



	<b>Experiment title:</b> Structural changes and	<b>Experiment number:</b> HD-396
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<b>Shifts:</b> 18	<b>Local contact(s):</b> Dr. L. Simonelli	<i>Received at ESRF:</i>
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## Report:

Parts of this experiment have been published in:

F. Lehmkuhler, A. Sakko, I. Steinke, C. Sternemann, M. Hakala, Ch.J. Sahle, T. Buslaps, L. Simonelli, S. Galambosi, M. Paulus, T. Pylkkänen, M. Tolan, and K. Hämäläinen, Temperature induced structural changes of tetrahydrofuran clathrate and of the liquid water/tetrahydrofuran mixture, *Journal of Physical Chemistry C* **115**, 21009 (2011).

**Abstract:** We present two complementary inelastic X-ray scattering studies on the structure of tetrahydrofuran (THF) clathrate hydrate and the supercooled stoichiometric liquid mixture of water and THF. Compton scattering experiments of the liquid mixture show that formation of hydrate precursors is unlikely. By comparing experimental spectra of THF hydrate and water/THF mixtures at temperatures above 250 K with density functional theory calculations, structural changes that manifest in OH bond length changes are observed. X-ray Raman scattering measurements of the oxygen K-edge in the same temperature range corroborate these results. The experimental results of THF hydrate at temperatures between 20 and 244 K can be modeled best by assuming thermal expansion only. Therefore, dependency on the system's temperature different structural behavior of THF hydrate is reported.