



	<b>Experiment title:</b> The phase relations and PVT EoS of NaMnF <sub>3</sub> : novel analogue to MgSiO <sub>3</sub> in the lowermost mantle	<b>Experiment number:</b> ES259
<b>Beamline:</b>	<b>Date of experiment:</b> from: 12 June 2015 to: 16 June 2015	<b>Date of report:</b>
<b>Shifts:</b>	<b>Local contact(s):</b> Wilson Crichton	<i>Received at ESRF:</i>
<b>Names and affiliations of applicants</b> (* indicates experimentalists): <b>David Dobson, University College London (UCL),</b> <b>Edward Bailey, UCL</b> <b>Andrew Thompson, UCL</b> <b>Alexander Lindsay-Scott, UCL</b>		

## Report:

The physical properties of the post-perovskite phase of MgSiO<sub>3</sub> control the dynamics of the lower thermal boundary layer of the Earth's mantle in the D'' region. Unfortunately, many of these properties cannot be measured at the extreme pressures (120 GPa) of stabilisation of this phase. The best chance of constraining these properties is through a combination of measurements on low-pressure analogue materials (which have the same crystal structure but a different chemical composition) and ab initio simulations of the analogue and natural systems. The NaBF<sub>3</sub> systems (B=Mg, 2+ transition metal) have proven to be good analogues, showing a range of properties which are similar to MgSiO<sub>3</sub> post-perovskite and also displaying new properties (which cannot be measured directly in the silicate system) which might be important for the D'' region.

The NaMnF<sub>3</sub> system shows a rich phase diagram with an unquenchable phase existing at pressures above ~6 GPa (based on ex-situ diffusion studies which show first-order partitioning behaviour above this pressure and further phase transitions at ~12 GPa, from the literature).

We have performed in situ multi-anvil cell experiments to delineate the phase diagram in this system (Figure 1). There are two reversible phase transitions at pressures close to 6-7 GPa at 500-600K: these have strongly negative clapeyron slopes such that the lower-temperature transition intersects the NaMnF<sub>3</sub> liquidus close to 3 GPa.

The structure of these two phases is not yet clear but it is not any of the post-post-perovskite phases proposed by Umamoto and Wentzcovitch, for the NaMgF<sub>3</sub> system, and seen in NaCoF<sub>2</sub>, NaFeF<sub>3</sub> and NaNiF<sub>3</sub>. There is a further, recoverable, dissociation reaction at 10 GPa and 1500 K.

Figure 1. Powder pattern of NaMnF<sub>3</sub> during heating from 300K to 1100K at 8.5 GPa. The sample is initially highly strain broadened but this anneals out before the first transition. The loss of the strong perovskite (020) reflection at the first transition is clear, as is the appearance of a weak low-angle reflection. At the second transition, there is a discontinuous change in the position of the 'perovskite triplet' and a new low-angle reflection appears.

