



Contribution ID: 14

Type: not specified

Inelastic Neutron Scattering Measurements of Clathrate Hydrates for the HighNESS Project

Tuesday, 19 October 2021 17:30 (10 minutes)

Clathrate hydrates are crystalline water-based solids (similar to ice), which form cages that are able to host guest molecules. The guests are trapped in cavities of the hosts, that are composed of hydrogen-bonded water molecules. Tetrahydrofuran (THF) clathrate hydrates (fully or partially deuterated) seem particularly well suited as a moderation medium for neutron, as they possess low-energy modes with sufficiently large inelastic neutron scattering cross sections [1].

Since THF only occupies the large cages in the clathrate structure, the twice more abundant smaller cages can still be filled with other molecules. This allows a binary clathrate, consisting of two guest molecules within the water structure to be constituted [2]. Of particular interest is oxygen as a second guest molecule. It offers an additional path for moderation via a cooling cascade mechanism that exploits the zero-field splitting of the magnetic triplet ground state of molecular oxygen [3].

In the context of the European project HighNESS [4, 5], whose main mission is the “Development of an High Intensity Neutron Sources at the European Spallation Source (ESS)”, we present the first results of measurements of the neutron scattering function $S(q, \omega)$ for clathrate hydrates in absolute units. Both the simple and the binary structure are investigated on the time-of-flight (TOF) spectrometer Panther and IN5 at the ILL. The results include measurements with neutron-wavelengths from 0,1 nm to 0,3 nm, for fully and partially deuterated clathrate samples. With this variation contrast we show the contribution of the different constituents.

References

- [1] H Conrad, W. F Kuhs, K N`unighoff, C Pohl, M Prager, and W Schweika. Inelastic scattering and spectral measurements of advanced cold moderator media. *Physica B: Condensed Matter*, 350(1, Supplement):E647–E650, July 2004.
- [2] Hongjun Yang, Shuanshi Fan, Xuemei Lang, and Yanhong Wang. Phase equilibria of mixed gas hydrates of oxygen + tetrahydrofuran, nitrogen + tetrahydrofuran, and air + tetrahydrofuran. *Journal of Chemical & Engineering Data*, 56, 10 2011.
- [3] Oliver Zimmer. Neutron conversion and cascaded cooling in paramagnetic systems for a high-flux source of very cold neutrons. *Physical Review C*, 93(3):035503, March 2016. Publisher: American Physical Society.
- [4] HighNESS. Project Description. <https://highnessproject.eu/mission-and-objectives/>, 2020. [Online].
- [5] V Santoro, KH Andersen, DD DiJulio, Esben Bryndt Klinkby, TM Miller, David Milstead, G Muhrer, M Strobl, A Takibayev, L Zanini, et al. Development of high intensity neutron source at the European Spallation Source. *Journal of Neutron Research*, (Preprint):1–11, 2020.

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Session Classification: Poster session