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 via the User Portal:

https://wwws.esrf.fr/misapps/SMISWebClient/protected/welcome.do

Reports supporting requests for additional beam time

Reports can 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:** Combined effects of pressure and temperature on thaumasite: implications for six-fold silicon coordination and degradation of Portland cements	**Experiment number**: **CH- 3499**
Beamline: ID27	**Date of experiment**: from: 30 May 2012 to: 02 June 2012	**Date of report**: 27 February 2015
Shifts: 9	**Local contact(s)**: Gaston GARBARINO	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

*CRUCIANI Giuseppe – University of Ferrara, Dep of Physics and Earth Sciences

ARDIT Matteo – University of Ferrara, Dep of Physics and Earth Sciences

*DONDI Michele – CNR-ISTEC, Faenza

ZANELLI Chiara – CNR-ISTEC, Faenza

Report:

Published paper:
Title: Phase transitions during compression of thaumasite, $Ca_3Si(OH)_6(CO_3)(SO_4)\cdot 12H_2O$: A high-pressure synchrotron powder X-ray diffraction study
Authors: Ardit M., Cruciani G., Dondi M., Garbarino G.L., Nestola F.
Journal: Mineralogical Magazine, vol.78, p.1193-1208, 2014
DOI: http://dx.doi.org/10.1180/minmag.2014.078.5.07

Abstract:
The high-pressure behaviour of the thaumasite structure was investigated using synchrotron powder X-ray diffraction, up to 19.5 GPa. Based on Rietveld refinements, thaumasite retained the room-pressure $P6_3$ space group throughout the whole investigated pressure range while the pressure dependence of the refined unit-cell parameters can be cast into three different compression regimes, each corresponding to a different thaumasite phase (th-I, th-II and th-III) related by isosymmetric phase transitions. In particular, the phase transition in the 7.40 – 15.02 GPa P-range (i.e.from th-II to th-III) is associated with an inversion of the axial bulk moduli which, by analogy with ettringite, can be rationalized as due to a change in the relative strengths of the iono-covalent bonds along the $[Ca_3Si(OH)_6(H^2O)_{12}]^{4+}$ columns parallel to the c axis vs. the O– H bonds linking the columns within the ab plane. The linear inverse relationship between the low- and high-temperature data from the literature with those collected under high-pressure conditions reveals that the same bonding regime governs the anisotropic expansion and contraction of thaumasite up to ~1.4 GPa and 400 K (*HP-HT* stability limits of th-I phase).