High-pressure growth of BaPrO₃ single crystal

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The family of ABO₃ type Perovskite materials remains perfectly cubic due to the smaller B site compared to A site atom which was discovered in 1839. However, in the case of a larger ionic size B site, displacement of the oxygen atom results in orthorhombic or rhombohedral distortion. In the case of BaPrO₃, orthorhombic distortion has been observed involving a cooperative buckling of these corner-sharing octahedra. This B-ion sits at the centre of the slightly distorted octahedron formed by the six near-neighbour oxygen atoms. The octahedra are linked in a 3-d corner-sharing network which can act as a super-exchange pathway, permitting interactions between the B-ions through the intervening oxygen atoms.

The Pr⁴⁺ (4f¹) ions are magnetic, however despite numerous studies to determine their magnetic order, there has been no agreement in the literature as to the nature of the magnetic ordering. For instance, one neutron powder diffraction study found BaPrO₃ remains paramagnetic down till 2 K. In contrast another powder neutron diffraction study has shown that the system develops Γ-point antiferromagnetic order along a below 11.7 K. While yet another study indicates that the PrBaO₃ samples appear to have an oxygen excess of about 2%, and a difference in colours may be attributed to the different oxygen concentration of the samples. Furthermore, owing to the large magnetic susceptibility measured on this compound, it was proposed, although never experimentally measured, that these systems also contain a ferromagnetic component along c. This is by symmetry and the assumption that the magnetic structure transforms by a single irreducible representation of the *Pbnm* space group.

Here we are reporting the growth of BaPrO₃ single crystal for the first time using high pressure optical floating zone technique. The availability of bulk crystals opens a new avenue to understand the quantum physics of this material.