American Mineralogist, Volume 90, pages 1157–1162, 2005

P-V equation of State, thermal expansion, and *P-T* stability of synthetic zincochromite ($ZnCr_2O_4$ spinel)

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Abstract

The elastic properties and thermal behavior of synthetic zincochromite ($ZnCr_2O_4$) have been studied by combining room-temperature high-pressure (0.0001–21 GPa) synchrotron radiation powder diffraction data with high-temperature (298–1240 K) powder diffraction data. Elastic properties were obtained by fitting two Equations of State (EoS) to the *P-V* data. A third-order Birch-Murnaghan model, which provides results consistent with those from the Vinet EoS, yields: K_0 = 183.1(±3.5) GPa, K' = 7.9(±0.6), K'' = –0.1278 GPa^{-1} (implied value), at V_0 = 577.8221 $Å^3$ (fixed). Zincochromite does not exhibit order-disorder reactions at high temperature in the thermal range explored, in agreement with previous studies. The volume thermal expansion was modeled with $\alpha_V = \alpha_0 + \alpha_1 T + \alpha_2/T^{-2}$, where only the first coefficient was found to be significant [α_0 = 23.0(4) 10^{-6} K^{-1}]. Above 23 GPa diffraction patterns hint at the onset of a phase transition; the high pressure phase is observed at approximately 30 GPa and exhibits orthorhombic symmetry. The elastic and thermal properties of zincochromite were then used to model by thermodynamic calculations the *P-T* stability field of $ZnCr_2O_4$ with respect to its oxide constituents (Cr_2O_3 and rocksalt-like ZnO). Spinel is expected to decompose into oxides at about 18 GPa and room temperature, in absence of sluggish kinetics.