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:** DECIPEHRING THE ROLE OF HALOGEN INTERACTIONS IN THE MULTICOLOR THERMOCHROMISM BY COORDINATION ISOMERISM OF XNMCLM COMPLEXES: A COMPLEX INORGANIC ALL-SOLID-STATE EQUILIBRIUM	**Experiment number**: **CH- 3887**
Beamline: ID31	**Date of experiment**: from: 05 December 2013 to: 09 December 2013	**Date of report**: 14 February 2014
Shifts: 8	**Local contact(s)**: Yves Watier	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Runchevski Tomche* – Max Planck Institute for Solid State Research

Robert E. Dinnebier – Max Planck Institute for Solid State Research

Report:

The decision on this proposal stated that it was well received but there was insufficient beam time available for allocation in this round. To our great pleasure, beamtime was awarded to us at the end of round. Unfortunately, the thermochromic samples need several Months prior experiments to be prepared, and they are not stable for long period. Therefore, only part of the samples proposed were studied.

The rest of the beamtime was used for studying similar thermochromic metal organic sample, with the accent on its remarkable property of self-actuation or exhibiting the thermosalient (TS) phenomenon - an extremely rare propensity of certain crystalline solids for self-actuation by elastic deformation or by a ballistic event.

With (phenylazophenyl)palladium hexafluoroacetylacetonate, we obtained a direct evidence for the driving force behind this impressive crystal motility. PHA crystals can switch between five crystal structures that are related by four phase transitions including one TS transition. Upon these phase transitions the single crystals do not survive, and they get disintegrated in powder samples. Therefore, powder X-ray diffraction using synchrotron radiation is the perfect method of choice for profound structural studies. The collected data, in addition, confirmed that the mechanical effect is driven by a remarkable uniaxial negative expansion compensated by exorbitantly large positive axial expansion ($> 100 \times 10^{-6}$ K^{-1}), with volumetric expansion coefficients ($\approx 250 \times 10^{-6}$ K^{-1}) that are among the highest values reported in molecular solids thus far.