



	Experiment title: Hydrate formation studied by x-ray Raman scattering	Experiment number: HD-296
Beamline: ID16	Date of experiment: from: 29/10/2008 to: 03/11/2008	Date of report: 09/02/2010
Shifts: 15	Local contact(s): Dr. Laura Simonelli	<i>Received at ESRF:</i>
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Report:

The results of the beam time are published in:

(1) H. Conrad, F. Lehmkuhler, C. Sternemann, A. Sakko, D. Paschek, L. Simonelli, S. Huotari, O. Feroughi, M. Tolan, and K. Hämäläinen, Phys. Rev. Lett. **103**, 218301 (2009).

Abstract:

We report on the formation of tetrahydrofuran clathrate hydrate studied by x-ray Raman scattering measurements at the oxygen K edge. A comparison of x-ray Raman spectra measured from water-tetrahydrofuran mixtures and tetrahydrofuran hydrate at different temperatures supports stochastic hydrate formation models rather than models assuming hydrate precursors. This is confirmed by molecular dynamics simulations and density functional theory calculations of x-ray Raman spectra. In addition, changes in the spectra of tetrahydrofuran hydrate with temperatures close to the hydrate's dissociation temperature were observed and may be connected to changes in hydrate's local structure due to the formation of hydrogen bonds between guest and water molecules.

(2) H. Conrad, F. Lehmkuhler, C. Sternemann, O. Feroughi, L. Simonelli, S. Huotari, and M. Tolan, Rev. Sci. Instrum. **80**, 026103 (2009).

Abstract:

We present a new sample cell for measuring nonresonant inelastic x-ray scattering spectra of a tetrahydrofuran THF -water liquid mixture and THF hydrate. The hydrate is formed inside the cell after nucleation seeds have been offered by a special magnetic stirring mechanism. Hydrate formation was verified by wide angle x-ray scattering and nonresonant x-ray Raman

scattering spectra at the oxygen K-edge. A broad range of scattering angles can be studied with this cell which is necessary for momentum transfer dependent inelastic x-ray scattering. This cell is ideal to examine other liquid hydrate formers or other liquid samples, which have to be mixed in situ during the measurements.