

Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office using the **Electronic Report Submission Application:**

<http://193.49.43.2:8080/smis/servlet/UserUtils?start>

Reports supporting requests for additional beam time

Reports can now be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

**Experiment title:**

Compton scattering of semiconductor clathrates

Experiment number:

HE-1365

Beamline:**Date of experiment:**

from: 05.02.2003 to: 11.02.2003

Date of report:**Shifts:****Local contact(s):****N. Hiraoka, T. Buslaps***Received at ESRF:***Names and affiliations of applicants** (* indicates experimentalists):

C. Sternemann*, M. Volmer*, M. Paulus*

Fakultät Physik/DELTA, Technische Universität Dortmund, Germany

J.S. Tse, D.D. Klug

Stacie Institute of Molecular Science, NRCC, Ottawa, Canada K1A 0R6

P.F. McMillan

Department of Chemistry, University College London, London, UK

C.Bull

Davy Faraday Research Laboratories, London, England

Report:

The results of this experiment have been published as:

M. Volmer, C. Sternemann, J.S. Tse, T. Buslaps, N. Hiraoka, C. L. Bull, J. Gryko, P.F. McMillan, M. Paulus, and M. Tolan, *Charge transfer in silicon clathrates studied by Compton scattering*, Phys. Rev. B **76**, 233104 (2007)

High-resolution Compton profiles of the clathrates $\text{Na}_8\text{Si}_{46}$, $\text{K}_{7.6}\text{Si}_{46}$, and Si_{136} were measured to study the charge transfer of the alkali-metal guest atoms to the clathrates silicon host lattice. The experiment was accomplished utilizing the Compton spectrometer at beamline ID15B of the European Synchrotron Radiation Facility with an incident energy of 56.7 keV and a momentum space resolution of 0.16 a.u. The valence electron contribution to the total Compton profile of the sodium and potassium guest atoms was extracted and is compared with calculations employing density-functional theory using Becke exchange and Perdew-Wang correlation. Good overall agreement between experiment and theory is found and proves the quality of the underlying wave functions used for the theoretical predictions. On this basis, the charge transfer in these systems is estimated by a Mulliken population analysis and discussed for the different guest atoms.