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ABSTRACT BOOK

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Structure and thermal equation of state of $Ca_3KNa(CO_3)_4$ carbonate

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The presence of alkali-carbonates in the Earth's mantle is suggested by the occurrence of these minerals as diamond inclusion. We expect that alkali-carbonates may play a significant role in carbon-related processes (volcanism, mantle metasomatism, diamond formation…) in upper mantle and transition zone. High-pressures and temperatures experiments have recently revealed the possible occurrence of new class of Ca-alkali-carbonates above 4 GPa. We report the crystal structure of $Ca_3NaK(CO_3)_4$ synthesized at 4 GPa. It appears in equilibrium with carbonatitic liquids. It presents a similar topology wih the reported $Ca_3Na_2(CO_3)_4$ high-pressure phase (Gavryushkin et al., 2014) but a different unit cell and symmetry. Irregular coordination sites for Ca, K and Na cations and a partially disordered CO_3 group arrangement reveal an anomalous elastic behaviour for the different cation sites, suggesting an interesting capability of trace element incorporation in the structure.

Thermal equation of state of $Ca_3NaK(CO_3)_4$ is determined by single crystal synchrotron X-ray diffraction with resistive heated DAC (ESRF, Grenoble, ID15a beamline) and the results are used to model the possibility for these phases to differentiate from liquids and stagnate in the upper mantle.

Gavryushkin P.N., Bakakin V.V., Bolotina N.B., Shatskiy A.F., Seryotkin Y.V. & Litasov K.D. (2014) - Synthesis and crystal structure of new carbonate $Ca_3Na_2(CO_3)_4$ homeotypic with orthoborates $M_3Ln_2(BO_3)_4$ (M= Ca, Sr, and Ba). Crystal Growth & Design, 14(9), 4610-4616.

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