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:** Crystal structure determination of the complex metallic compounds XPt$_3$Be$_6$ (X = Th, U, La)	**Experiment number**: HC-3331
Beamline: BM20	**Date of experiment**: from: Nov. 3, 2017 to: Nov. 7, 2017	**Date of report**: 27.07.2018
Shifts: 12	**Local contact(s)**: Christoph Hennig	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

High resolution powder X-ray diffraction patterns of the ternary X-Pt-Be phases have been successfully recorded at the BM20 Rossendorf beamline with a wavelength of λ = 0.459317(1) Å. The diffractograms of X = Th, U, La could be indexed with a body-centered cubic unit cell with the lattice parameters $a \approx 13.70$ Å (T = 300 K). On cooling the lattice parameters showed a continuous decrease by about 1 % for T = 140 K, respectively, with no indication of a phase transition in this temperature range (Figure 1).
The data were indexed as a cubic body-centered unit cell and used to solve the crystal structure in the cubic space group $I\bar{4}3d$ and refine the structure model. The high quality data enabled the localization of the light Be atoms next to the heavy atoms. The final structure model agreed nicely with the experimental powder pattern (Figure 2). The isostructural compounds constitute new complex intermetallic compounds with over 200 atoms per unit cell (Figure 3). The obtained structural data will enable a deeper understanding of the physical properties and serve as input to calculate the electronic structure of these compounds.

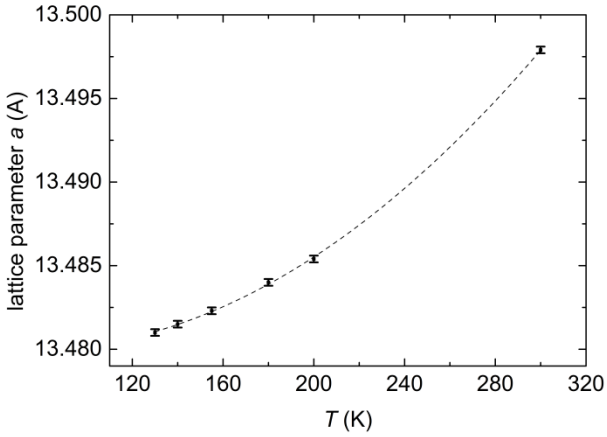

Figure 1. Lattice parameter *a* of the U compound as a function of temperature. The dashed line serves as a guide to the eye.

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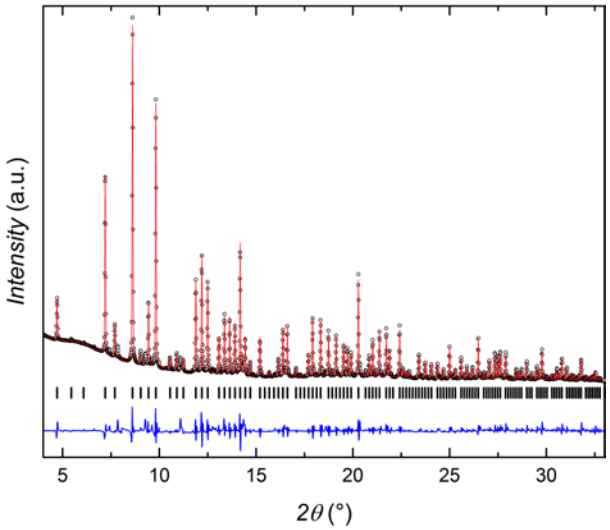

Figure 2. Synchrotron powder diffraction pattern of the La compound recorded at BM20. Measured data points pattern (black circles), calculated pattern (red line), difference (blue line) and indexation in $I\bar{4}3d$ (black ticks).

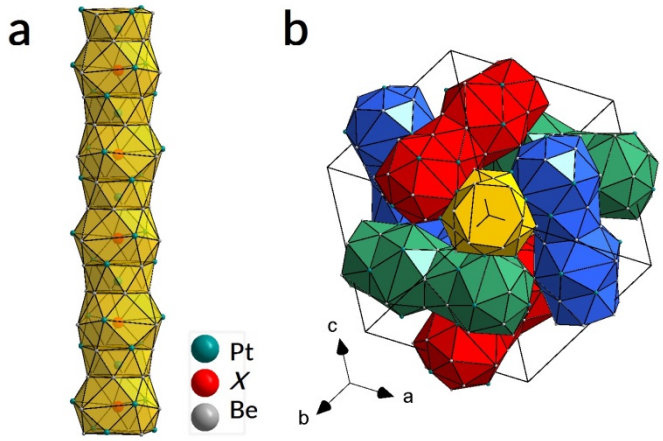

Figure 3. Exemplary crystal structure . (a) Pt and Be atoms form channels around a chain of alternating *X* and Pt atoms. (b) The channels form a cubic rod packing in the unit cell.