MS16-P4 Symmetry reduction in anti-perovskites at high pressure

Morten B. Nielsen[1], Martin Bremholm[1]

1. Aarhus University

email: mbnielsen@chem.au.dk

Anti-perovskites of AXB_3 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]. Few high pressure structural studies on anti-perovskites exist, and it is worth investigating whether this class of materials follows the same structural trends at high pressure as the oxide perovskites.

A famous anti-perovskite is $CeSiPt_3$, a heavy fermion superconductor that crystallises in the non-centrosymmetric *P4mm* space group. Its properties have been investigated under pressure to a few GPa, but no structural studies on this or related compounds have been reported. In this study, we investigated the structure of $CeSiPt_3$ and the newly synthesized isostructural $YBPt_3$ to high pressures. Surprisingly, we observed a second-order structural phase transition in $YBPt_3$ at 24 GPa that lowered the symmetry even further. It is interesting that pressure drives further structural distortion in this anti-perovskite system, since the oxide perovskite $PbVO_3$ (which also displays the *P4mm* structure with similar *c/a* ratio at ambient pressure) undergoes a first-order transition at ~3 GPa with a large volume collapse (10.6%) to the ideal cubic *Pm-3m* perovskite structure[4]. $CeSiPt_3$ on the other hand does not undergo any changes in structure up to 45 GPa. We will present our structural results and rationalise the difference between the two otherwise chemically similar compounds through DFT calculations.

References:

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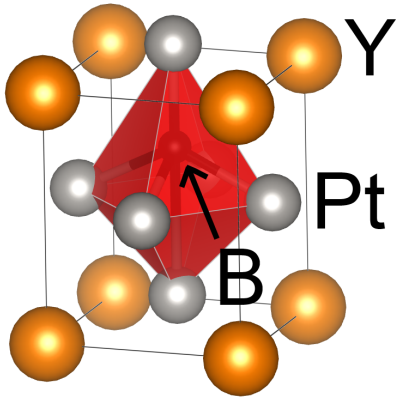

Figure 1. The non-centrosymmetric *P4mm* structure of $YBPt_3$

Keywords: Anti-perovskite, phase transition, symmetry reduction, intermetallic