

Evaluation of yttrium hydride thermal neutron scattering data over a broad temperature range

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Motivation

- **Isotope and reactions to update**

- H and Y in YH_2 TSL from 5 to 1200 K

- **Motivation? Deficiencies in the current ENDF/B-VIII.0?**

- YH_x is planned moderator for Oak Ridge National Laboratory (ORNL) Transformational Challenge Reactor (TCR). YH_x exhibits strong anharmonicity at higher temperatures that are not modeled in ENDF/B-VIII.0.

- **What new data/theory motivate a new evaluation/update?**

- TDEP (Temperature Dependent Effective Potential) method and new inelastic scattering measurements at the Spallation Neutron Source (SNS).

- **What validation testing has been/will be done?**

- Double differential scattering cross section comparison between the SNS experiments and MCNP model (that utilizes newly created libraries) has been performed. We plan to perform total cross section measurements at higher temperatures for further validation.

s-TDEP Phonon spectrum

- For each vibrational mode s phonon Density of States (DOS) is equal to:

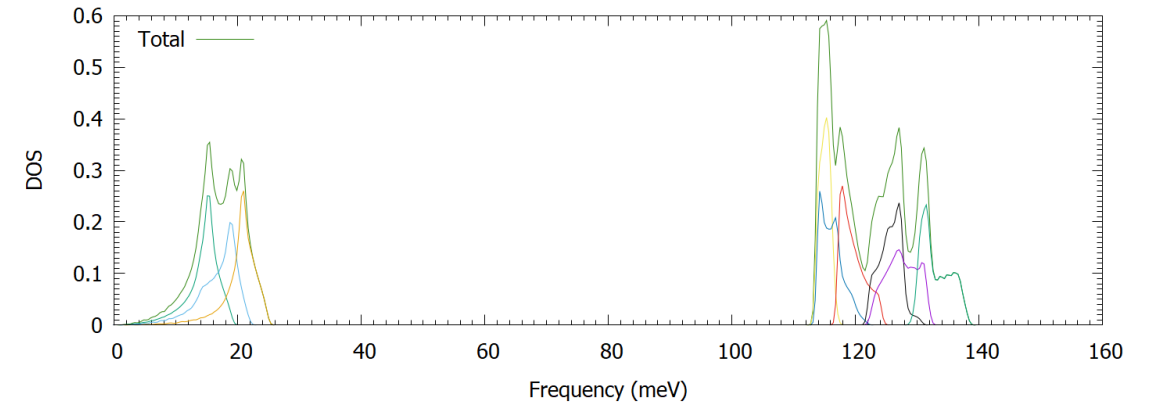
$$g_s(\omega) = \frac{2\pi}{V^3} \int_{BZ} \delta(\omega - \omega_{qs}) d\mathbf{q}.$$

- The atomic contribution for each atom i :

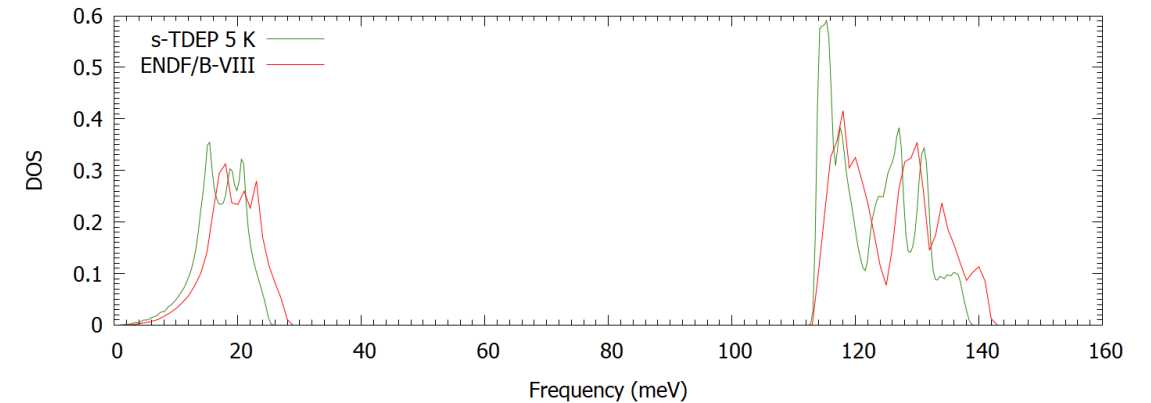
$$g_i(\omega) = \frac{2\pi}{V^3} \sum_s \int_{BZ} |\epsilon_{qs}^i|^2 \delta(\omega - \omega_{qs}) d\mathbf{q}.$$

- The total DOS is summed over all atomic contributions.

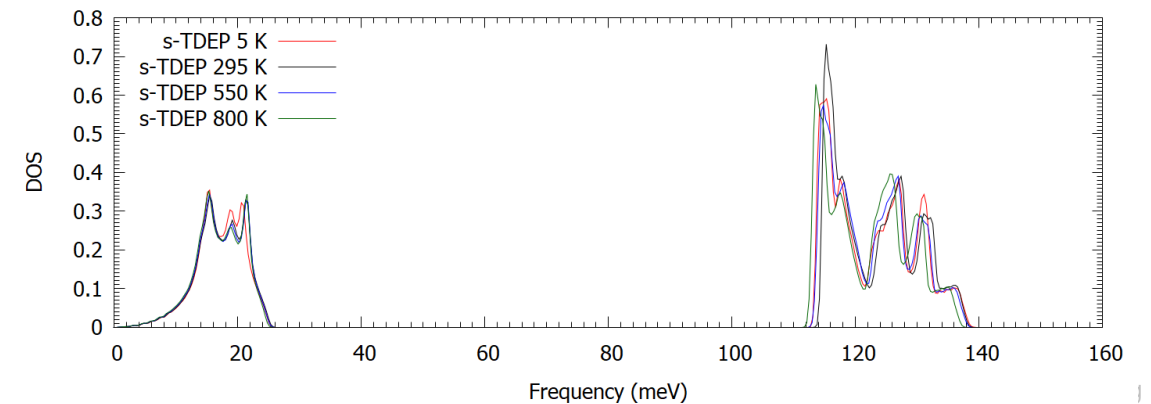
a) Total DOS with vibrational mode-projections



b) Total DOS comparison



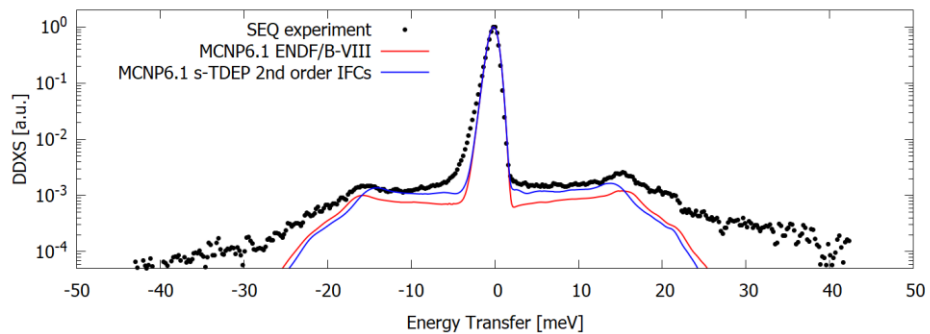
c) Total DOS comparison at different temperatures



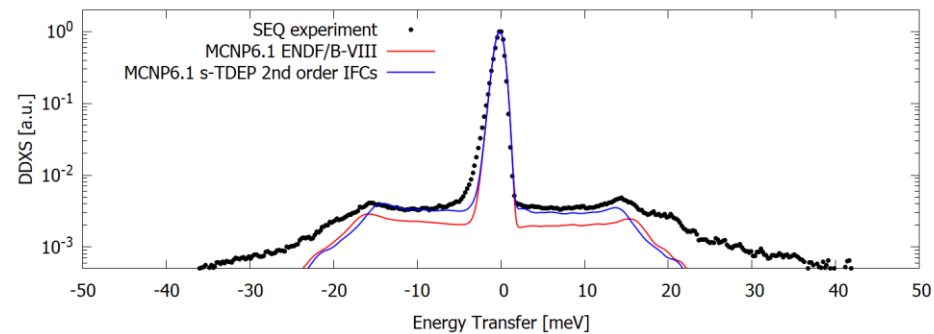
data over a broad temperature range

MCNP Double Differential Scattering Cross Section (DDXS)

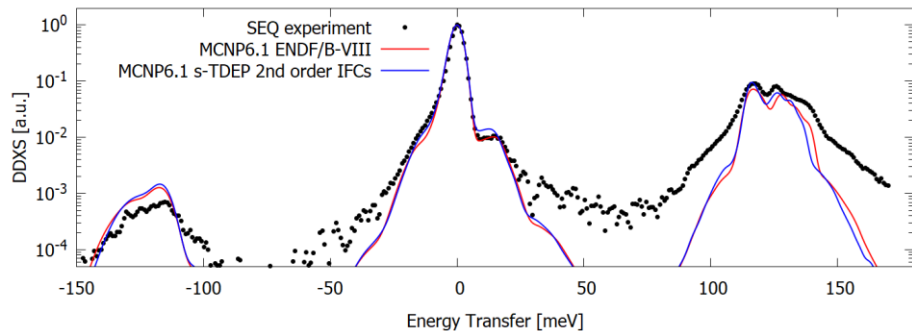
a) Comparison - $E_i=45$ Theta= 25° T=295 K



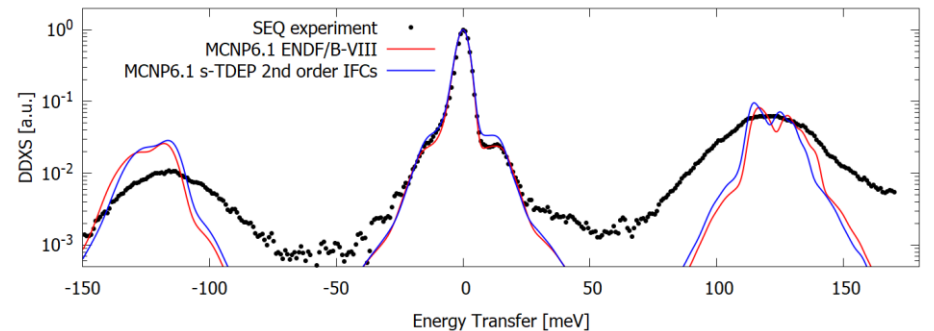
a) Comparison - $E_i=45$ Theta= 25° T=800 K



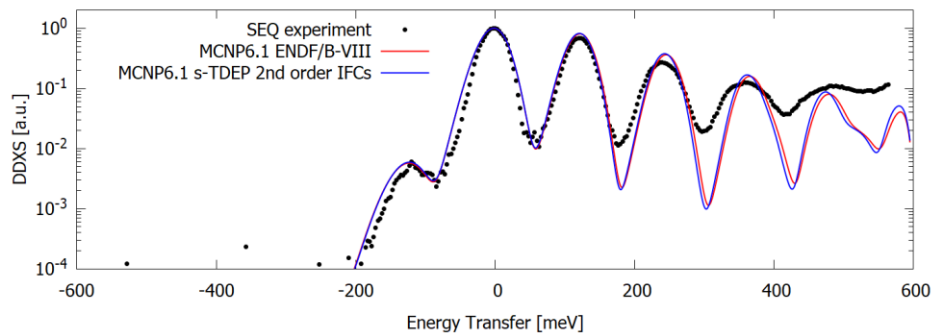
b) Comparison - $E_i=180$ Theta= 25° T=295 K



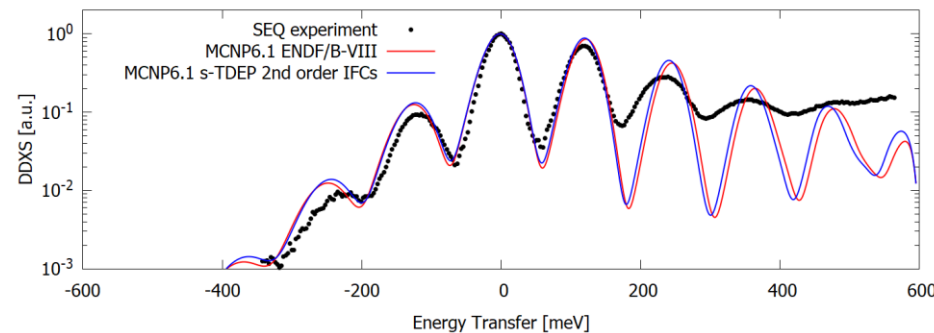
b) Comparison - $E_i=180$ Theta= 25° T=800 K



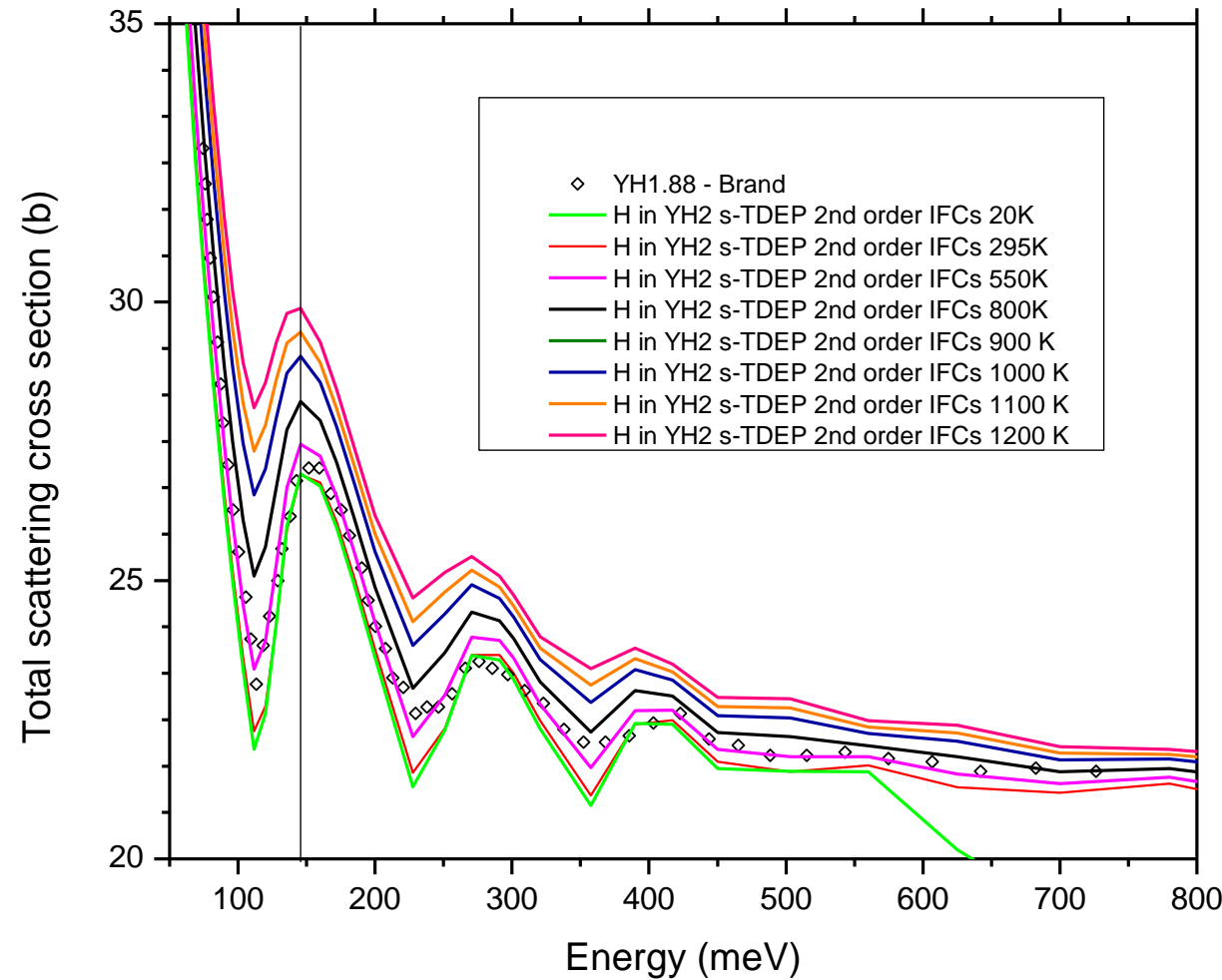
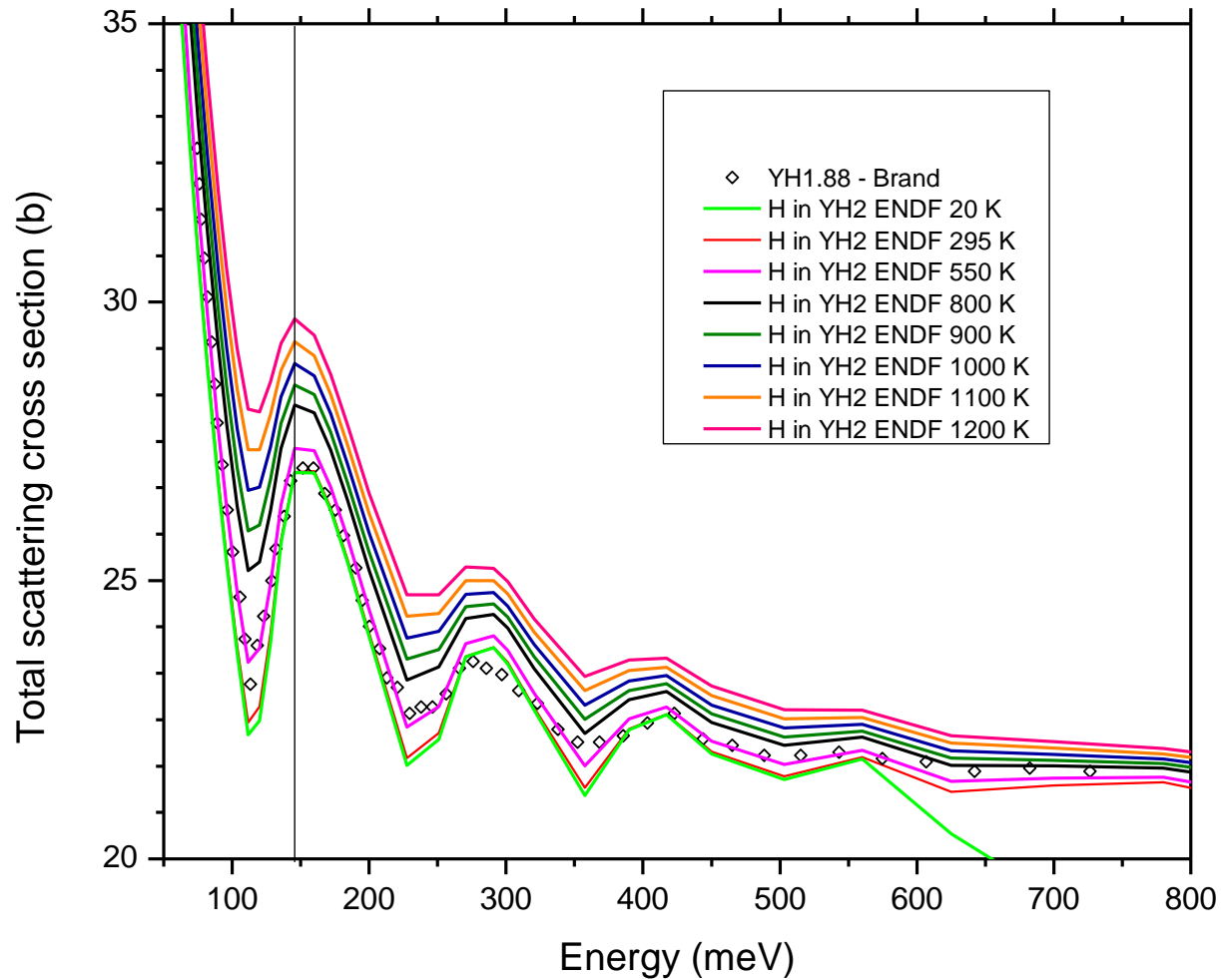
c) Comparison - $E_i=600$ Theta= 25° T=295 K



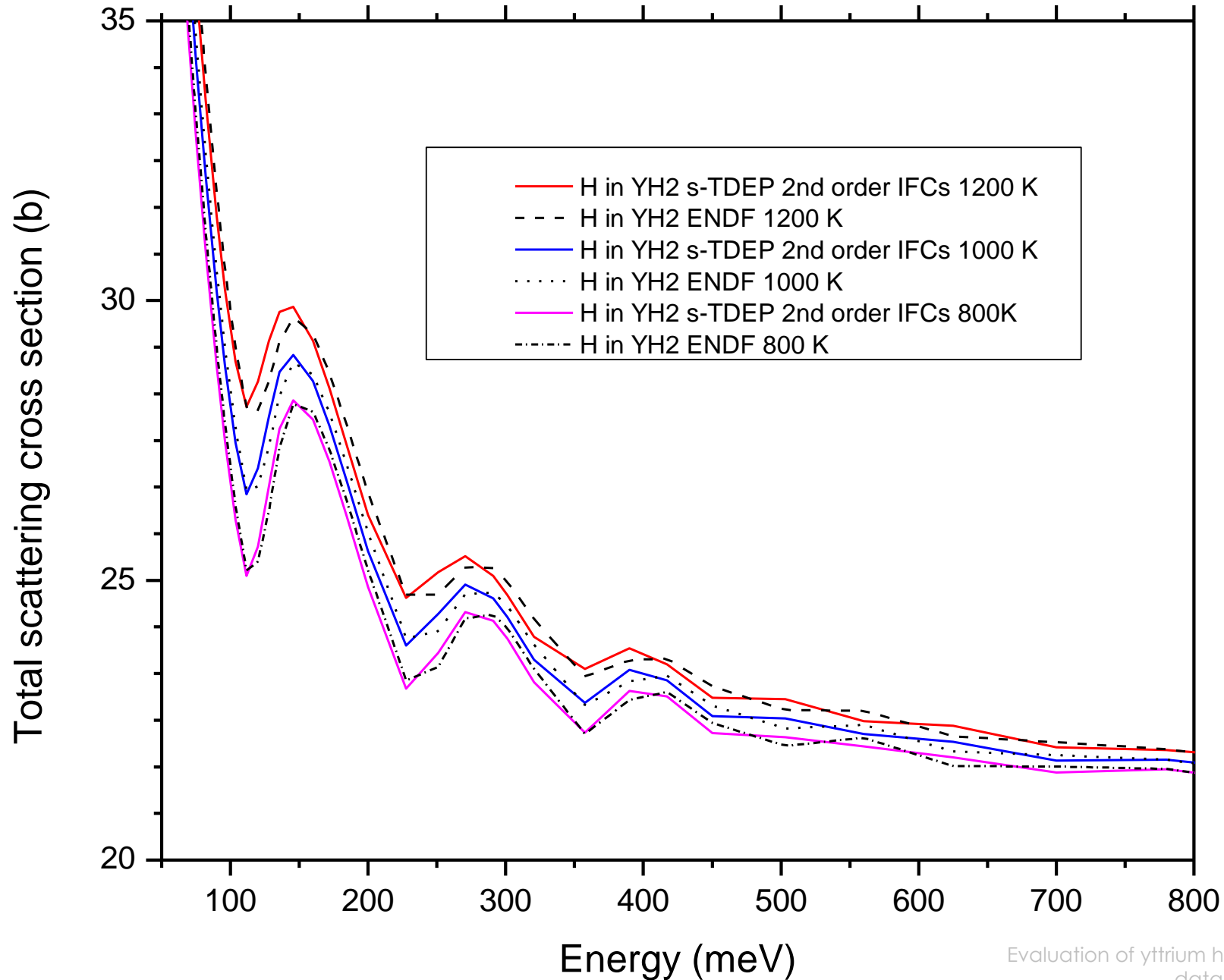
c) Comparison - $E_i=600$ Theta= 25° T=800 K



Total cross section comparison



Total cross section comparison



Acknowledgments

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- Chris Chapman's presentation: "Thermal Neutron Scattering Measurements at the ORNL Spallation Neutron Source"
- More information on the experiments and modeling: https://tcr.ornl.gov/wp-content/uploads/2020/10/TNS_evaluation_of_YHx_FY2020_Progress.pdf

• Questions?