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Inelastic Neutron Scattering Measurements of ClathrateHydrates for the HighNESS Project

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Clathrate hydrates are 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

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