

**Experiment title:**

Ba<sub>8</sub>Si<sub>46</sub> and Si under high pressure studied with non-resonant x-ray Raman scattering

**Experiment number:**  
HE-3157

**Beamline:**

ID16

**Date of experiment:**

from: 14.04.2010 to: 20.04.2010

**Date of report:**

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**Shifts:**

18

**Local contact(s):**

Dr. V. Giordano

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**Names and affiliations of applicants (\* indicates experimentalists):**

C. Sternemann\*, A. Nyrow,\* Ch.J. Sahle\*

Fakultät Physik/DELTA, Technische Universität Dortmund, D-44221 Dortmund, Germany

J.S. Tse\*

Department of Physics, University of Saskatchewan, Saskatoon, Canada

**Report:**

Parts of this experiment have been published in:

J.S. Tse, L. Yang, S.J. Zhang, C.Q. Jin, Ch.J. Sahle, C. Sternemann, A. Nyrow, V. Giordano, J.Z. Jiang, S. Yamanaka, S. Desgreniers, and C.A. Tulk, Pressure-induced electron topological transitions in Ba-doped Si clathrate, *Physical Review B* **84**, 184105 (2011).

Abstract: Ba(8)Si(46) is the archetype of the Si clathrates family. X-ray diffractions have revealed an unusual homothetic isostructural transition at similar to 14-16 GPa. Raman experiments, however, suggested even more transitions at lower pressure. We present evidence showing that successive electronic topological transitions are responsible for the transformations. It is shown that the electronic structure of Ba(8)Si(46) is easily perturbed by the environment. Reverse Monte Carlo calculations and in-situ resistivity measurements revealed continual changes in the structure and electrical properties upon compression. This finding is corroborated by results of x-ray Raman scattering study in the vicinity of the Ba N(4,5) and Si L(2,3) absorption edges.