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Crystal structure, high-pressure, and high-temperature behavior of carbonates in the $K_2Mg(CO_3)_2$–$Na_2Mg(CO_3)_2$ join

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Abstract

Although alkali-alkali earth carbonates have not been reported from mantle-derived xenoliths, these carbonates may have a substantial role in mantle metasomatic processes through lowering melting temperatures. On the $Na_2Mg(CO_3)_2$–$K_2Mg(CO_3)_2$ join only the Na-end-member eitelite ($R\bar{3}$ space group), was reported in nature. The K-end-member ($R\bar{3}m$) readily hydrates even at low temperatures, therefore, only baylissite, $K_2Mg(CO_3)_2 \cdot 4H_2O$, has been observed. Because of the role of (K,Na)Mg-double carbonates in mantle metasomatism, we performed high *P-T* experiments on $K_2Mg(CO_3)_2$, $(K_{1.1}Na_{0.9})_2Mg(CO_3)_2$, and $Na_2Mg(CO_3)_2$. Structure refinements were done upon compression of single crystals from 0 to 9 GPa at ambient temperature employing synchrotron radiation. Fitting the compression data to the second-order Birch-Murnaghan EoS resulted in V_0 = 396.2(4), 381.2(5), and 347.1(3) Å^3 and K_0 = 57.0(10), 54.9(13), and 68.6(13) GPa for $K_2Mg(CO_3)_2$, $(K_{1.1}Na_{0.9})_2Mg(CO_3)_2$, and $Na_2Mg(CO_3)_2$, respectively. These compressibilities are lower than those of magnesite and dolomite. The KMg-double carbonate transforms into a monoclinic polymorph at 8.05 GPa; the high-*P* phase is 1% denser than the low-*P* polymorph. The NaMg-double carbonate has a phase transition at ~14 GPa, but poor recrystallization has prevented structure refinement. The parameters for a *V-T* EoS were collected at 25–600 °C and ambient pressure and are $\alpha_0 = 14.31(5) \times 10^{-5}$ K^{-1} and $16.73(11) \times 10^{-5}$ K^{-1} for $K_2Mg(CO_3)_2$ and $Na_2Mg(CO_3)_2$, respectively. Moreover, fitting revealed an anisotropy of thermal expansion along the *a*- and *c*-axis: $\alpha_0(a) = 2.84(6) \times 10^{-5}$ and $4.78(5) \times 10^{-5}$ K^{-1} and $\alpha_0(c) = 10.47(11) \times 10^{-5}$ and $8.72(5) \times 10^{-5}$ K^{-1} for $K_2Mg(CO_3)_2$ and $Na_2Mg(CO_3)_2$, respectively.

Keywords: Alkali-alkali earth double carbonates, synchrotron, high pressure, phase transition