Measurement of the total cross section of heavy water in the 0.1 meV - 1 eV energy range at 20 and 50 °C

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CONICET

- The Evaluated Nuclear Data Libraries contain two essentially different models for the thermal neutron scattering cross section for heavy water:
  - The model originally developed in General Atomics by Koppel and Young, which is purely incoherent (available in the ENDF/B-VI library), and
  - The model developed at IKE Stuttgart by Keinert and Mattes, which was calculated in the Sköld approximation (available in the ENDF/B-VII and JEFF-3.2 libraries).

- The IKE model is better, because it includes a correction for the coherent scattering in deuterium, but it shows and odd behaviour with temperature, as indicated to us by Dr. Danila Roubtsov from AECL.
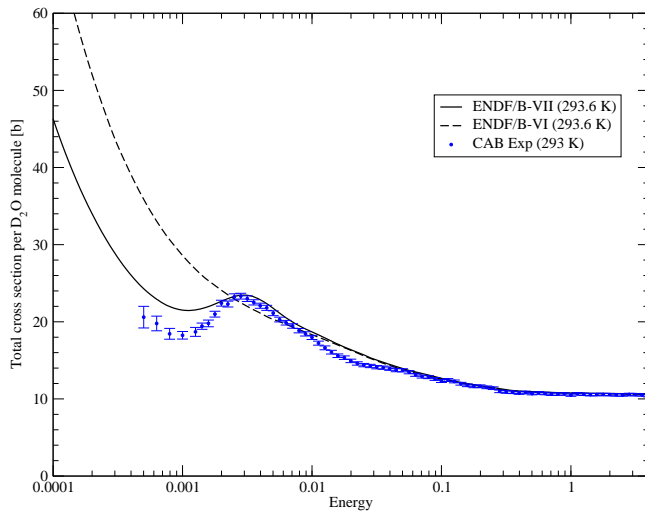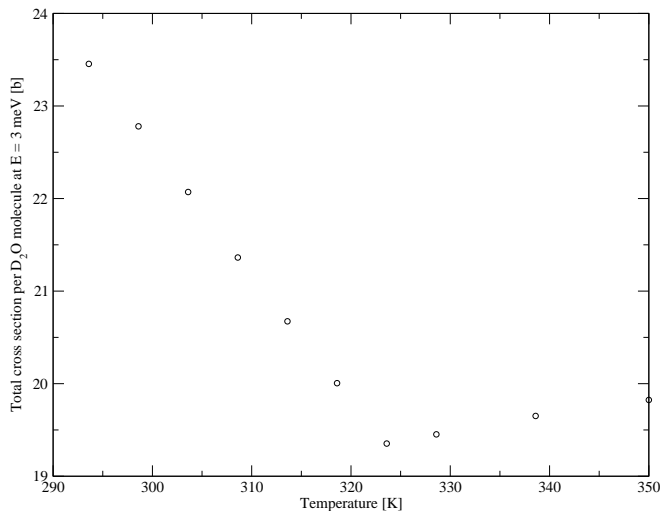
Total cross section of heavy water at room temperature, according to the GA Model (ENDF/B-VI) and IKE Model (ENDF/B-VII).
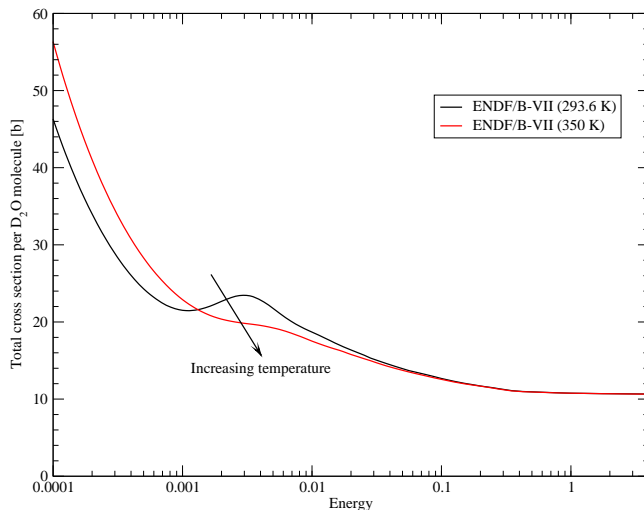
Total cross section of heavy water at 293 and 350 K, according to the IKE model.
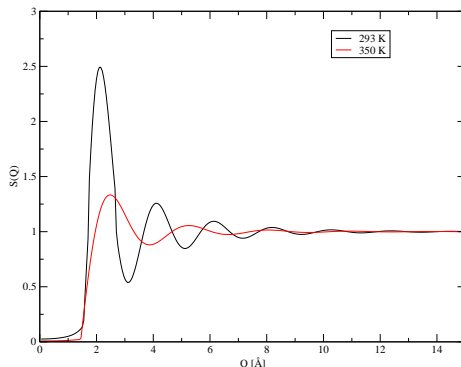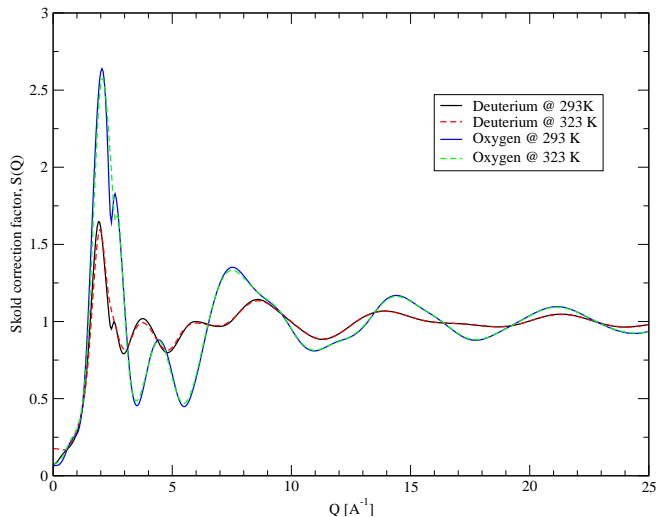
Total cross section of heavy water at $E = 3$ meV.

$$\frac{d\sigma^2}{d\hat{\Omega}dE} = \frac{\sigma_b}{4\pi k_B T}\sqrt{\frac{E'}{E}}S(\alpha, \beta) \tag{1}$$

$$S(\alpha, \beta) = S_{\text{inc}}(\alpha/S(Q), \beta)S(Q)$$

where $S(Q)$ is a correction function, which corresponds to the structure factor for atomic liquids. In the case of the IKE model, $S(Q)$ is computed from a Lennard-Jones model and decreases rapidly with temperature:

- Model for D and O in D_2O.
- Dynamics: convolution of three terms:
  1. Molecular diffusion, represented with the Egelstaff-Schofield model .
  2. Intermolecular stretching and bending of the hydrogen bond network and molecular librations, represented as a continuous spectrum. Continuous spectrum calculated from the generalized frequency distribution obtained from molecular dynamics, and substracting diffusion and the two internal modes.
  3. Internal vibrations, represented as discrete oscillators.
- Coherent component, calculated with the Sköld approximation, using partial structure factors published by Soper.

Sköld correction factors for deuterium and oxygen bound in heavy water at 293 and 323 K, used in the CAB model.
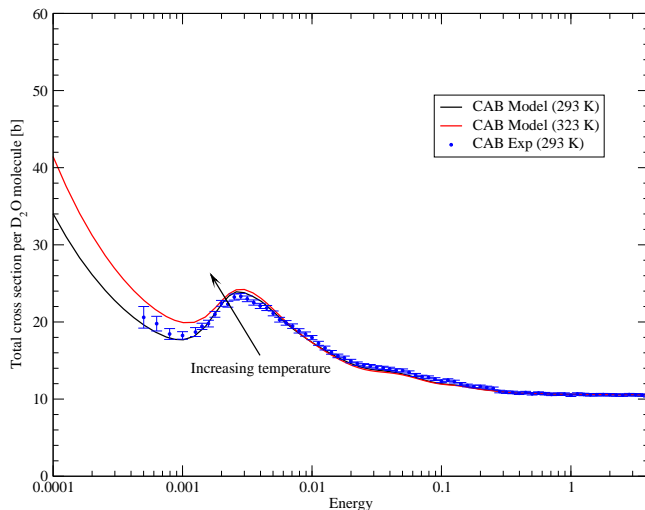
Total cross section of heavy water at 293 and 323 K, according to the CAB model.

- To settle this we needed a measurement of the total cross section of heavy water.
- Last measurement available in EXFOR was made 40 years ago in Bariloche. And only at room temperature.
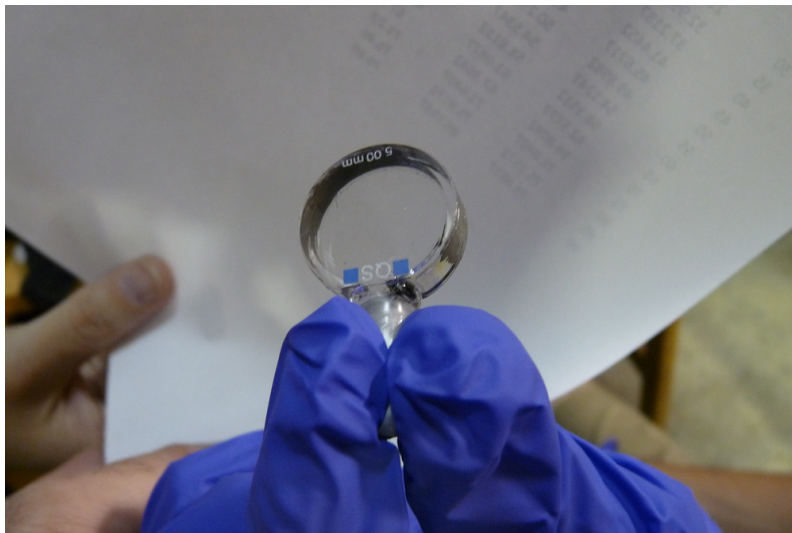- We asked David, and together we performed the measurement at LENS.

SANS beamline at LENS.

Sample area with transmission set up.

Sample holder.
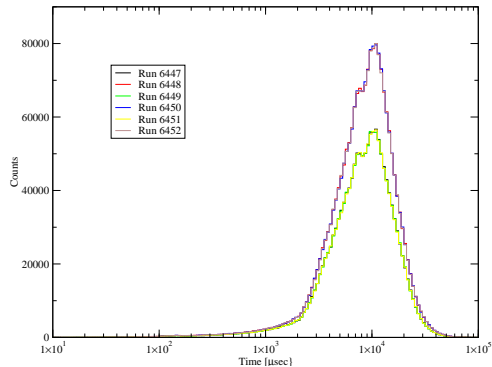
Experimental corrections:

- Mean emission time.
- Dead time.
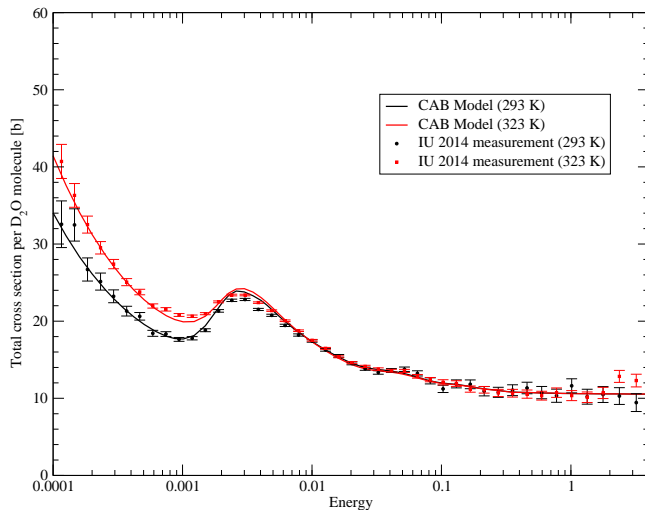
Measured total cross section of heavy water at 293 and 323 K, compared with CAB model calculations.

- There is a current need for total neutron cross sections in the thermal range.
- These cross sections can be measured in a broad energy range using the transmission technique in a pulsed neutron source.
- LENS is suitable for these measurements, specially for liquids.
- It was experimentally verified that the anomaly in the temperature dependence of the total cross section for heavy water, predicted by the scattering model present in the ENDF/B-VII and JEFF 3.2 libraries, does not exist.
- The new libraries can be downloaded from our website:

        http://www2.cab.cnea.gov.ar/~nyr/tsl_eng.html