ESRF	<b>Experiment title:</b> Na-Ca carbonates at high pressure: new hosts of deep carbon	Experiment number: ES-810
Beamline:	Date of experiment:	Date of report:
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## **Report:**

In several experimental series we studied compressibility of four Na-Ca carbonates:  $Na_2Ca_4(CO_3)_5$  and  $Na_4Ca(CO_3)_3$ , synthesized in multianvil press at 3 and 6 GPa, respectively, and  $Na_2Ca(CO_3)_2$  and  $Na_{1.64}K_{0.36}Ca(CO_3)_2$ , synthesized hydrothermally at 1 kbar and 450°C. During experiments, crystals of Na-Ca carbonates were compressed up to 10 or 20 GPa in helium and studied by single-crystal X-ray diffraction.

Na<sub>2</sub>Ca<sub>4</sub>(CO<sub>3</sub>)<sub>5</sub> shows regular compression without any structural changes (Fig. 1):

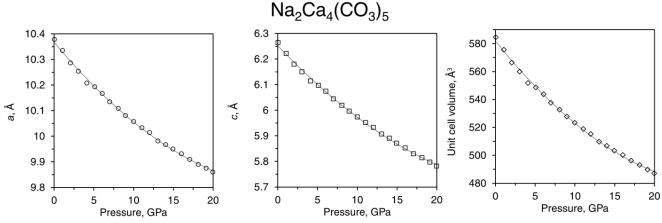


Figure 1. Dependence of Na<sub>2</sub>Ca<sub>4</sub>(CO<sub>3</sub>)<sub>5</sub> unit cell parameters and volume on pressure

 $Na_4Ca(CO_3)_3$  shows symmetry change from cubic to rhombohedral at pressures above 10 GPa, however without abrupt changes in *a* parameter and unit cell volume (Fig. 2):

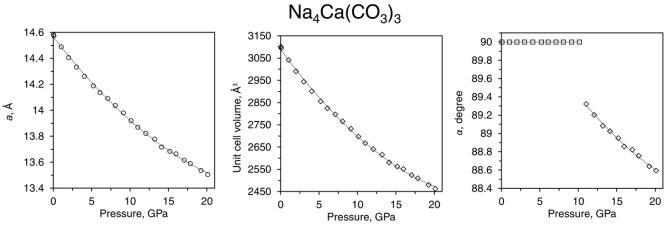
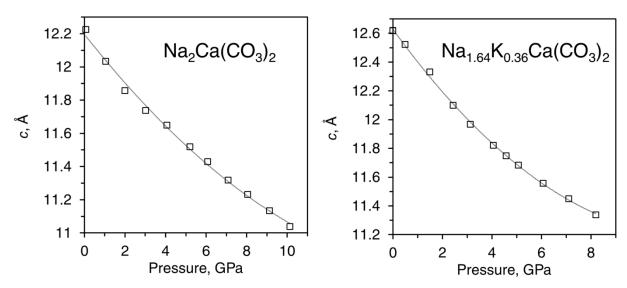


Figure 2. Dependence of Na<sub>4</sub>Ca(CO<sub>3</sub>)<sub>3</sub> unit cell parameters and volume on pressure

Crystals of Na<sub>2</sub>Ca(CO<sub>3</sub>)<sub>2</sub> and Na<sub>1.64</sub>K<sub>0.36</sub>Ca(CO<sub>3</sub>)<sub>2</sub> were compressed up to 10 GPa, and currently only *c* unit cell parameter is obtained from diffraction data due to complex twinning and modulation of the structure. No abrupt changes in this parameter, however, are observed in the studied pressure range (Fig. 3):



**Figure 3.** Dependence of unit cell parameter *c* on pressure for  $Na_2Ca(CO_3)_2$  and  $Na_{1.64}K_{0.36}Ca(CO_3)_2$