EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

ESRF

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.

ESRF	**Experiment title:** High P-T X-Ray Diffraction of Polymeric CO2 under Hydrostatic Conditions	**Experiment number**: HS-4211
Beamline:	**Date of experiment**: from: 31/05/2011 to: 04/06/2011	**Date of report**: 24/04/2012
Shifts:	**Local contact(s)**: A. Salamat	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

F. Datchi, B. Mallick and S. Ninet

IMPMC, UPMC and CNRS, 4 place Jussieu, 75252 Cedex 05

Report:

The results of this experiment have been published in the following journal article:

F. Datchi, B. Mallick, A. Salamat and S. Ninet. Structure of polymeric carbon dioxide (CO_2-V). *Phys. Rev. Lett.* **108**, 125701 (2012)

Abstract :

The structure of polymeric carbon dioxide (CO2-V) has been solved using synchrotron x-ray powder diffraction, and its evolution followed from 8 to 65 GPa.We compare the experimental results obtained for a 100% CO2 sample and a 1 mol% CO2=He sample. The latter allows us to produce the polymer in a pure form and study its compressibility under hydrostatic conditions. The high quality of the x-ray data enables us to solve the structure directly from experiments. The latter is isomorphic to the β-cristobalite phase of SiO2 with the space group I -42d. Carbon and oxygen atoms are arranged in CO4 tetrahedral units linked by oxygen atoms at the corners. The bulk modulus determined under hydrostatic conditions, B0= 136(10) GPa, is much smaller than previously reported. The comparison of our experimental findings with theoretical calculations performed in the present and previous studies shows that density functional theory very well describes polymeric CO2.