

Experimental Report for Regular Proposal ES-1061

We have performed 4 sets of single-crystal diffraction experiments on synthetic carbonates with different K:Ca ratio (= 2:3, 2:2, 2:1, 8:3) compressed in He medium up to 20 GPa. The data quality is high enough to characterise the compressibility and structural behaviour of these compounds. In particular, interesting features of the high-pressure structure evolution have been revealed in $K_2Ca(CO_3)_2$, analogue of mineral buetschliite, important constituent of the carbonate inclusions in deep minerals [Giuliani et al. 2012]. The trigonal-to-monoclinic phase transition at about 6.5 GPa is rather smooth in terms of the bulk compressibility (Fig. 1a); however the K structure polyhedron exhibits not only an abrupt increase of the distortion index, but also the volume expansion (Fig. 1b), which seems quite unusual. In the nearest future we intend to submit a paper on the high-pressure behaviour of $K_2Ca(CO_3)_2$ to the journal "Physics and Chemistry of Minerals".

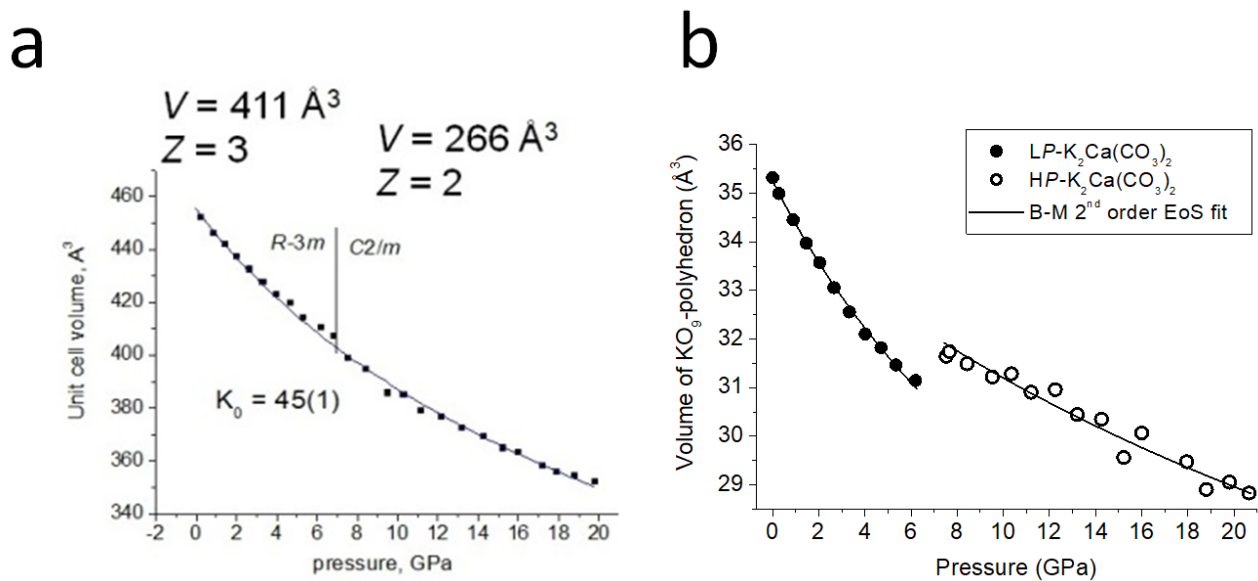


Fig. 1. Pressure dependence of the unit cell volume (a) and the volume of the structure polyhedron KO_9 (b) for the low-pressure (LP) and high-pressure (HP) phase of $K_2Ca(CO_3)_2$.

Regarding the other binary carbonates studied, we can note different compression behaviour of ordered and disordered modification of $K_2Ca_3(CO_3)_4$ (Fig. 2), which demonstrates their independent structure evolution and the absence of mutual transitions at room temperature.

In general, the aim of the experiment is achieved and the collected data are sufficient for the preparation of several papers (roughly one paper per each of the listed compounds).

In addition to the binary K-Ca carbonates, we have studied synthetic K-bearing tourmaline (foitite) and prepared the paper "High-pressure structure evolution and compressibility of synthetic potassium-bearing foitite: the role of Fe in the stiffening of tourmaline structure" by Likhacheva et al. This manuscript has passed the first stage of reviewing in the journal "Physics and Chemistry of Minerals".

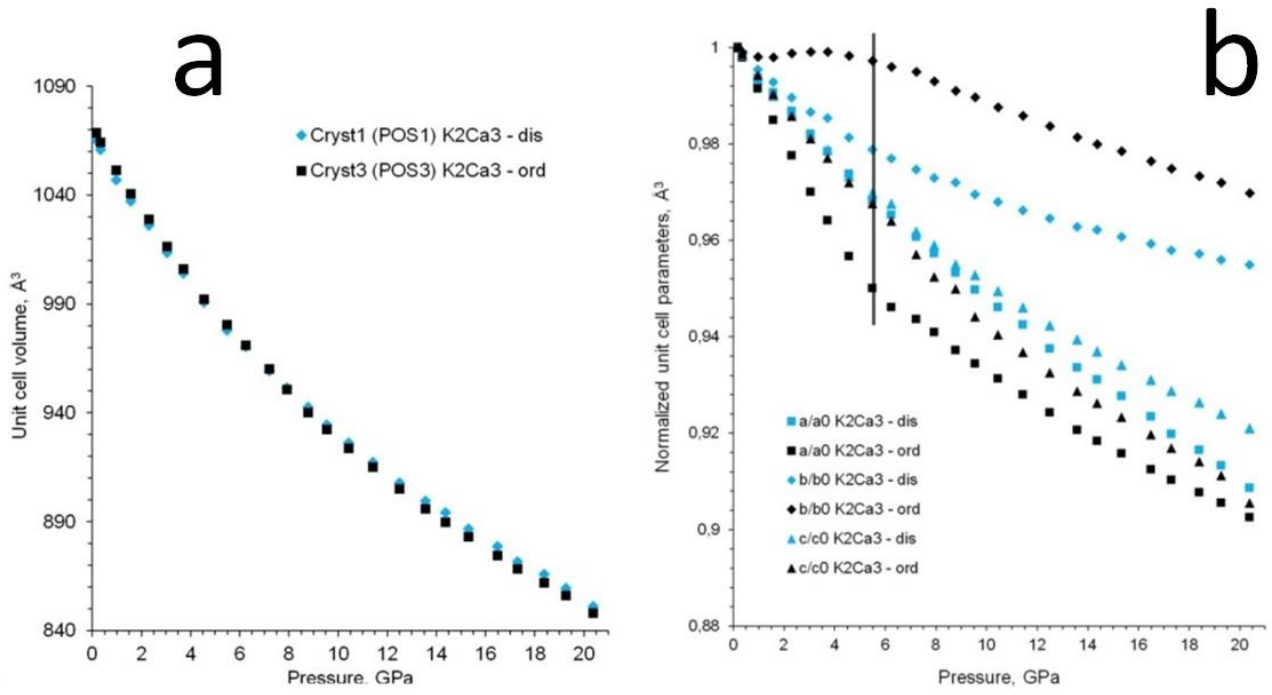


Fig. 2. Pressure dependence of the unit cell volume (a) and normalized unit cell parameters (b) for the disordered (dis, $Pnma$) and ordered (ord, $P2_12_12_1$) modification of $K_2Ca_3(CO_3)_4$ (K_2Ca_3). Vertical line marks the transition of ordered $K_2Ca_3(CO_3)_4$ to monoclinic phase defined by the bend on the compression curves.