



	<b>Experiment title:</b> Compton scattering of gas hydrates	<b>Experiment number:</b> HE-1366
<b>Beamline:</b>	<b>Date of experiment:</b> from: 13.11.2002 to:19.11.2002	<b>Date of report:</b> 07.09.2006
<b>Shifts:</b>	<b>Local contact(s):</b> N. Hiraoka and T. Buslaps	<i>Received at ESRF:</i>
<b>Names and affiliations of applicants</b> (* indicates experimentalists): C. Sternemann, M. Paulus, C. Gutt Department of Physics, University of Dortmund, D-44221 Dortmund, Germany J. S. Tse Stacie Institute for Molecular Science, National Research Council of Canada, Ottawa, Ontario, Canada K1A OR6 S. Huotari Division of X-ray Physics, Department of Physical Sciences, University of Helsinki, P.O. Box 64, FIN-00014 University of Helsinki, Finland		

## Report:

The results of this experiment have been published as:

C. Sternemann, S. Huotari, M. Hakala, M. Paulus, M. Volmer, C. Gutt, T. Buslaps, N. Hiraoka, D. D. Klug, K. Hämäläinen, M. Tolan, J. S. Tse, *Electronic structure of methane hydrate studied by Compton scattering*, Phys. Rev. B **73**, 195104 (2006)

## Abstract:

High-resolution Compton scattering spectra of methane, methane hydrate, and ice were measured using incident photon energy of 56.4 keV at beamline ID15B of the European Synchrotron Radiation Facility. The experimental Compton profiles are compared to calculations employing density-functional theory using model atomic clusters. The hydrate has a cagelike structure built up from water molecules and the related Compton profile is observed to change apparently when compared to hexagonal ice. Furthermore, the influence of the guest-host interactions between the methane molecules and the water molecules of the cages on the Compton profile is discussed.