Thermal equation of state of CaGeO₃ perovskite

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ABSTRACT

Pressure-volume-temperature data have been obtained for CaGeO₃ perovskite up to 9.6 GPa and 1100 K using a cubic anvil, DIA-type high-pressure apparatus in conjunction with synchrotron X-ray diffraction. The data were analyzed using Birch-Murnaghan equation of state and thermal pressure approach with the bulk modulus at ambient pressure, K_{T0} , and its pressure derivative, K'_{T0} , constrained by previous measurements. A fit of the unit-cell volume data to the high-temperature Birch-Murnaghan (HTBM) equation of state gives $(\partial K_T/\partial T)_P = -0.025 \pm 0.015$ GPa/K, $a = 1.047 \pm 0.356 \times 10^{-5}$ /K, and $b = 3.282 \pm 0.735 \times 10^{-8}$ /K² for the thermal expansion α expressed by a + bT. The thermal pressure approach yields $\alpha K_T = 4.04 \pm 0.37 \times 10^{-3}$ GPa/K and $(\partial^2 P/\partial T^2)_V = 6.17 \pm 1.28 \times 10^{-6}$ GPa/K². The energy dispersive X-ray diffraction data reveal no indication of a structural phase transition over the *P*-*T* range of the current experiment. A systematic relationship, $K_{s0} = 6720/V$ (molar) – 13.07 GPa, has been established based on these isostructural analogues, which predicts $K_{s0} = 261(15)$ for MgSiO₃ perovskite and 225(8) for CaSiO₃ perovskite, respectively.

Keywords: CaGeO₃ perovskite, equation of state, thermal pressure, high pressure and high temperature, X-ray diffraction