

Comparative high-pressure crystal chemistry of karrooite, MgTi_2O_5 , with different ordering states

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ABSTRACT

Two karrooite crystals, one with a disorder parameter ($X = \text{Ti}$ content in the M1 site) of 0.070(5) and the other with $X = 0.485(5)$, were mounted together in one diamond-anvil cell and studied by single-crystal X-ray diffraction at several pressures up to 7.51 GPa. The most noticeable effect of increasing cation disorder on the high-pressure behavior of the structure is to increase the compressibilities of the mean $\langle \text{M2-O} \rangle$ bond length from 0.00148(2) GPa⁻¹ in the ordered sample to 0.00163(7) GPa⁻¹ in the disordered one and decrease those of the mean $\langle \text{M1-O} \rangle$ bond length from 0.00243(5) to 0.00193(12) GPa⁻¹. These changes are responsible for the compressibility difference between the two phases observed by Hazen and Yang (1997). Both compressibilities of the mean $\langle \text{M-O} \rangle$ bond lengths and the octahedral volumes in two phases decrease linearly with increasing the Ti contents in the octahedral sites. All octahedra in two samples become less distorted as pressure increases, but those in the more disordered structure exhibit larger decreases in terms of the octahedral angle variance than the corresponding ones in the more ordered structure. The influence of pressure on the interatomic angles is small compared to the interatomic distances, suggesting that compression of the karrooite structure is controlled primarily by the bond-length shortening, rather than by bond-angle bending. The strong compressional anisotropy of the structure is a consequence of the differential compressibilities of the weaker $\text{Mg}^{2+}\text{-O}$ and stronger $\text{Ti}^{4+}\text{-O}$ bonds and the complex edge-sharing linkage involving the M1 and M2 octahedra.