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P-V-T equation of state of $Ca_3Cr_2Si_3O_{12}$ uvarovite garnet by using a diamond-anvil cell and in-situ synchrotron X-ray diffraction

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Abstract

The pressure-volume-temperature (*P-V-T*) equation of state (EoS) of synthetic uvarovite has been measured at high temperatures up to 900 K and high pressures up to 16.20 GPa, by using in situ angle-dispersive X-ray diffraction and diamond-anvil cell. Analysis of room-temperature *P-V* data to a third-order Birch-Murnaghan EoS yielded: $V_0 = 1736.9 \pm 0.5$ Å^3, $K_0 = 162 \pm 2$ GPa, and $K_0' = 4.5 \pm 0.3$. With K_0' fixed to 4.0, we obtained: $V_0 = 1736.5 \pm 0.3$ Å^3 and $K_0 = 164 \pm 1$ GPa. Fitting of our *P-V-T* data by means of the high-temperature third-order Birch-Murnaghan equations of state, given the thermoelastic parameters: $V_0 = 1736.8 \pm 0.8$ Å^3, $K_0 = 162 \pm 3$ GPa, $K_0' = 4.3 \pm 0.4$, $(\partial K/\partial T)_P = -0.021 \pm 0.004$ GPa/K, and $\alpha_0 = (2.72 \pm 0.14) \times 10^{-5}$ K^{-1}. We compared our elastic parameters to the results from the previous studies for uvarovite. From the comparison of these fittings, we propose to constrain the bulk modulus and its pressure derivative to $K_0 = 162$ GPa and $K_0' = 4.0$–4.5 for uvarovite. Present results were also compared with previous studies for other ugrandite garnets, grossular and andradite, which indicated that the compression mechanism of uvarovite might be similar with grossular and andradite. Furthermore, a systematic relationship, K_0 (GPa) = 398.1(7)–0.136(8) V_0 (Å^3) with a correlation coefficient R^2 of 0.9999, has been established based on these isostructural analogs. Combining these results with previous studies for pyralspite garnets—pyrope, almandine, and spessartine—the compositional dependence of the thermoelastic parameters (bulk modulus, thermal expansion, and the temperature derivative of the bulk modulus) were discussed.

Keywords: Uvarovite, equation of state, high pressure and high temperature, X-ray diffraction, diamond-anvil cell