



## 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.



	<b>Experiment title:</b> Structural behavior under pressure of MX <sub>2</sub> compounds with molecular-like X <sub>2</sub> dumbbells (X=C, N, or O)	<b>Experiment number:</b> HS 3933
<b>Beamline:</b>	<b>Date of experiment:</b> from: 13 Nov 2009 to: 17 Nov 2009	<b>Date of report:</b> 30 Aug. 2010
<b>Shifts:</b>	<b>Local contact(s):</b> M. Hanfland	<i>Received at ESRF:</i> 30 Aug. 2010
<b>Names and affiliations of applicants</b> (* indicates experimentalists):  K. Syassen G. Vazhenin (G. Vajenine) I. Efthimiopoulos		

## Report:

A manuscript on BaO<sub>2</sub> under pressure has been submitted to Physical Review B on 28 July 2010. The abstract is shown below. Two more manuscripts on the structural properties of LaC<sub>2</sub> and BaC<sub>2</sub> under pressure are getting close to be submitted. Their abstracts will be posted separately.

## Structural transformation and vibrational properties of BaO<sub>2</sub> at high pressure

I. Efthimiopoulos,<sup>1</sup> K. Kunc,<sup>1, \*</sup> S. Karmakar,<sup>1</sup> K. Syassen,<sup>1</sup> M. Hanfland,<sup>2</sup> and G. Vajenine<sup>1, 3, y</sup>

<sup>1</sup>Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

<sup>2</sup>European Synchrotron Radiation Facility, F-38043 Grenoble, France

<sup>3</sup>Institut fuer Anorganische Chemie, Universitaet Stuttgart, Pfaffenwaldring 55, D-70569 Stuttgart, Germany

(Dated: July 24, 2010)

The tetragonal ambient-pressure phase of BaO<sub>2</sub> (CaC<sub>2</sub>-type, space group I 4/mmm) with sixfold coordination of Ba atoms and O<sub>2</sub> dumbbells was found to transform reversibly to an orthorhombic modification (space group Cmmm) near 33 GPa. The eight-coordinated high-pressure phase represents a new structure type. It is related to the CsCl-type structure, but can also be viewed as a distorted variant of the hexagonal AlB<sub>2</sub> type, suggesting possible polymerization of the isolated O<sub>2</sub> dumbbells to a 2D network at higher pressure. In addition to in situ x-ray diffraction, Raman measurements were performed to study the lattice dynamics of the BaO<sub>2</sub> phases under pressure. The experimental observations are compared to the results of ab initio calculations of the structural stability and dynamical properties. Raman spectra of barium monoxide BaO are reported in an Appendix; these results were found useful for the interpretation of the Raman scattering of BaO<sub>2</sub>.

PACS numbers: 62.50.-p, 64.70.kp, 71.15.Nc, 78.30.Am



