IRSN
INSTITUT
DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

Faire avancer la sûreté nucléaire

Investigation of frequency spectrum of light water to generate thermal scattering law

WPEC meeting
SG-42

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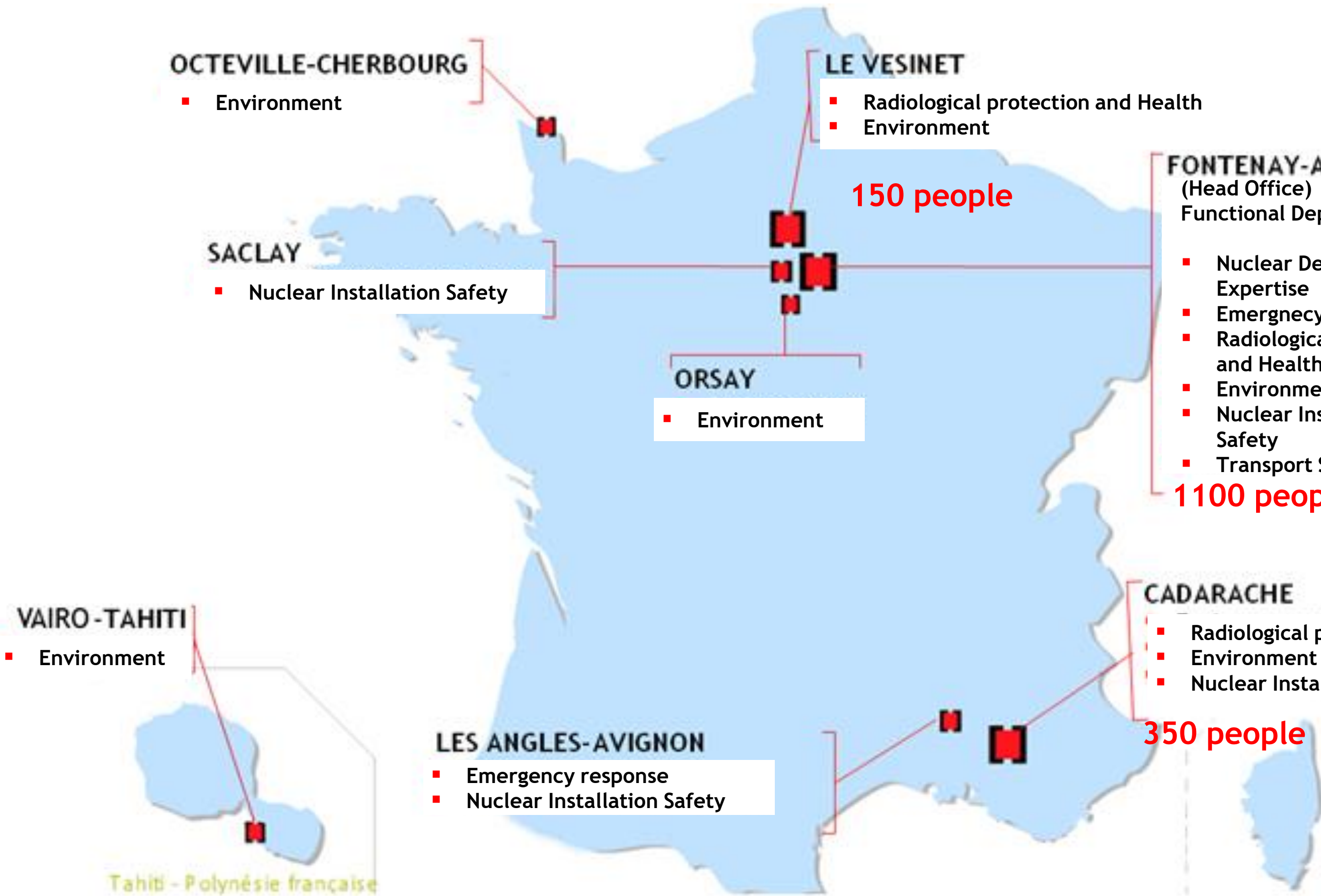
1800 personnel at 8 sites



Agenda

- **Motivation**
- **TSL generation methodologies**
- **TOF experiment to generate frequency spectrum of light water**
- **Results**
- **Conclusions**

"Neutron Man*"

* Neutron Scattering: A Primer by Roger Pynn

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- To improve the design and safety of thermal reactors:
  - It is necessary to perform high-precision neutron transport calculations (MCNP, MORET, etc.)
  - Estimate results and uncertainties

- These calculations are based on neutron interaction data (cross-sections) which are available in evaluated nuclear data libraries (JEFF, ENDF, etc.)

- Light water is the most common moderator in nuclear reactor applications (PWRs)

Pressurized Water Reactors (PWRs) operate with light water at high temperature and pressure (Temperature ~600 K and Pressure ~150 bar)

We need reliable thermal scattering cross-section data often termed as Thermal scattering law (TSL) for Light water !!

Existing TSL libraries for light water

Existing libraries are based upon:

- Experiments performed in the sixties with limited resolution and information about their uncertainties.

- LEAPR module of the NJOY code which uses numerous approximations (Gaussian and incoherent).

- S(α, β) is reduced to an **analytic function of g(ω) or ρ(β), the frequency spectrum** (most common approach used presently):

- **If one chooses to work within the LEAPR framework**, the main issue becomes the **accurate determination of the frequency spectrum**.

Thermal scattering law (TSL)

- The double differential cross-section (DDXS) for neutrons with incident energy E, secondary energy E', μ is the neutron scattering cosine and scattering angle Ω is related to S(α,β) by :

$$\frac{d^2\sigma_T}{d\Omega dE'}(E \to E', \mu) = \frac{\sigma_b}{4\pi k_B T}\sqrt{\frac{E'}{E}}\, S(\alpha,\beta)$$

$$\alpha = \frac{E + E' - 2\mu\sqrt{EE'}}{Ak_B T} \qquad \beta = \frac{E' - E}{k_B T}$$

Momentum transfer *Energy transfer*

S(α, β)
Thermal Scattering Law

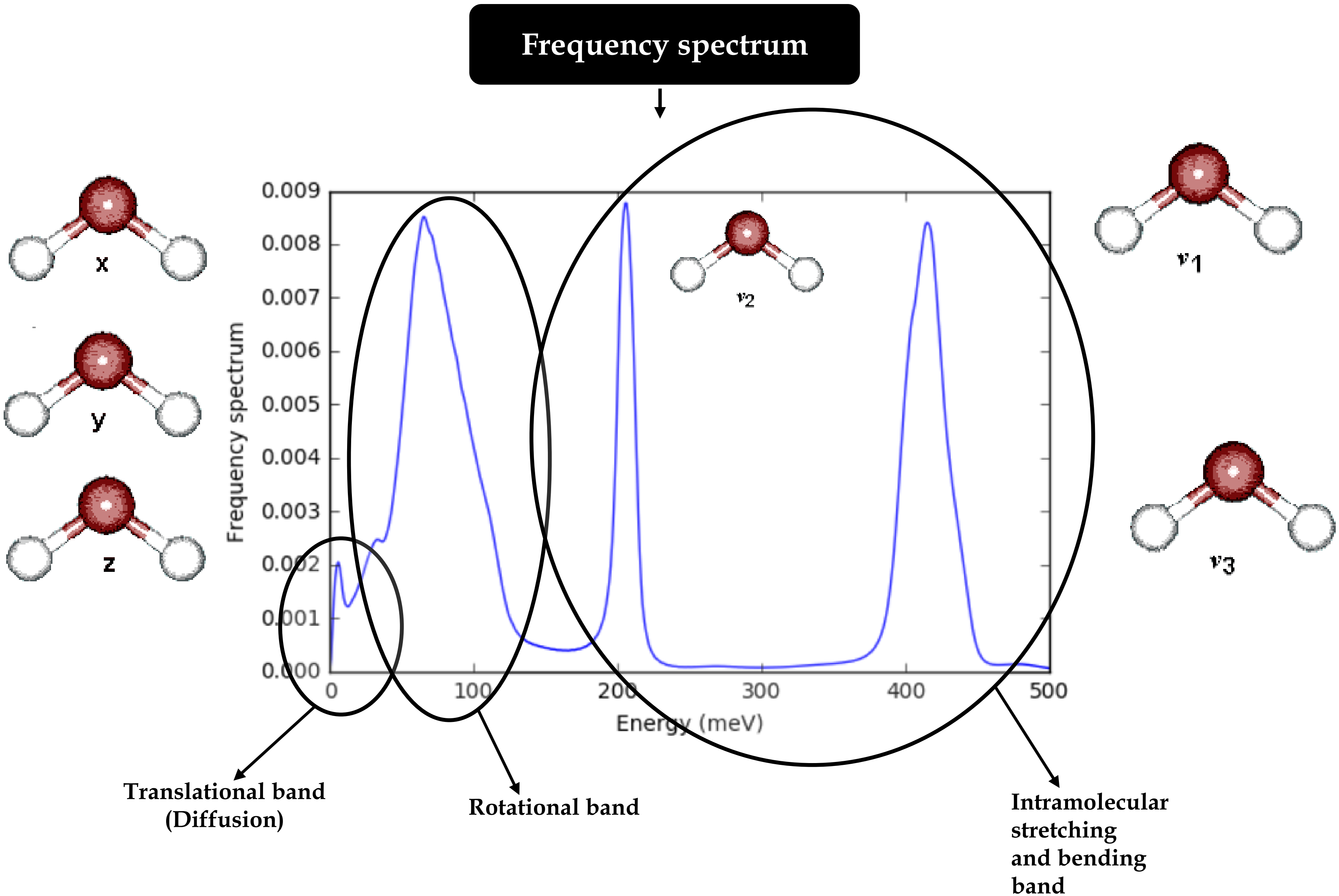
$$S(\alpha,\beta) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{\iota\beta\hat{t}}\, e^{-\gamma(\hat{t})} d\hat{t}$$

$$\gamma(\hat{t}) = \alpha\int_{-\infty}^{+\infty} P(\beta)(1 - e^{-\iota\beta\hat{t}})\, e^{-\beta/2} d\beta$$

$$P(\beta) = \frac{\rho(\beta)}{2\beta\sinh(\beta/2)}$$

$\rho(\beta)$ ← **Frequency spectrum**

Frequency spectrum of light water



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TSL models of light water

Based on TOF Experiments

We use neutrons to measure the structural properties of light water.

Quantum thermal scattering law (Asymmetric)

Based on MD simulations

We use classical potentials to indirectly obtain the structural properties of light water.

Classical thermal scattering law (Symmetric)

TSL libraries

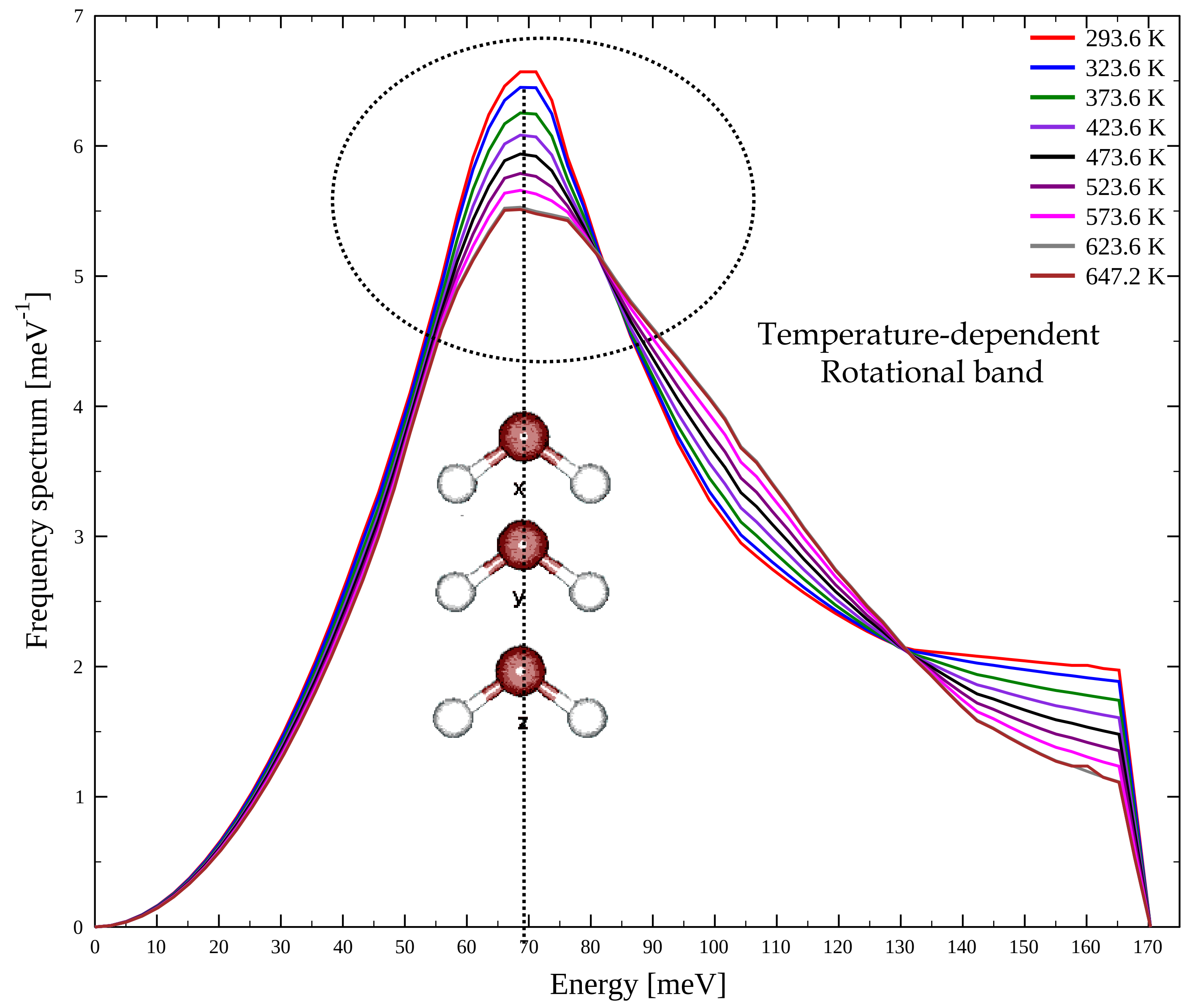
IKE Model

JEFF-3.1
JEFF-3.2
JEFF-3.3
ENDF/B-VII.1

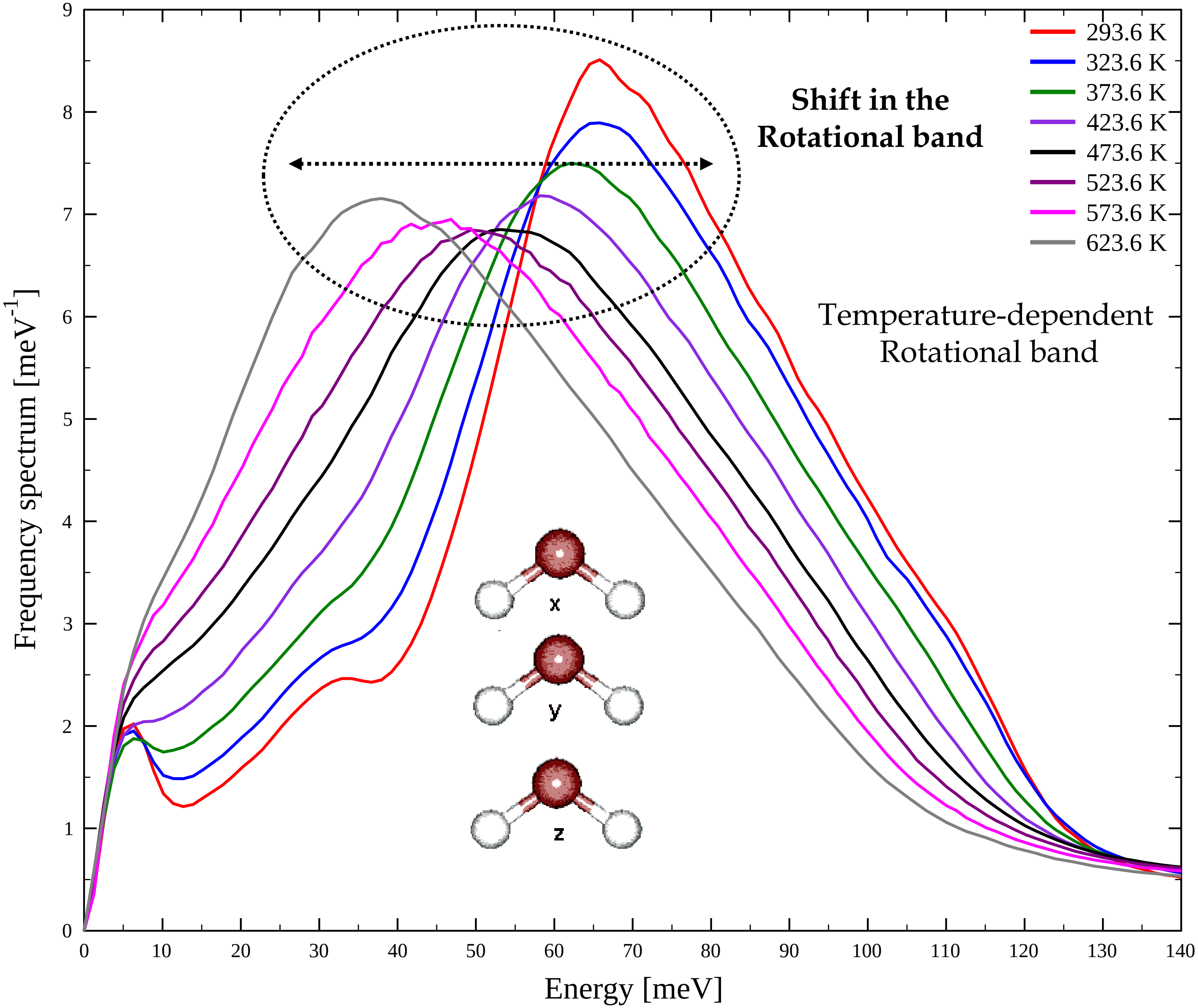
CAB Model

ENDF/B-VIII.0

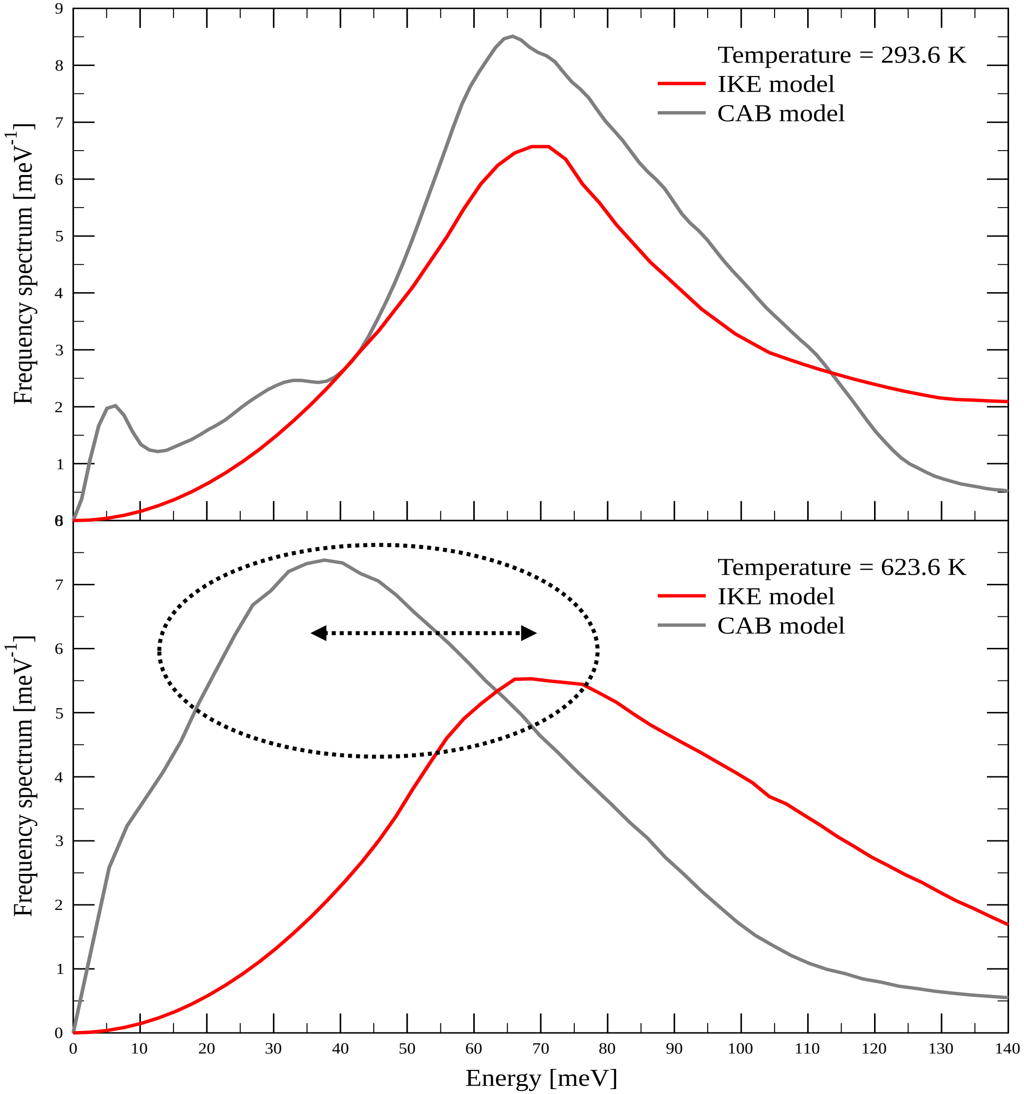
Frequency spectrum of light water: JEFF-3.3 (IKE model)



Frequency spectrum of light water: ENDF-B/VIII.b5 (CAB model)



Comparison of frequency spectrum: CAB & IKE Model

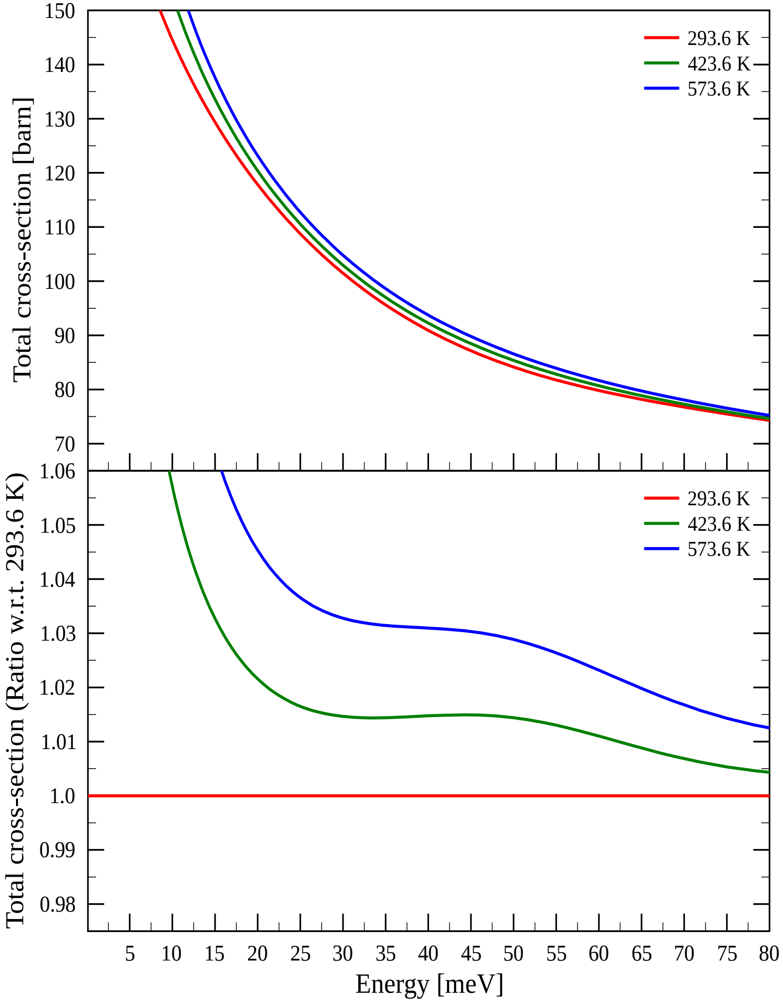


Shift in the Rotational band

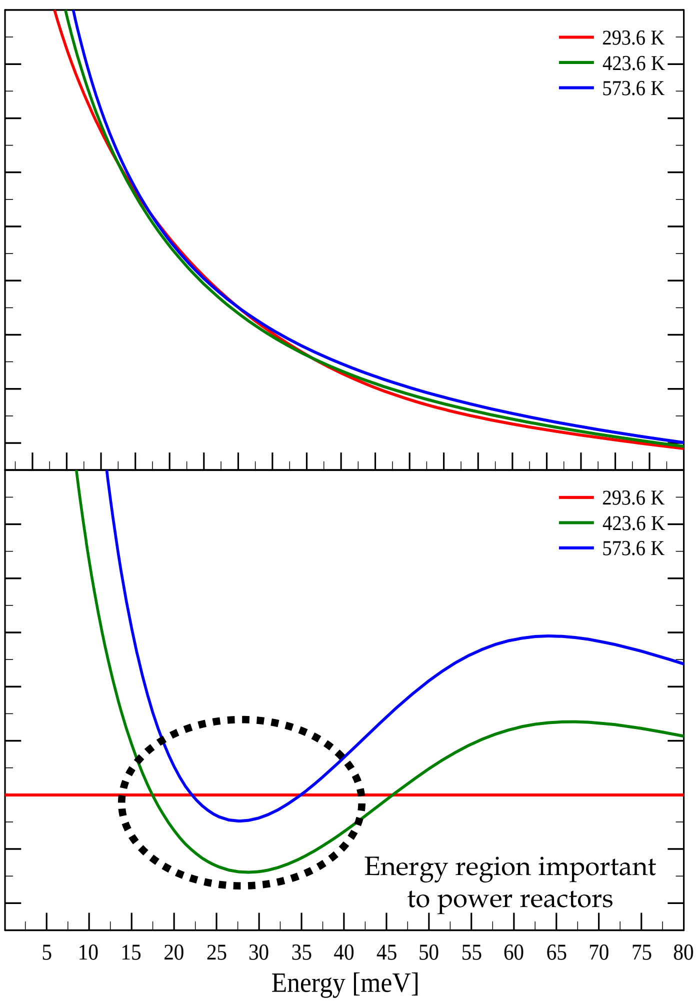
Shift in the Rotational band

Comparison of total cross-section: CAB & IKE Model

JEFF-3.3 (IKE Model)



ENDF/B-VIII.b5 (CAB Model)



New experimental data for the verification of recent evaluations are very scarce.

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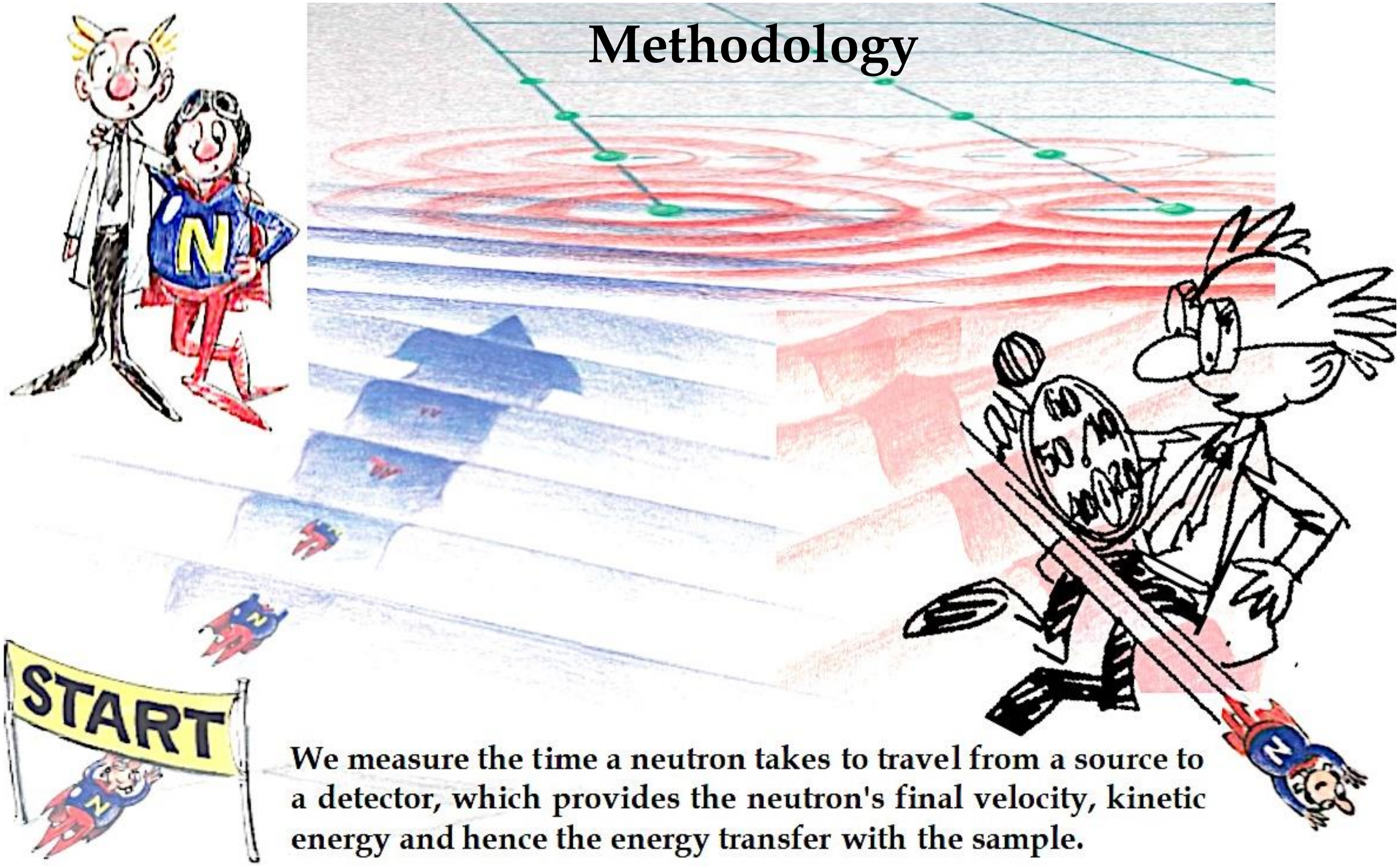
TOF experiments with light water using two spectrometers **IN4c** and **IN6** at Institut Laue-Langevin (ILL), Grenoble .



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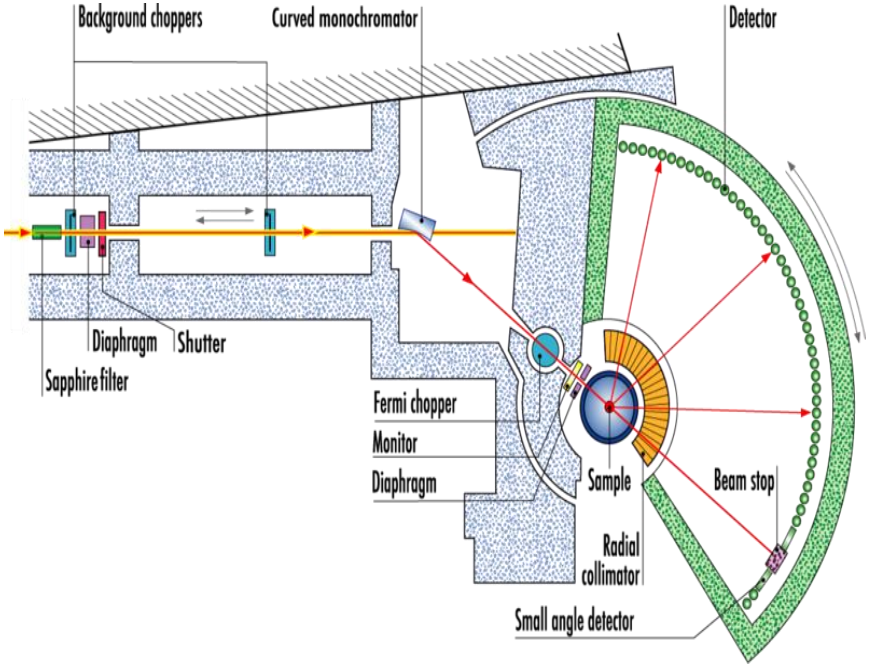
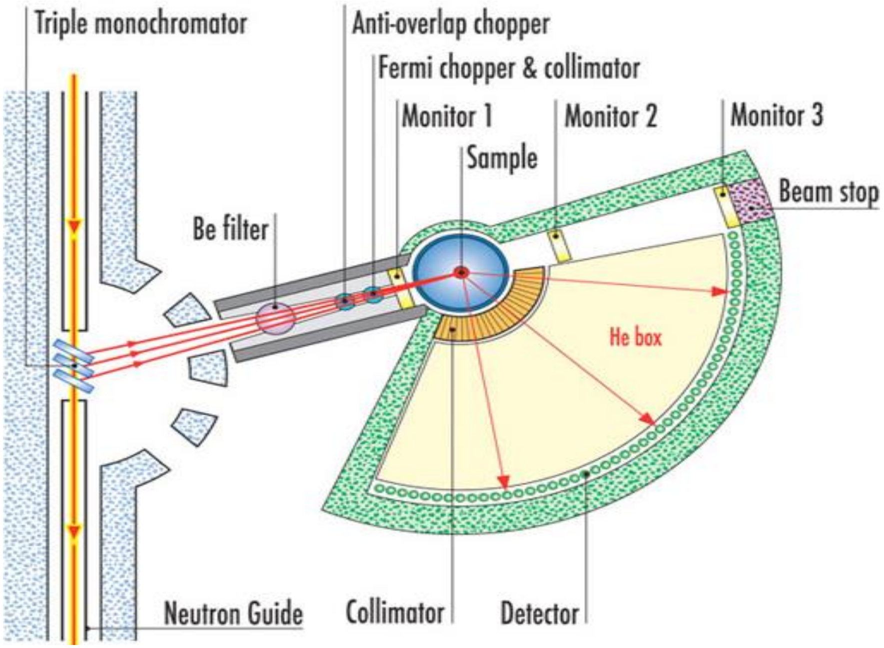
IN4c

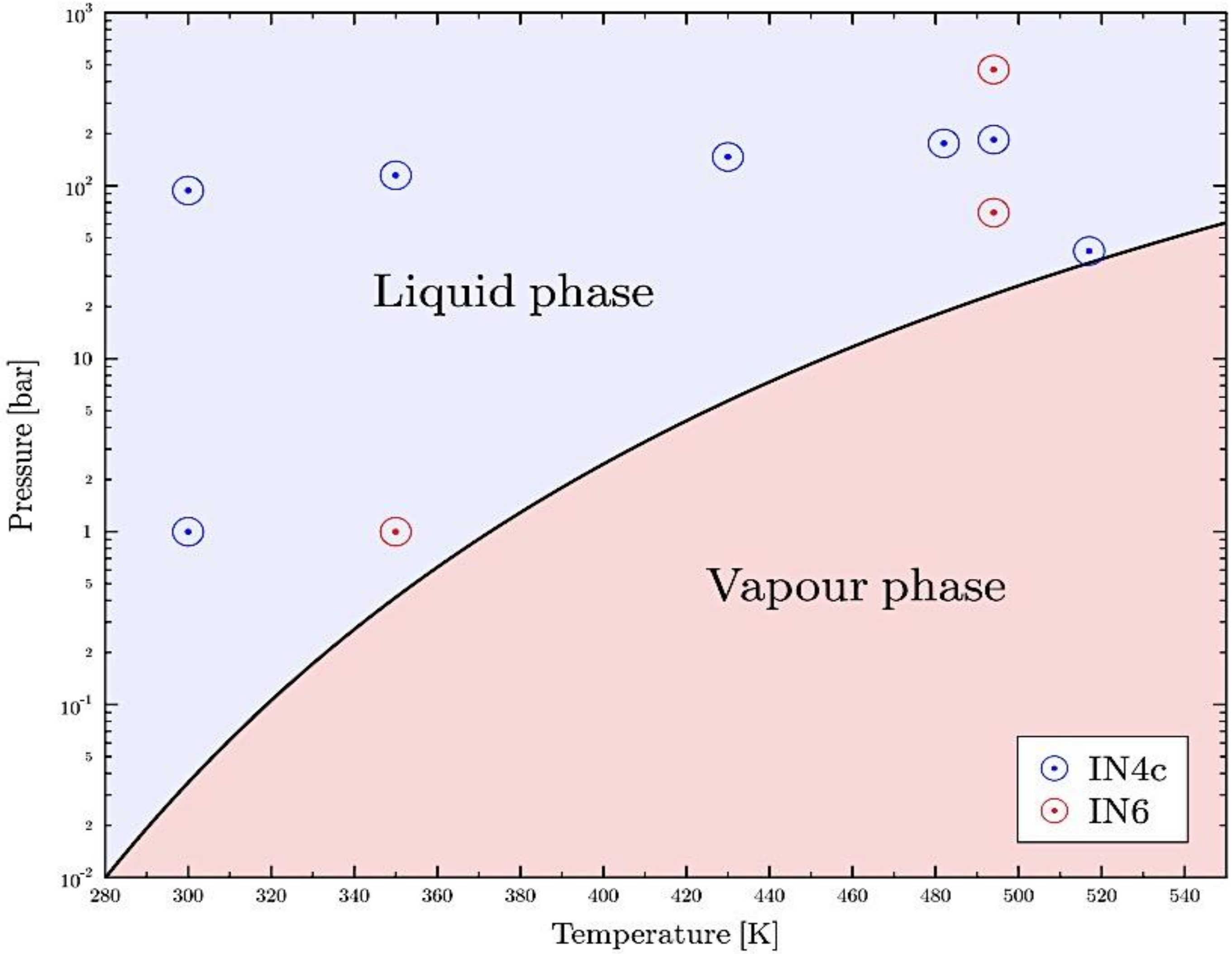


- Wavelength of the incident neutron = 2.41 Å
- This wavelength corresponds to a neutron energy of 14.2 meV
- Energy resolution at this incident neutron energy = 4 %
- Scattering angle range θ = 15°-120°

IN6



- Wavelength of the incident neutron = 5.1 Å
- This wavelength corresponds to a neutron energy of 3.15 meV
- Energy resolution at this incident neutron energy = 2 %
- Scattering angle range θ = 15°-110°



Thermodynamic states (experimental conditions) of light water for the data measurement.

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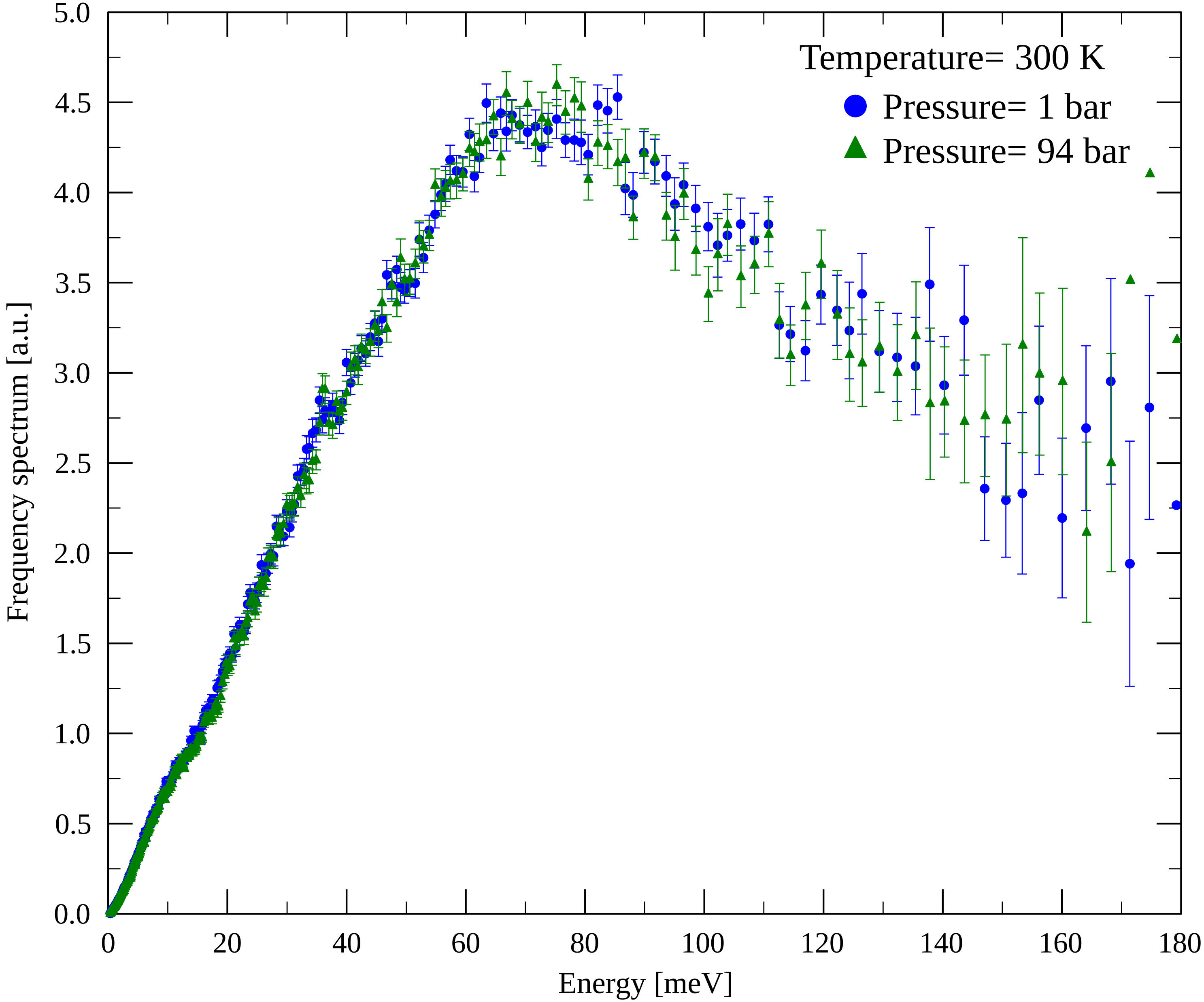
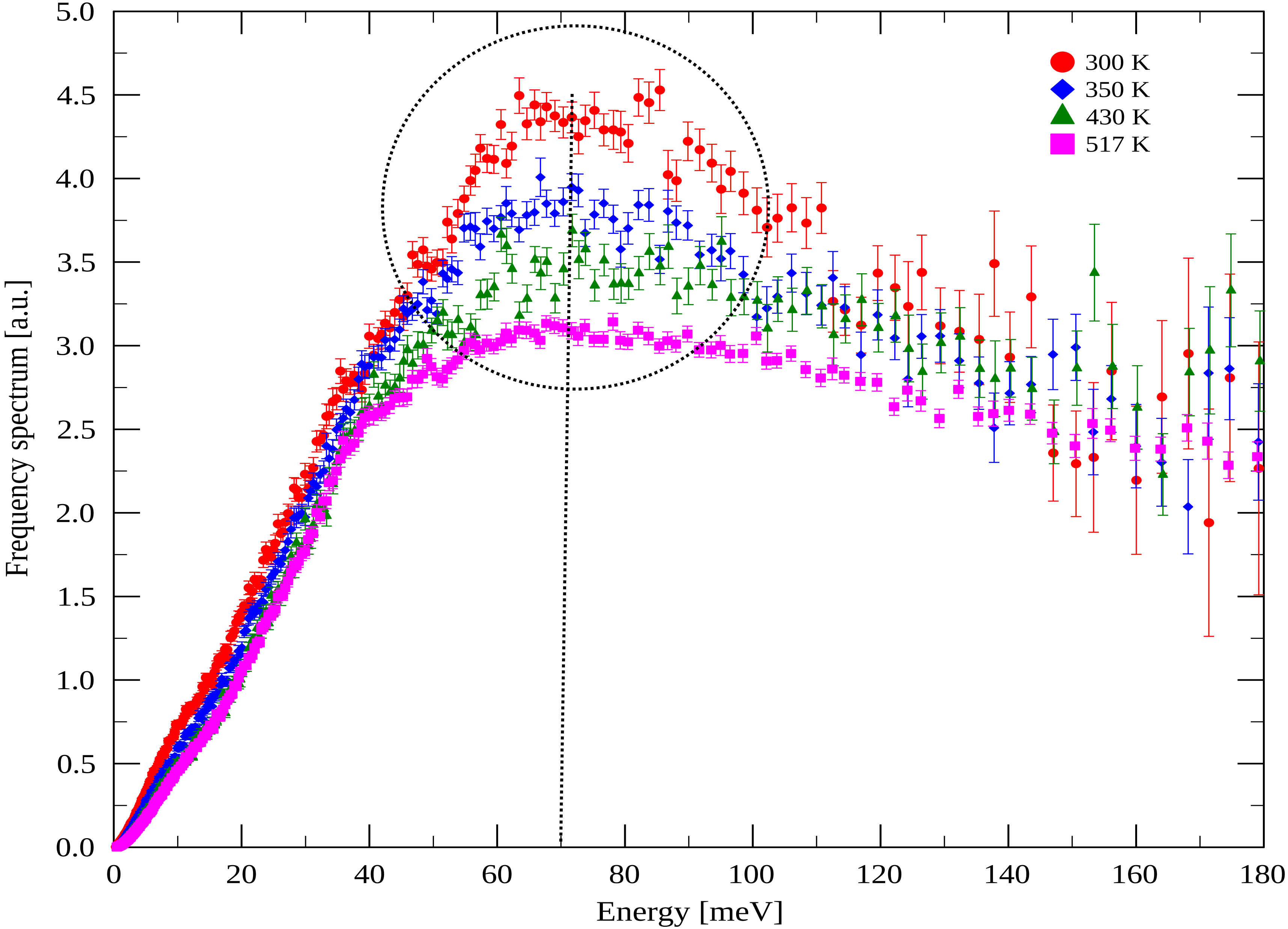
Pressure dependence on frequency spectrum: IN4c

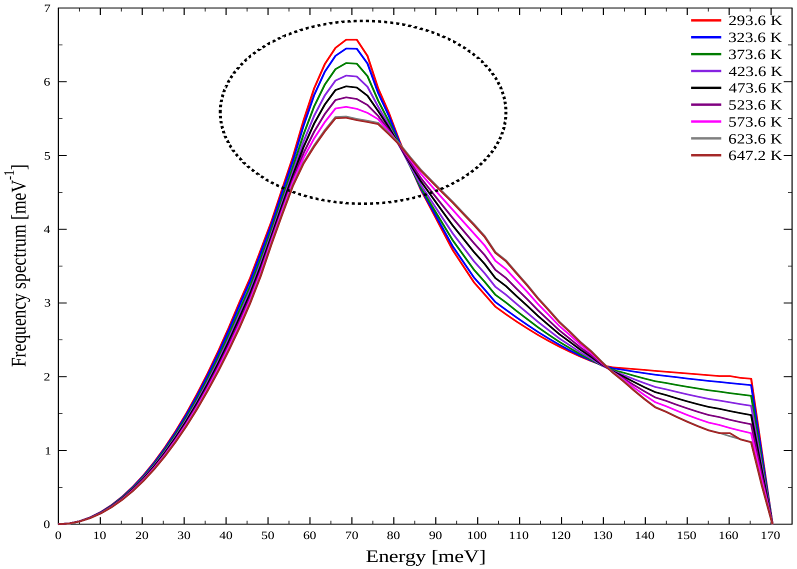


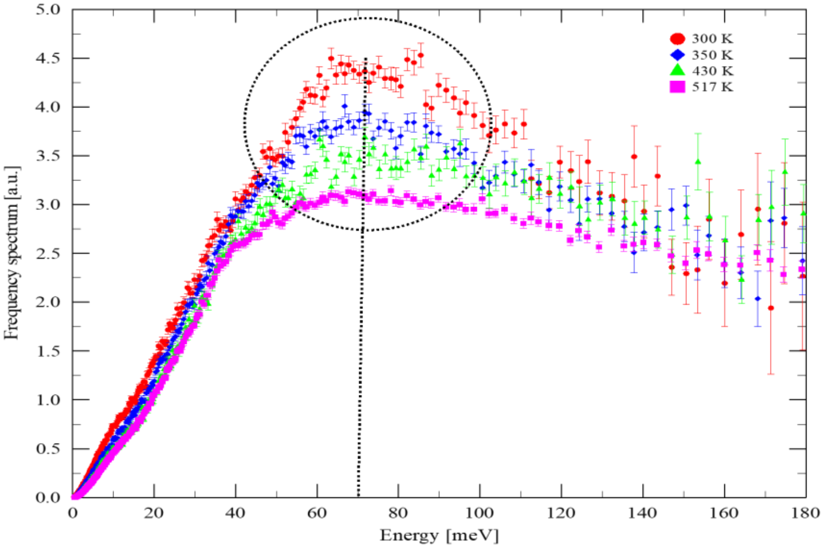
Temperature dependence on frequency spectrum: IN4c



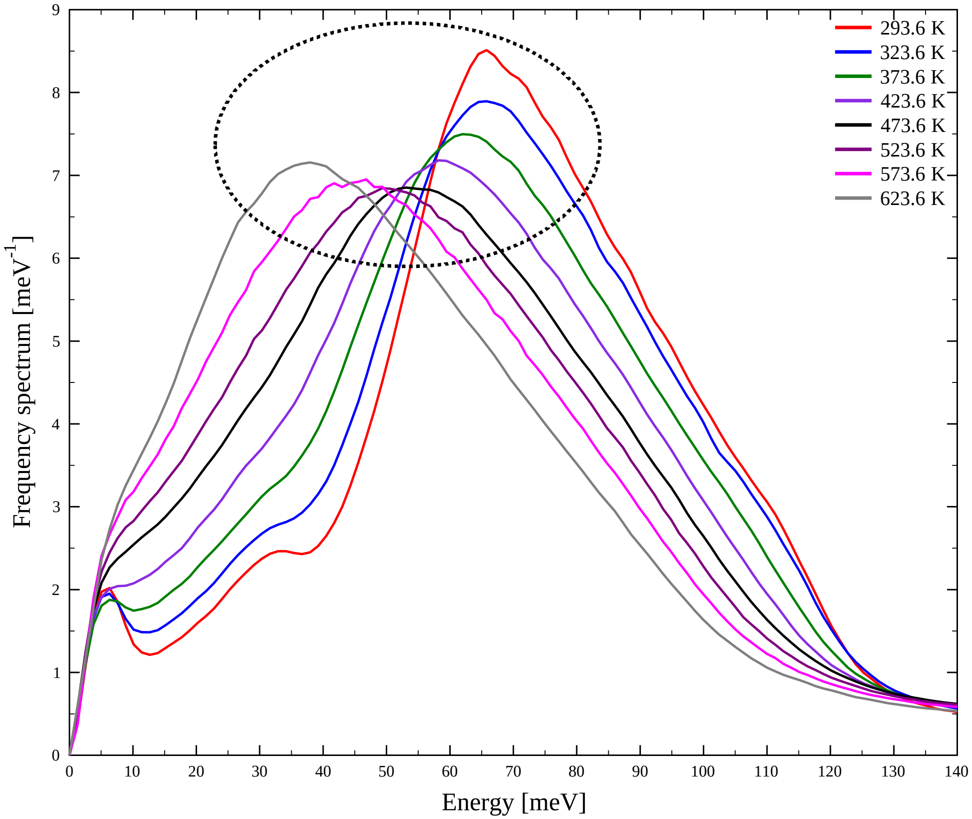
Discussion

Based on TOF Experiments





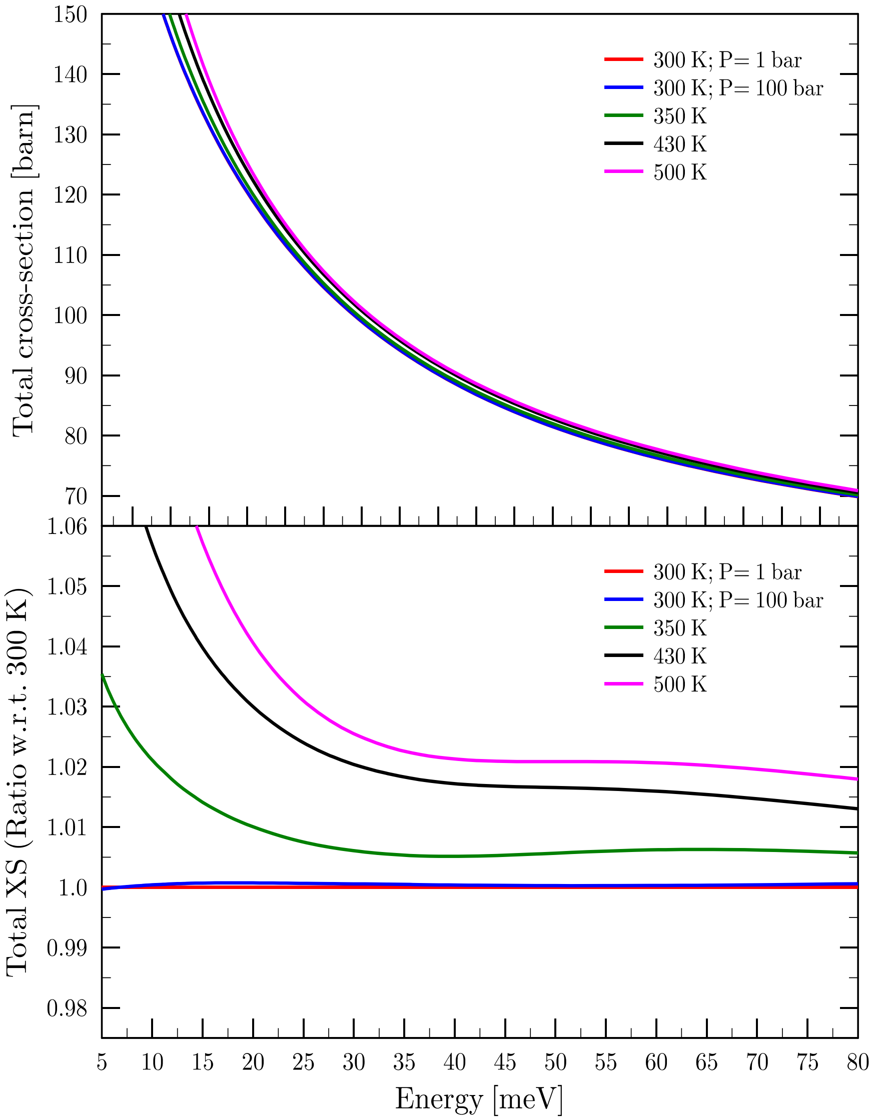
Based on MD simulations



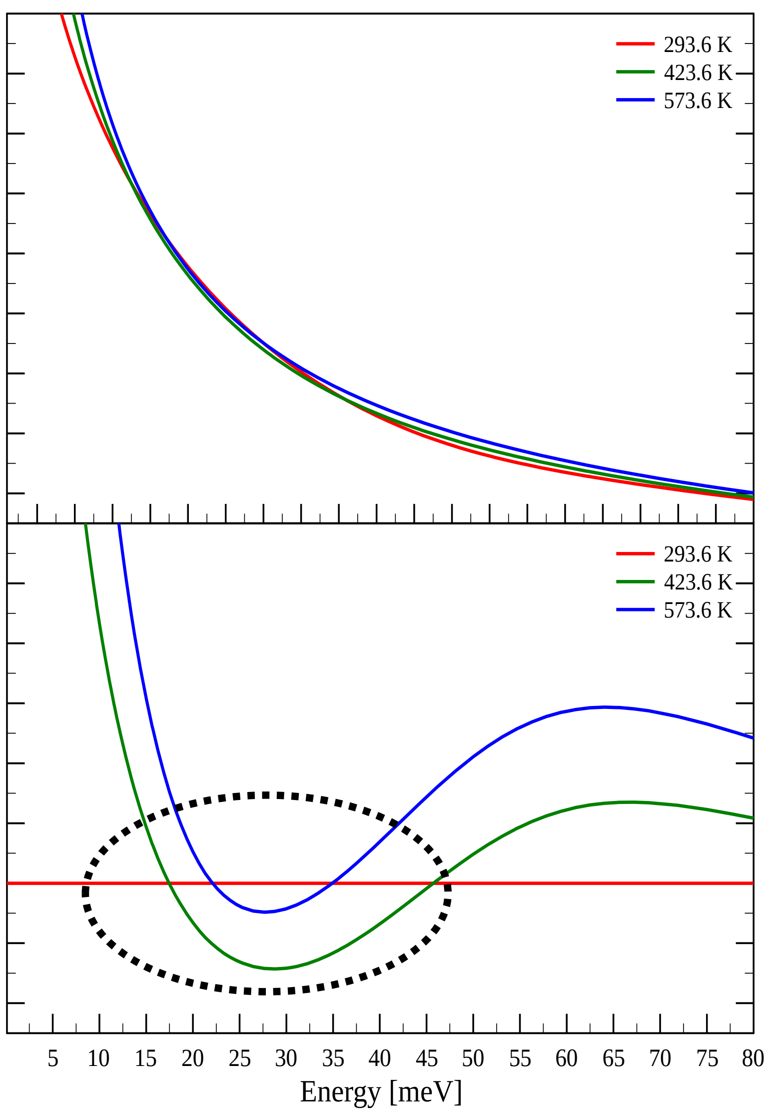
Behavior of water potentials at high temperature ??

Comparison of total cross-section: CAB model & ILL data

IRSN-lib (ILL data)(Preliminary)



ENDF/B-VIII.b5 (CAB Model)



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Conclusions

- Measurement of the dynamic structure factor and hence the frequency spectrum of light water at several high temperatures and pressures were carried out at ILL.

- We observed some discrepancies in the shape of the frequency spectrum obtained from the experiments and those utilized by the CAB model based on classical MD simulations with TIP4P/2005f flexible water potential.

- Choosing a water potential without testing its limitations is not a viable option for the reactor physics community.

- Using a water potential for reactor physics applications implies its test for all the thermodynamic properties of water at the required temperatures and pressures, failure to do so would lead to misleading results and conclusions.

Hey, I have a question.. !

Yes! Go ahead!!
Will be happy to answer