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Re-investigation of the crystal structure of enstatite under high-pressure conditions

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Abstract

A synthetic single crystal of pure orthoenstatite ($MgSiO_3$, space group *Pbca*) has been investigated at high pressure for structural determinations by in situ single-crystal X-ray diffraction using a diamond-anvil cell. Ten complete intensity data collections were performed up to 9.36 GPa. This study significantly improved the accuracy of structural parameters in comparison to a previous high-pressure structural study, allowing a more detailed examination of structural behavior of orthoenstatite at high pressures and a comparison to other more recent structural studies performed on orthopyroxenes with different compositions. The structural evolution determined in this work confirms the high-pressure evolution found previously for other orthopyroxenes and removes some ambiguities originating from the less accurate published data on the $MgSiO_3$ structure at high pressure. The structural compression is mostly governed by significant volume decrease of the Mg1 and Mg2 octahedra, affecting in turn the kink of the tetrahedral chains, especially the TB chain of larger SiO_4 tetrahedra. The Mg2 polyhedron undergoes the largest volume variation, 8.7%, due especially to the strong contraction of the longest bond distance (Mg2-O3B), whereas Mg1 polyhedral volume decreases by about 7.4%. The compressional behavior of the tetrahedral sites is quite different from previously published data. The TA and TB tetrahedral volumes decrease by about 2.8 and 1.8%, respectively, and no discontinuities can be observed in the pressure range investigated. Using the data on the pure orthoenstatite as reference, we can confirm the basic influences of element substitutions on the evolution of the crystal structure with pressure.

Keywords: Enstatite, crystal structure, X-ray diffraction, high pressure, diamond-anvil cell