



	<b>Experiment title:</b> High-pressure structural transition in heavy fermion superconductor anti-perovskites CeSiPt <sub>3</sub> and YBPt <sub>3</sub>	<b>Experiment number:</b> HC-2482
<b>Beamline:</b> ID27	<b>Date of experiment:</b> from: 03/03/2016 to: 06/03/2016	<b>Date of report:</b>  <i>Received at ESRF:</i>
<b>Shifts:</b> 9	<b>Local contact(s):</b> Volodymyr Svitlyk	
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## Report:

Anti-perovskites of AXB<sub>3</sub> stoichiometry with A = early period cation, X = group 13-15 anion and B = transition metal have in recent years been found to host as many interesting physical and structural properties as the vast perovskite family. While the anti-perovskites are much less common than their normal counterparts, they display superconductivity in the presence of ferromagnetic ions[1], topologically insulating states[2] and heavy fermion superconductivity[3].

The goal for this beamtime was to study the high pressure transition in the anti-perovskite compound YBPt<sub>3</sub>, which were identified at an earlier preliminary high pressure screening, using X-ray powder diffraction. We also investigated the pressure behaviour of the isostructural compounds YSiPt<sub>3</sub> and CeBPt<sub>3</sub>.

During the experiment on ID27 we verified the transition on YBPt<sub>3</sub> by compressing the compound to 32 GPa. The diffraction data obtained during both compression and decompression can be seen in Figure 1. As the pressure increases, a sudden splitting of several peaks appears at after 20.9 GPa. The splitting is most pronounced for the {h00} reflection family such as the 200 reflection at  $2\theta = 7^\circ$ . Following this, new strong peaks grow in intensity, while most of the original peaks retain their original intensity. The corresponding data obtained upon the slow decompression of the sample

essentially mirrors the compression data, with the intensity of the new peaks decreasing rapidly as pressure is released, combined with a merging of peaks related to the  $a$  and  $b$  axes of the  $P4mm$  crystal structure. The new peaks completely disappear at a pressure between 19.8 and 17.6 GPa.

Two complimentary approaches were used to predict the possible structure of  $YBPt_3$  above the phase transition pressure. The structure of the new phase have been solved and the result will be included in a future publication.

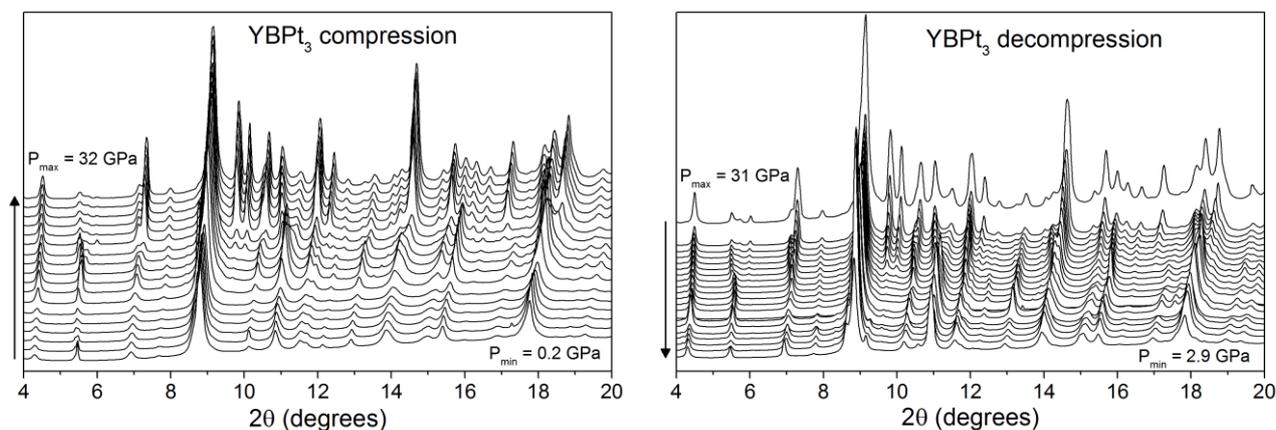


Figure 1: Left: Diffraction data obtained on  $YBPt_3$  upon compression from 0.2 GPa to 32 GPa, displaced with increasing pressure (not to scale). Phase transition onset is marked by a series of peaks splitting (5.5, 7.0, 11, 14.3 and 18.5°), followed by the slow growth of new peaks, especially noticeable near 10°. Right: Diffraction data obtained during decompression of the same sample down to 2.9 GPa. Note the similarity to the compression data, indicating the reversibility of the phase transition.

It is interesting that pressure drives further structural distortion in this anti-perovskite system, compared for instance to the regular non-centrosymmetric perovskite  $PbVO_3$ , which also displays the  $P4mm$  structure with similar  $c/a$  ratio at ambient pressure, but undergoes a first-order transition at  $\sim 3$  GPa with a large volume collapse (10.6%) to the ideal cubic  $Pm-3m$  perovskite structure[4].

We also measured diffraction data on  $CeSiPt_3$  and  $CeBPt_3$  to even higher pressures (45 and 34 GPa respectively), but did not observe any phase transitions in either compound. This is somewhat puzzling, especially for  $CeBPt_3$  which has the same  $c/a$  ratio with an only marginally larger volume. Exploring the possible cause of this disparity is likely to lead to useful insights.

Theoretical calculations are presently in progress and to corroborate the solution of crystal structure the high pressure phase. They will also be compared to the observed transition pressure, lattice parameters and so on. It is hoped that they will also be able to shed light on the nature of the interactions responsible for the transition and to explain why no phase transition was observed in the explored pressure range of  $CeBPt_3$  and  $CeSiPt_3$ .

In conclusion, the  $YBPt_3$  anti-perovskite displays vastly different behaviour from its isostructural oxide analogues. This suggests that different structural trends are to be expected for this class of compounds. More experiments on anti-perovskites, especially ones that display distorted versions of the ideal structure would be useful in further clarifying the differences (and similarities) between normal and anti-perovskites.

## References

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