Deuterated Clathrate Hydrates as Novel Moderator Material for a Source of Very Cold Neutrons

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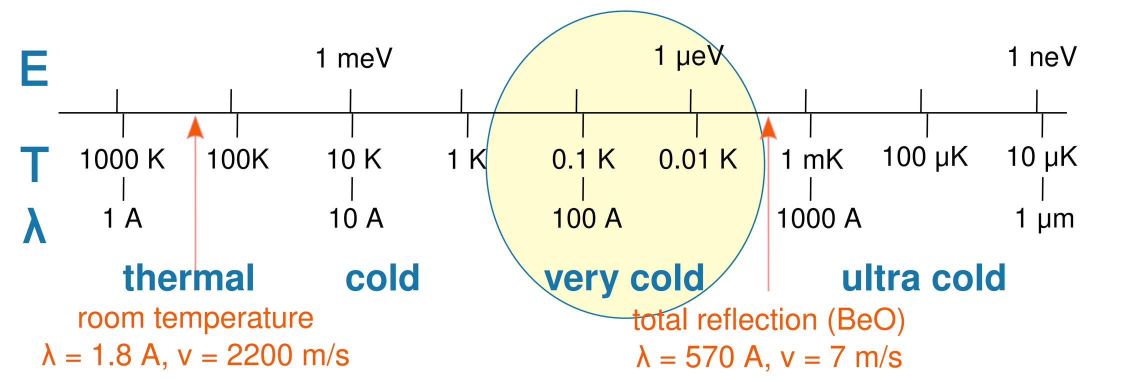
A Case for VCN

- Intense sources of Very Cold Neutrons (**VCN**) could be a game changer for neutron **scattering techniques** and **fundamental physics** research with neutrons
- VCNs increase the instrumental **resolution** at **fixed geometry**, and the **intensity** at a **fixed resolution** [a]
- Particle-physics experiments take advantage of higher VCN fluxes:
  - → search for neutron anti-neutron oscillations (**nnbar**)
    Figure of merit: FOM $\propto \lambda^2$ [b]
  - → In-beam neutron (**EDM**) search [c]
  - → In-beam **UCN sources**
  - → Experimental search for new fundamental forces [d]



- Feasibility study of a dedicated **VCN moderator** at the ESS
  - → HighNESS project [e]
- Deuterated **Clathrate Hydrates** are a promising candidate

[a] J. M. Carpenter and B. J. Micklich, Proceedings (2005)
[b] D.G. Phillips et al., Phys. Rep. V. 612, p. 1-45 (2016)
[c] F. M. Piegsa, Phys. Rev. Lett., 108.181801 (2012)
[d] F. M. Piegsa, American Phys. Soc., 88.045502 (2013)
[e] V. Santoro et al., arXiv:2204.04051v1 (2022).

Scattering Function $S(q,\omega)$

- Scattered intensity is measured as a function of both wave-vector transfer q and energy transfer $\hbar\omega$
- Slices of $S(q,\omega)$ along q and ω contain information about the structure and dynamics of the material

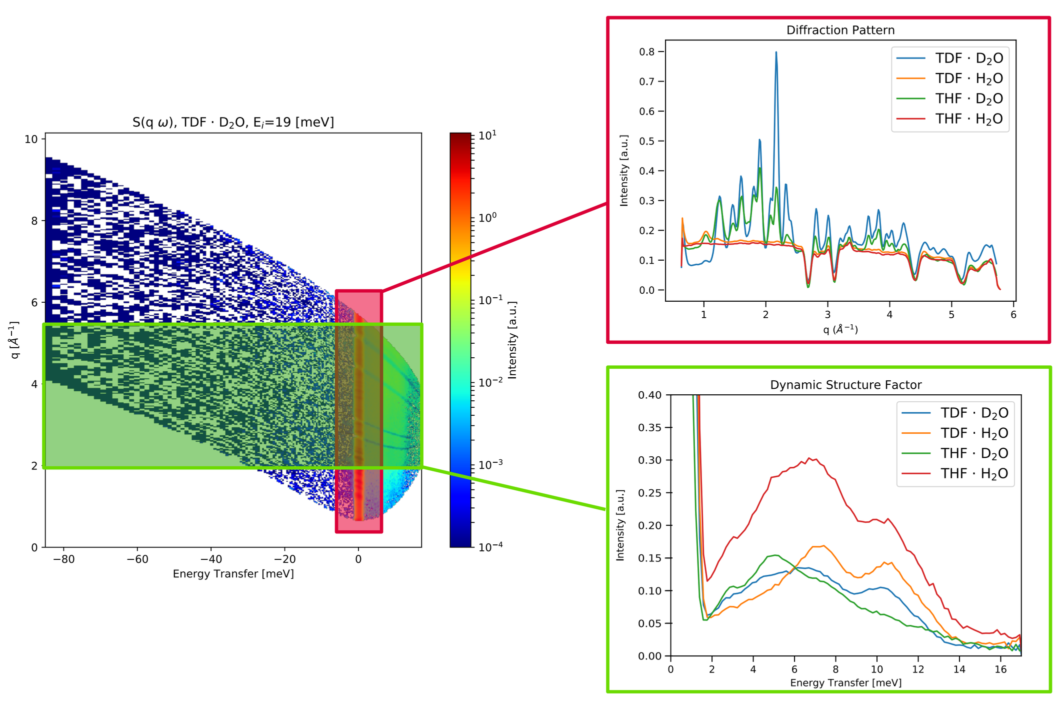


Fig. 1: $17D_2O \cdot TDF$ measured on Panther

Acknowledgements

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Clathrate Hydrates

- Inclusion compounds that are able to host guest molecules in cages that are formed by networks of hydrogen-bonded water molecules
- Unusually-large crystalline structures: → large **Bragg cut-off** wavelengths λ
  → **high albedo** for the whole cold neutron-range
- Stable up to high temperatures (gas hydrates: ∼140 K, THF hydrates: ∼280 K)

	Clathrate I	**Clathrate II**
Structure	cubic	fc cubic
Unit cell (UC)	a = 12.03 Å	a = 17.31 Å
Space group	$Fd\bar{3}m$	$Pm\bar{3}n$
# H_2O per UC	46	136
Cages per UC	6 L + 2 S	8 L +16 S
Bragg cut-off λ	24 Å	20 Å
Guest molecules e.g.	CH_4, H_2, O_2	O_2 + C_4H_8O (THF)

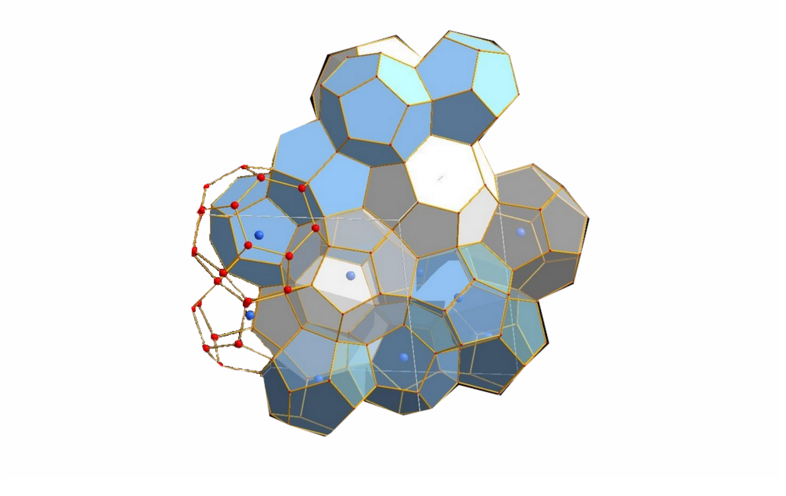

Fig. 2: C-II clathrate hydrate

VCN Transmission Experiments

- Study of reflectivity and transmittivity in the cold and VCN range for fully deuterated samples
- ToF setup on ILL's PF2-VCN beam (results below)
  → Reiteration after the upgrade
- Further experiments are to be conducted on beams of cold neutrons (ILL-PF1B and PSI-BOA)

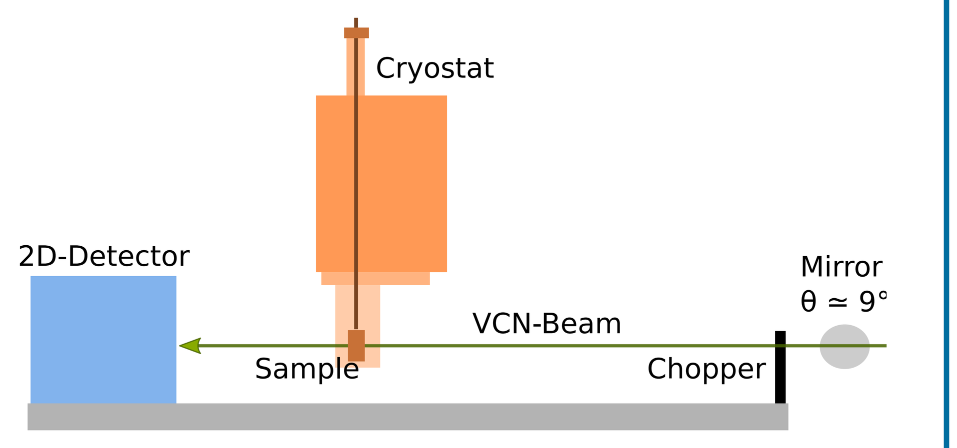

Fig. 3: Experimental Layout PF2-VCN

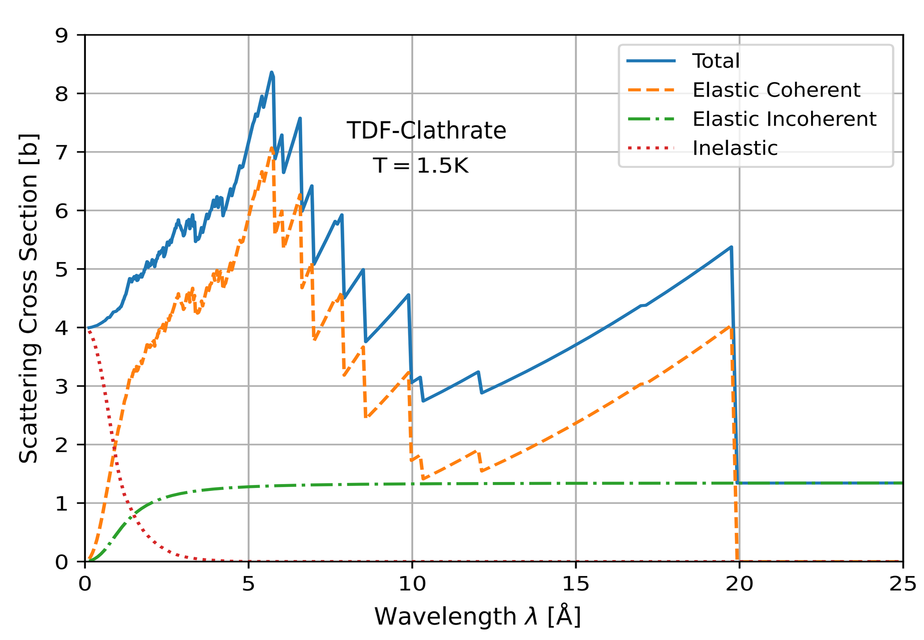

Fig. 4: Computed cross section of TDF-Clathrate (by Sara Isaline Laporte (MIB) & Shuqi Yvan Xu (ESS))

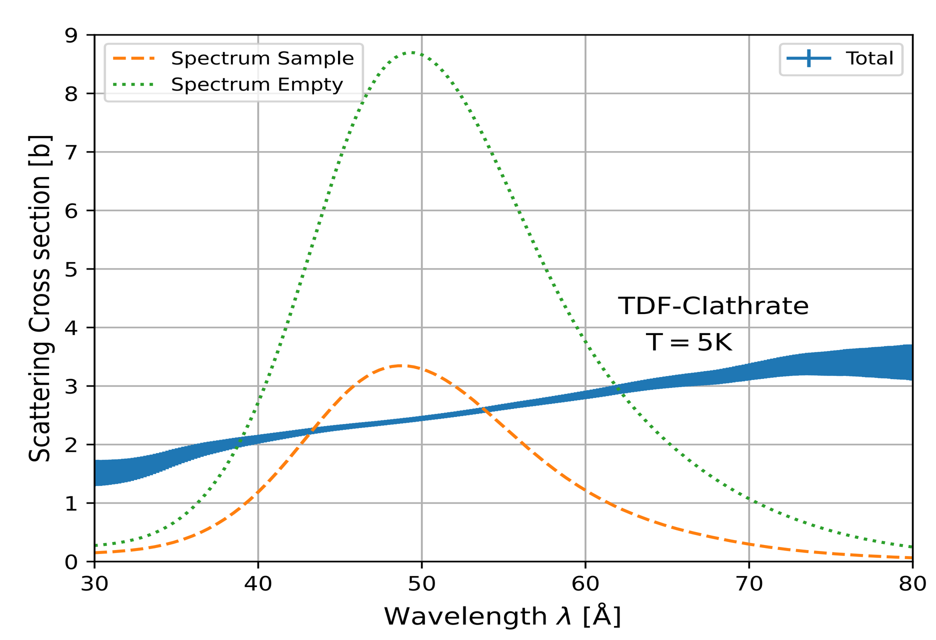

Fig. 5: Preliminary experimental results of the total cross section on PF2-VCN

Time of Flight Spectroscopy on Panther & IN5

- Incident beam properties:
  IN5: 2 Å (E_i = 19 meV), 3 Å (E_i = 9 meV)
  Panther: 1 Å (E_i = 76 meV), 2 Å (E_i = 19 meV)
- Contrast variation – protonated & deuterated sample variants: $17D_2O \cdot TDF$, $17H_2O \cdot TDF$, $17D_2O \cdot THF$, $17H_2O \cdot THF$
- Vanadium samples (normalization to absolute units)
- Data from the neutron **scattering function** $S(q,\omega)$ serve as a benchmark for new scattering kernels in **NCrystal** and MD-Simulations

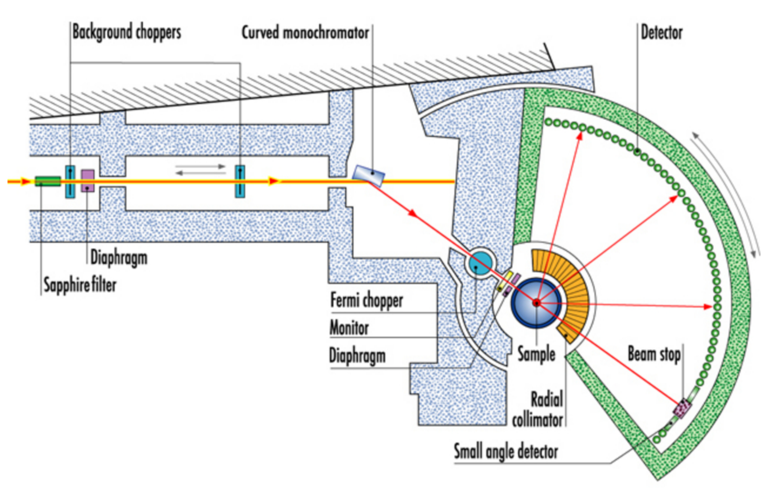

Fig. 6: Instrument-Layout: Panther

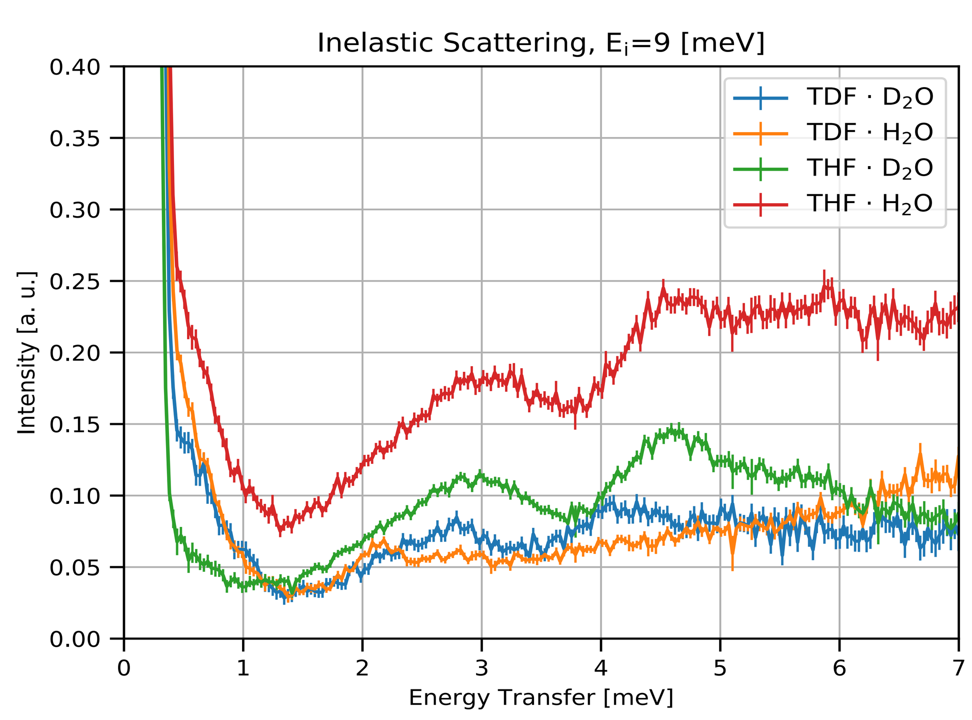

Fig. 7: E_i = 9 meV, T = 1.5K, **IN5**

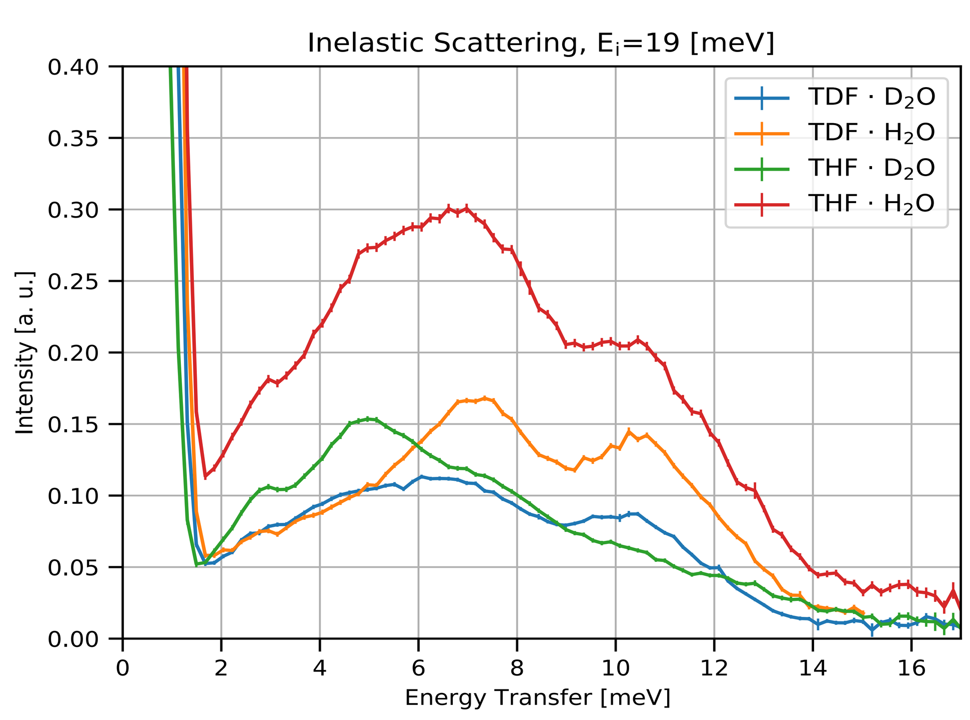

Fig. 8: E_i = 19 meV, T = 1.5K, **Panther**