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A high-pressure structural transition of norsethite-type $BaFe(CO_3)_2$: Comparison with $BaMg(CO_3)_2$ and $BaMn(CO_3)_2$

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Abstract

Investigations on the phase stability of the norsethite-type family [$BaMg(CO_3)_2$, $BaMn(CO_3)_2$, $BaFe(CO_3)_2$] under high-pressure conditions are of great significance for understanding the structure and metal cationic (Mg^{2+}, Fe^{2+}, Mn^{2+}) substitution mechanism in double divalent metal carbonates. The structural evolution and equation of state of $BaFe(CO_3)_2$ were studied at high pressure up to ~7.3 GPa by synchrotron X-ray diffraction (XRD) in diamond-anvil cell (DAC) in this study. $BaFe(CO_3)_2$ undergoes a reversible phase transition from $R\bar{3}m$ (α-phase) to $C2/c$ (γ-phase) space groups at ~3.0 GPa. The fitted elastic parameters are V_0 = 377.79(2) Å^3 and K_0 = 40.3(7) GPa for α-$BaFe(CO_3)_2$, V_0 = 483.24(5) Å^3 and K_0 = 91.2(24) GPa for γ-$BaFe(CO_3)_2$ using second-order Birch-Murnaghan equation of state (BM2-EoS). Besides, the vibrational properties and structural stability of complete norsethite-type minerals were also investigated first by Raman spectroscopy combined with DAC up to 11.1 GPa. Similar structural phase transitions occur in $BaMg(CO_3)_2$, $BaFe(CO_3)_2$, $BaMn(CO_3)_2$ at 2.2–2.6, 2.6–3.7, and 3.7–4.1 GPa, respectively. The onset phase transition pressures of the norsethite-type family are much lower than that of dolomite-type $Ca(Mg,Fe,Mn)(CO_3)_2$ and calcite-type $(Mg,Fe,Mn)CO_3$ carbonates. These results provide new insights into the divalent cation substitution effects on the stability and structural evolution of carbonates under high-pressure conditions.

Keywords: Norsethite-type minerals, synchrotron X-ray diffraction, Raman spectroscopy, phase transition, diamond anvil cell; Earth Analogs for Martian Geological Materials and Processes