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Single-crystal compression and crystal structure of clinopyroxene up to 10 GPa

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ABSTRACT

The hydrostatic compression of synthetic single crystals of diopside, $CaMgSi_2O_6$, and hedenbergite, $CaFeSi_2O_6$, was studied at 33 pressures up to 10 GPa by X-ray diffraction. In addition, intensity data for hedenbergite were collected at 12 pressures up to 10 GPa. For determination of the elasticity two crystals were loaded together in a diamond cell. The axial compressibilities β_a, β_b, and β_c of diopside and hedenbergite are 2.36(4), 3.17(4), and 2.50(4) $\times$ 10^{-3} GPa^{-1}, and 1.93(5), 3.38(6), and 2.42(8) $\times$ 10^{-3} GPa^{-1}, respectively. The bulk moduli (K_{T_0}) and their pressure derivatives (K'_{T_0}) were determined simultaneously from a weighted linear fit of a third order Birch-Murnaghan equation of state to the volume data at elevated pressures. K_{T_0} and K'_{T_0} are 104.1(9) GPa and 6.2(3) for diopside and 117(1) GPa and 4.3(4) for hedenbergite, respectively.

The unit-cell parameters decrease continuously with pressure. The larger polyhedra show more compression than the smaller ones. Between 0.1 MPa and 10 GPa the polyhedral volumes of CaO_8, FeO_6, and SiO_4 decrease by 8.4, 6.6, and 2.9%, respectively. The longest bonds of CaO_8 and FeO_6 show most compression. Significant compression in the two shortest Si-O1 and Si-O2 bond lengths of the SiO_4 tetrahedra was observed at relatively low pressures, resulting in a tetrahedral volume compression of 1.6% between 0.1 GPa and 4 GPa and 1.3% between 4 and 10 GPa. The compression of the unit cell can be described by the volume compression of the individual CaO_8 and FeO_6 polyhedra, with the SiO_4 tetrahedron playing a minor role. Diopside is more compressible than hedenbergite as shown by their axial and volume compressibilities because the FeO_6 octahedron is significantly more rigid than MgO_6 at high pressures. This observation implies that octahedrally coordinated Fe^{2+} behaves differently from Mg at high pressures, in contrast to their behavior at ambient conditions.