



	Experiment title: 'Stereochemically' active / non-active lone pair in HP lead-containing phases	Experiment number: ES-1060
Beamline: ID15b	Date of experiment: from: 25.01.2022 to: 27.01.2022	Date of report: 01.03.2022 <i>Received at ESRF:</i>
Shifts: 6	Local contact(s): Michael Hanfland	
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Report:

During our work at the beamline ID15b from 25.01.2022 to 27.01.2022 we have conducted the following high-pressure synchrotron diffraction experiments:

- Two single crystals of $\text{BaAs}_2\text{Zn}_2\text{O}_8 \cdot \text{H}_2\text{O}$ has been studied upon compression and decompression in the pressure range 0–13 GPa with the pressure step about 2–5 GPa (8 pressure points)
- One single crystal of HfB_2O_5 has been studied in the pressure range 0–155 GPa with the pressure step 5–20 GPa (16 pressure points)
- One single crystal of dmisteinbergite $\text{CaAl}_2\text{Si}_2\text{O}_8$ has been studied up to 21 GPa with the pressure step 2–5 GPa (8 pressure points)
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Sample preparations, preparation of diamond anvil cells (DACs) and DAC loadings for all samples were performed in the ESRF.

As a result, diffraction data were obtained. The first investigations demonstrated, that:

- The crystal structure of $\text{BaAs}_2\text{Zn}_2\text{O}_8 \cdot \text{H}_2\text{O}$ amorphized at the pressure above 10 GPa and this transformation is not reversible.
- The crystal structure of HfB_2O_5 is stable in the whole pressure range. The experiment was stopped due to the impossibility to further increase the pressure. We plan to continue this experiment.
- Dmisteinbergite amorphizes at the pressure about 18 GPa. Probably it undergoes phase transition below this pressure, but the obtained data need more careful refinements.

The aim of the experiments has been achieved: three samples were studied in the quite wide pressure ranges.

All data collected during the beamtime are sufficient for publications. It would be interesting to study HfB_2O_5 at the pressure higher pressures.