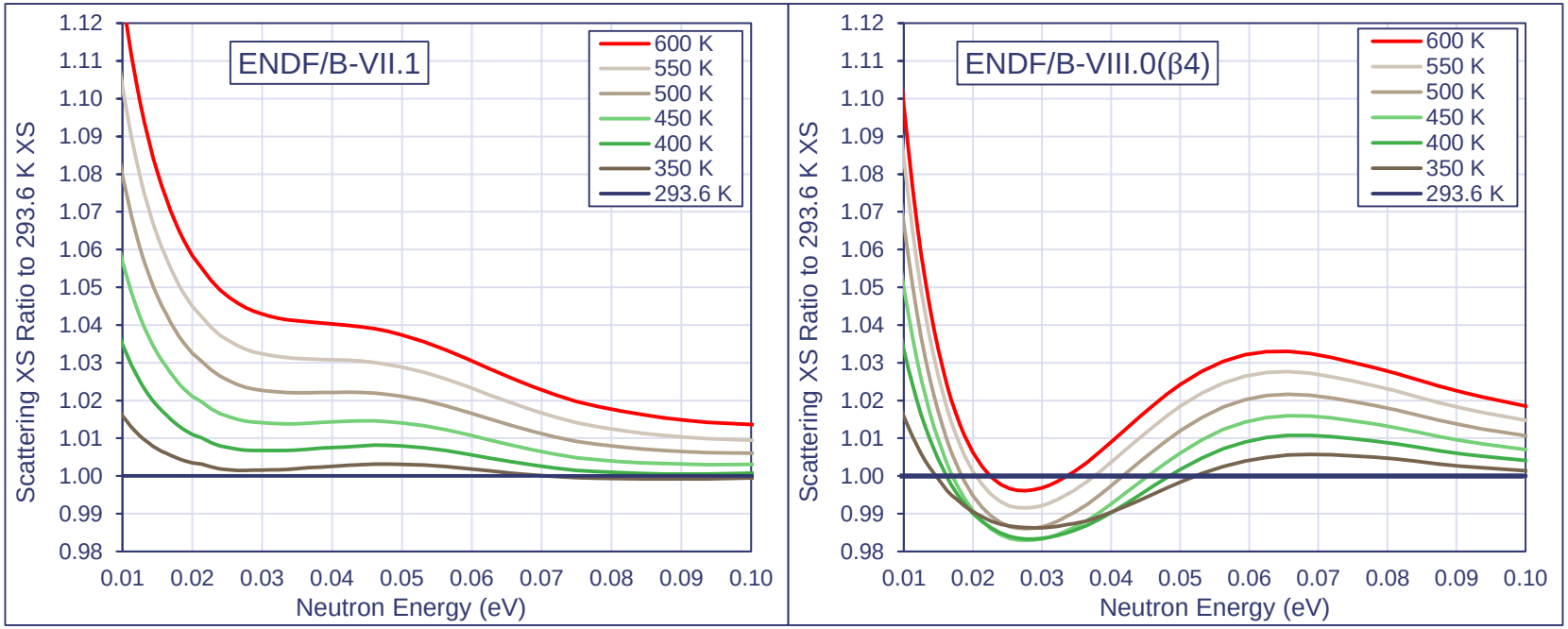

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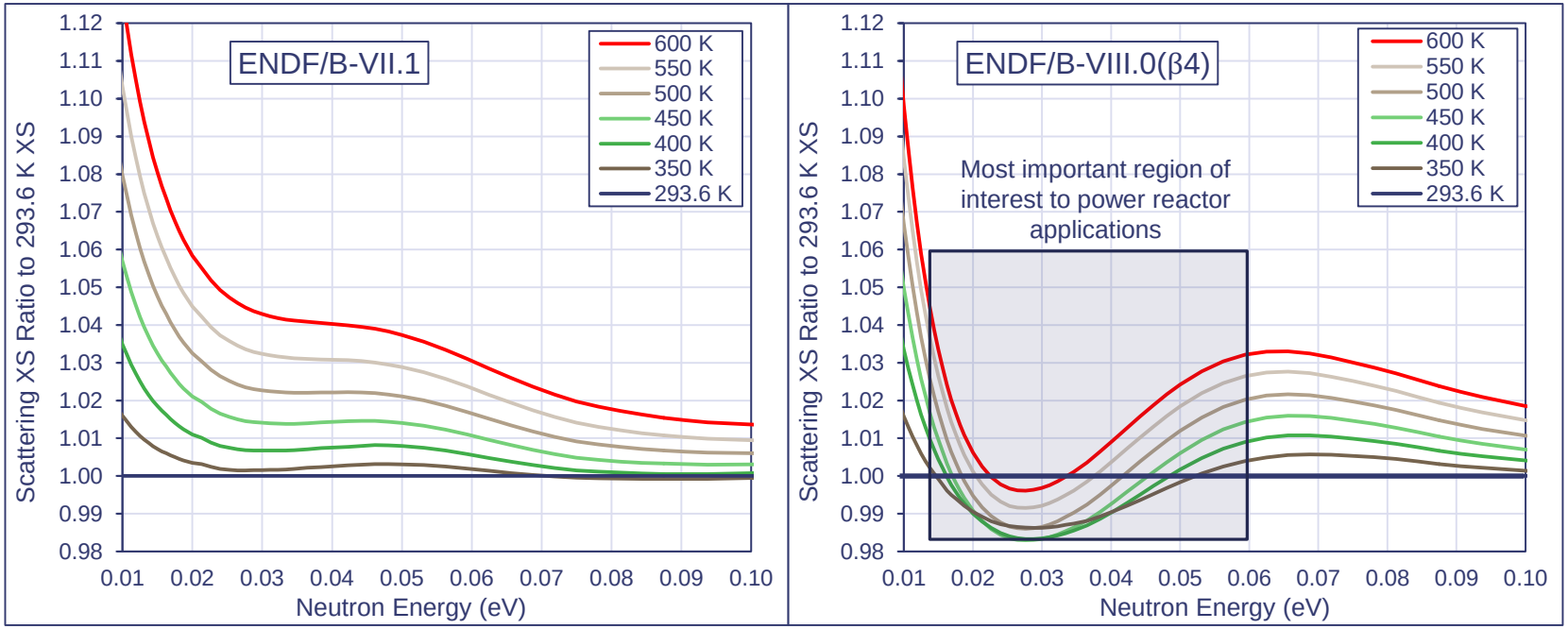

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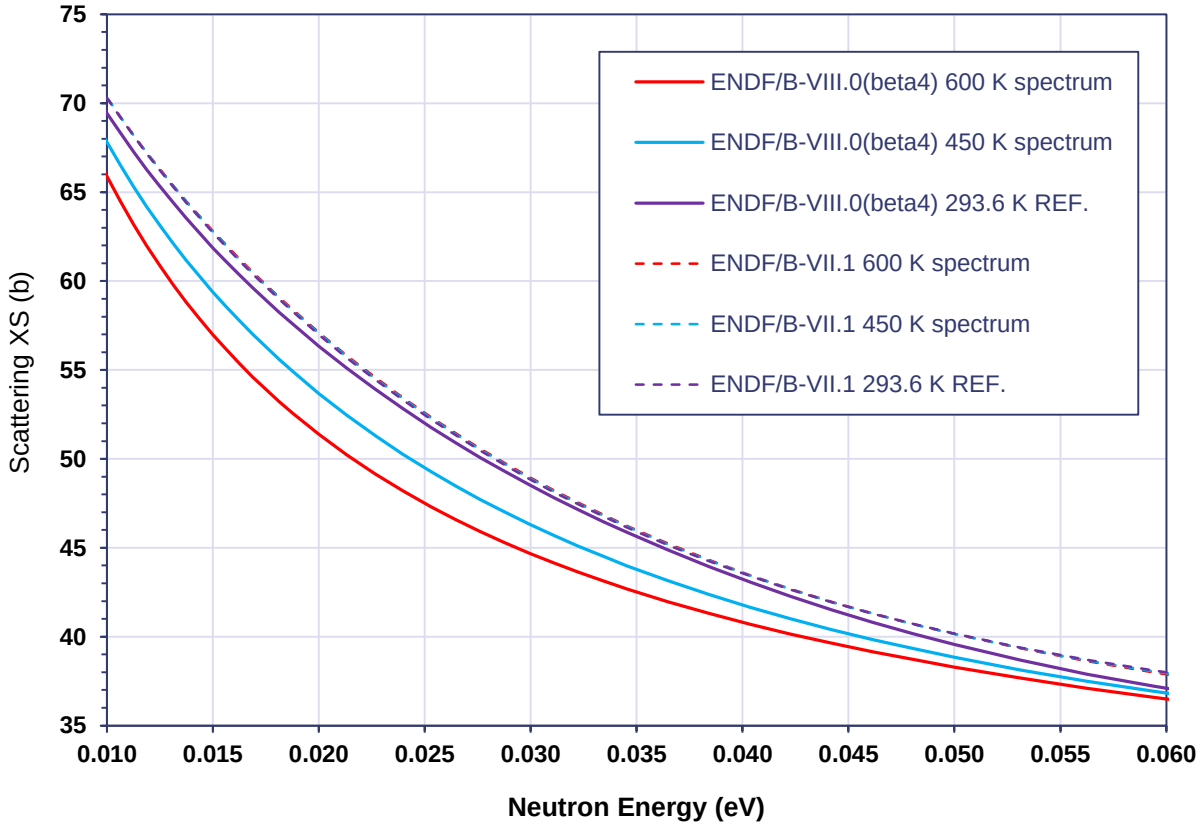
H-H_2O ENDF/B-VII.1 and ENDF/B-VIII.0(β4) Cross Section Sensitivity to Temperature-Dependent Phonon Spectra



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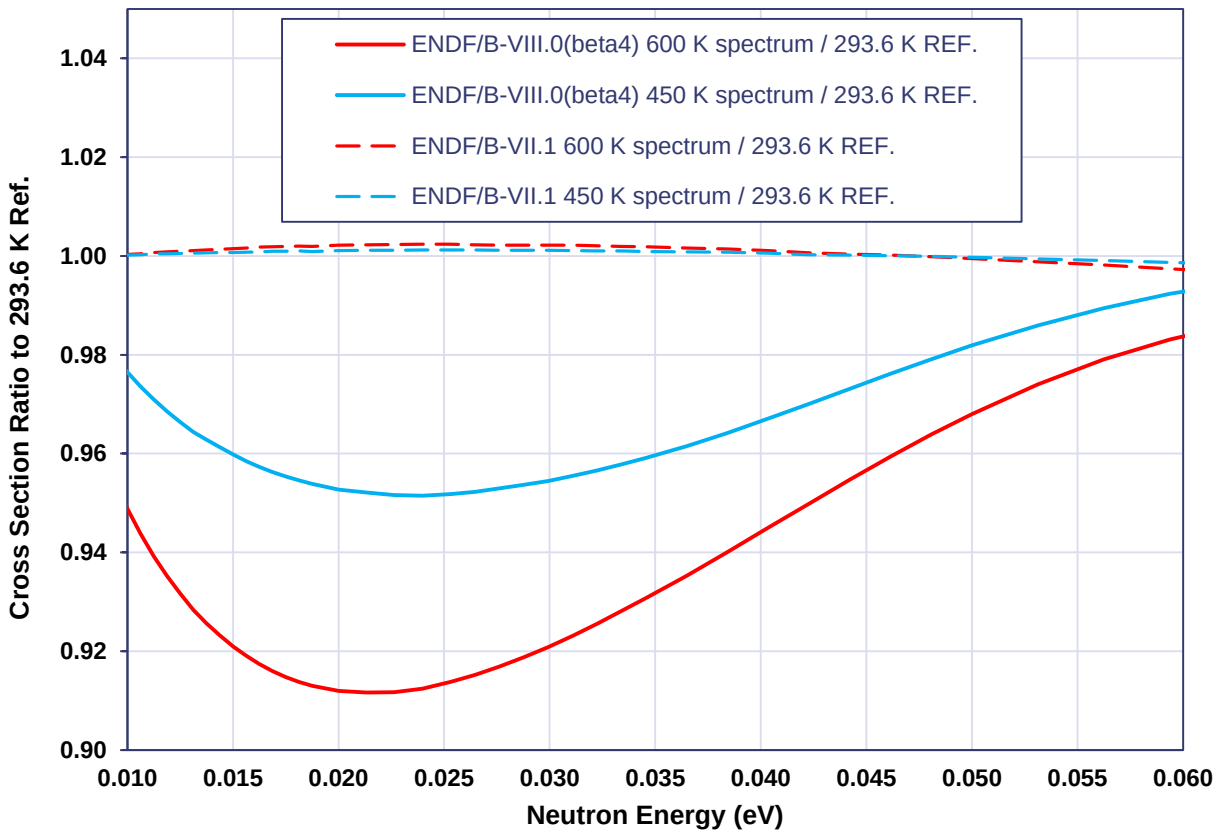
H-H_2O ENDF/B-VII.1 and ENDF/B-VIII.0(β4) Cross Section Ratio to 293.6 K Reference Changing Only Temperature-Dependent Phonon Spectra



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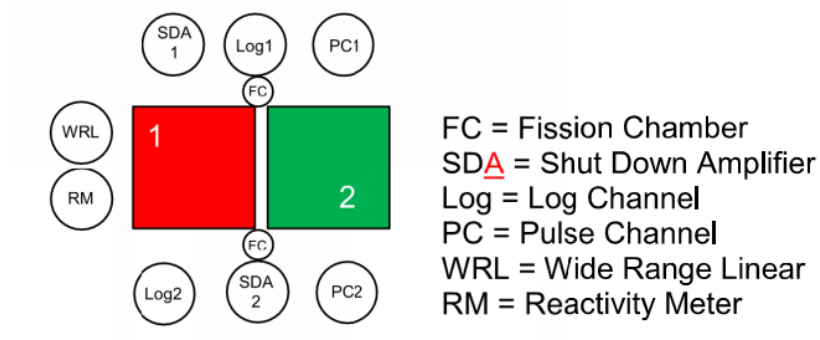
Validation at Elevated Temperatures

- In 2014 NNL and Rolls-Royce collaborated on a series of critical experiments at the Neptune facility to validate our ability to predict criticality for water isolated arrays as function of temperature
- Configurations were neutronically similar to spent fuel storage racks without poison inserts in flux trap
- In this configuration undermoderated fuel assemblies can have a positive temperature coefficient of reactivity
- Fuel loading in two assemblies adjusted to progressively increase the effective water gap between assemblies
- Water temperature varied from 20-50 °C

Schematic of Core and Detector Arrangement



Schematic of Fuel Arrangement Showing Increase in Effective Water Gap

Ref: S. Walley, et al., "Measurement of Positive Temperature Coefficients of Reactivity for Rack-like Arrangements of Reactor Fuel in the Neptune Zero Energy Facility," Proc. RRFM-2016, pp. 287-296, Berlin, March 13-17, 2016.

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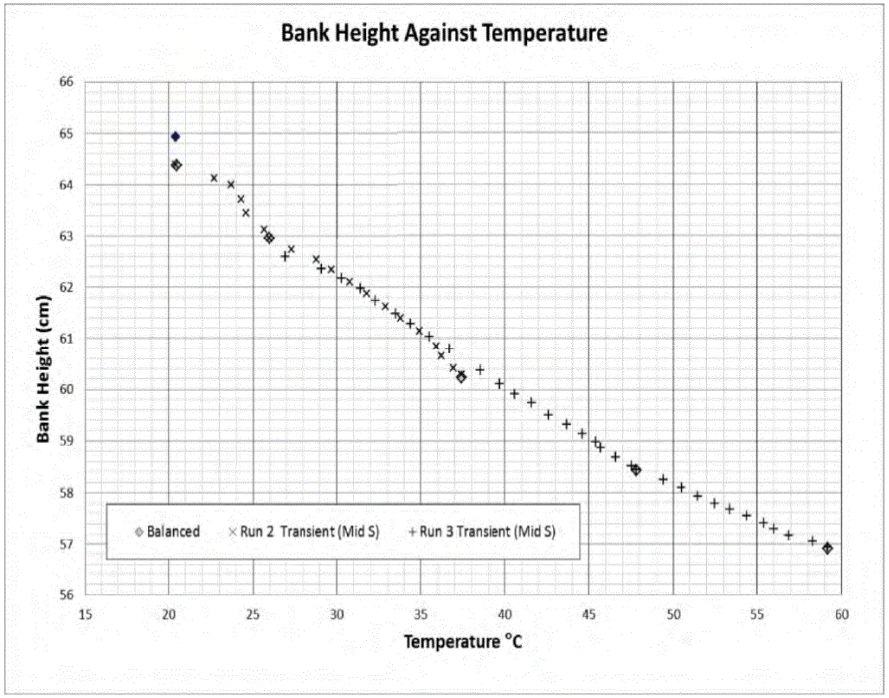
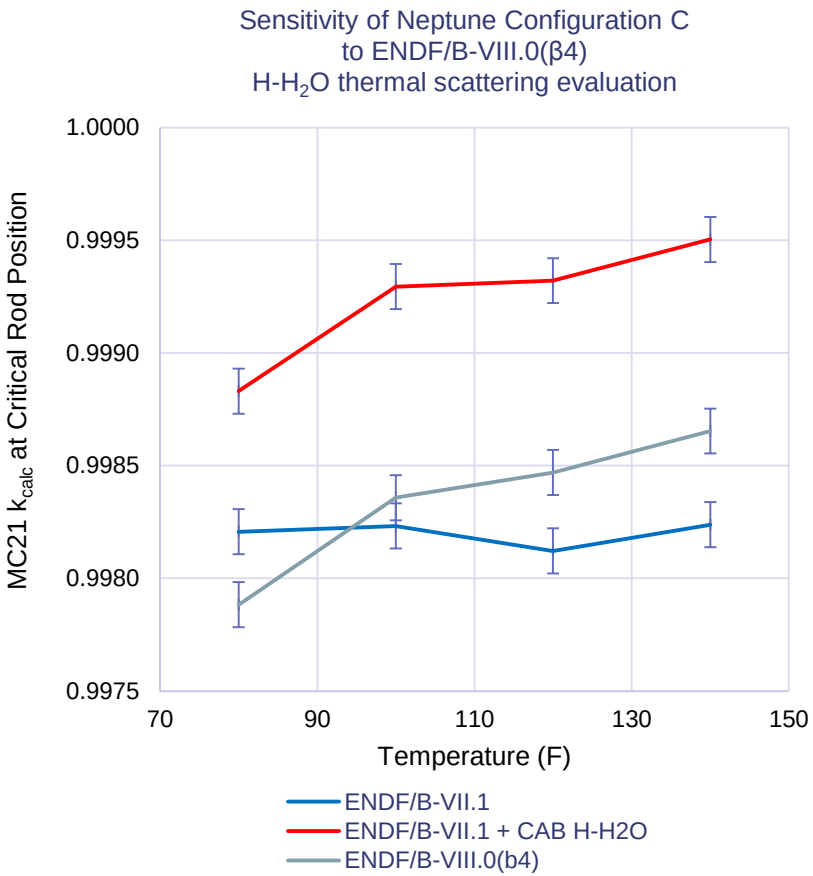
NEPTUNE Response to ENDF/B-VIII.0(β4) H-H_2O TSL vs. Temperature





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CAB LEAPR Model Observations

- H-H_2O, D-D_2O and O-D_2O
  - Suggest reducing maximum alpha and beta values to reduce maximum energy transfer from 10 eV to 5 eV, consistent with chemical bond energy
  - Suggest using uniform energy mesh for rotation mode PDOS to support preparation of application specific TSLs.
- O-H_2O
  - Consider including O-H_2O TSL to reduce the extent of tuning needed to match ultra-cold energy cross section data
- D-D_2O alpha values appear to be miscalculated
  - Based on A = 1 (H) instead of A = 2 (D)
  - Extends twice as high and with half the mesh density intended

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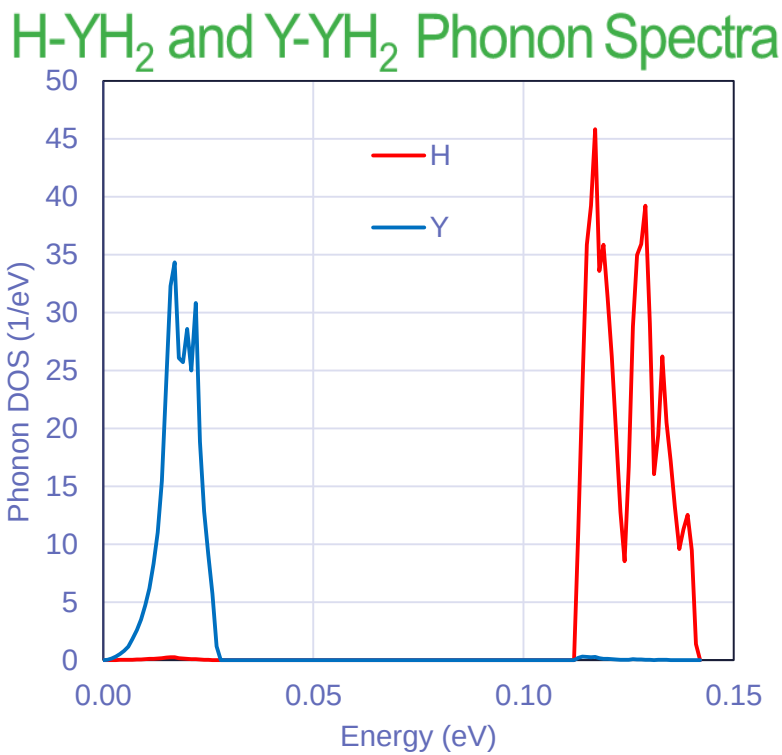
CAB LEAPR Mods

- CAB NJOY2012 mods raised S(α,β) floor in LEAPR from 10^{-75} to 2×10^{-38} (essentially single precision)
  - Impacts NJOY2012.82
  - Expect also impacts NJOY2016
- Mod adversely impacts processing of TSLs for materials with large bandgaps
  - H-ZrH
  - H-YH_2
  - H-PuH_2 and H-UH_3 (under development)
- Recommend mod be rolled back for NJOY2012 and NJOY2016 to support release of ENDF/B-VIII.0



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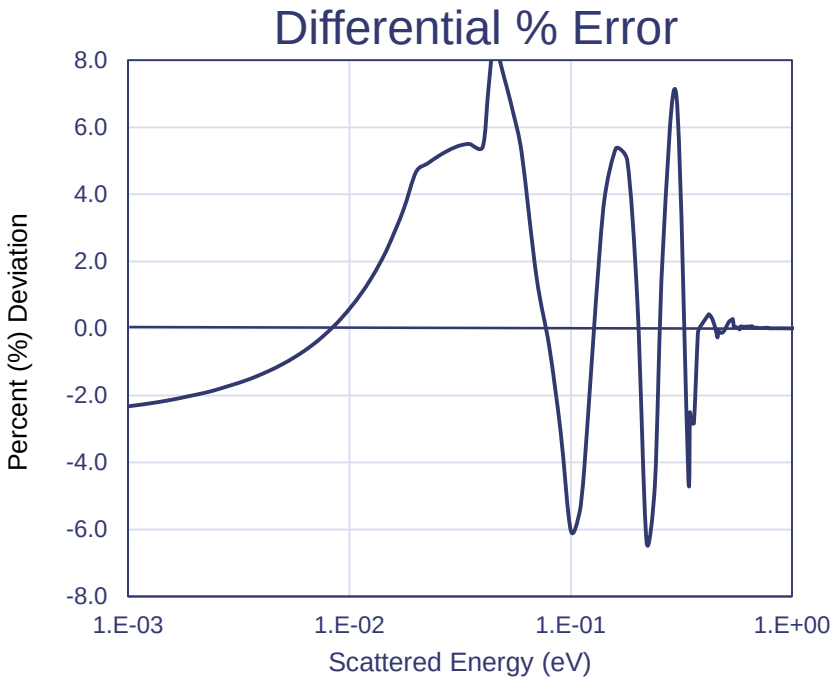
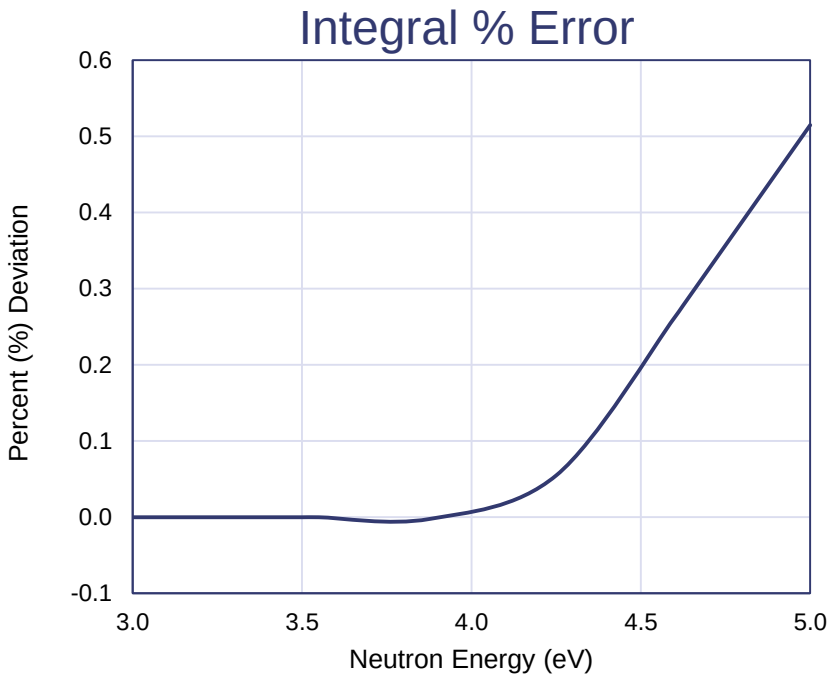
Percent Differential and Integral Cross Section Deviation for H-YH_2 at 293.6 K for Incident Neutron Energy = 4.46 eV Due to Implementation of a 10^{-38} Cutoff for S(α,β)





- At 293.6 K, for energy transfers > 4.2 eV, or β > 166, all S(α,β) information is truncated and the SCT is used (which overpredicts integral cross sections).
- Partial truncation begins for much lower β and progressively increases with β.

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Observations and Recommendations

- CAB H-H_2O performs well at room temperature
  - Improvements are primarily to ultra-cold temperature range, unimportant for reactor and criticality safety applications
- Reducing max temperature from 800 to 623.6 K may be an issue for commercial nuclear industry
  - Desire for temperatures up to 800 K (like available for ENDF/B-VII.1) to support severe accident analyses and SCWR studies
- Unexpected behavior at elevated temperatures
  - Have not previously seen trend with temperature for H-H_2O
  - Trend is disturbing for NNL

- Need to **slow down** and **understand** behavior at **elevated temperatures**
  - H-H_2O is most important moderator to industry
  - NNL will continue testing to understand behavior and provide recommendations
  - Need testing by commercial industry to ensure they understand impact to their applications and to provide additional feedback
- May need to delay ENDF/B-VIII.0 release or revert to ENDF/B-VII.1 H-H_2O

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