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High-pressure phases of cordierite from single-crystal X-ray diffraction to 15 GPa

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Abstract

High-pressure single-crystal X-ray diffraction experiments were conducted on natural cordierite crystals with composition $Mg_{1.907(18)}Fe_{0.127(6)}Al_{4.01(2)}Si_{4.96(3)}Na_{0.026(3)}O_{18.12(9)}$ using a synchrotron X-ray source. The samples were compressed at 300 K in a diamond-anvil cell to a maximum pressure of 15.22(15) GPa with a neon pressure-transmitting medium and a gold pressure calibrant. We observed a recently described orthorhombic to phase transition, as well as a further transition to a second triclinic phase. We solved and refined both new triclinic phases in space group *P*1, and designate them cordierite II and III. The structures of cordierite II and III were refined at 7.52(3) and 15.22(15) GPa, respectively. The lattice parameters at these pressures are a = 15.567(3), b = 9.6235(4), c = 9.0658(6) Å, α = 89.963(5)°, β = 86.252(10)°, and γ = 90.974(8)° for cordierite II, and a = 8.5191(19), b = 8.2448(3), c = 9.1627(4) Å, α = 85.672(4)°, β = 85.986(7)°, and γ = 70.839(10)° for cordierite III. Across the phase transitions there is a significant reduction in the length of the a-axis (~2 Å per phase transition), whereas both the b- and c-axis remain largely unchanged. Cordierite II has fourfold- and fivefold-coordinated Si and Al, while cordierite III has fourfold-, fivefold-, and sixfold-coordinated Si, fourfold- and fivefold-coordinated Al, and fivefold- and sixfold-coordinated Mg. The sequence of high-pressure phases shows increasing polymerization of coordination polyhedra. These results, together with other recent studies, suggest that mixed four-, five-, and sixfold coordination states may occur more commonly in silicate structures compressed at 300 K than previously recognized.

Keywords: Cordierite, phase transition, crystallography, high pressure, single-crystal X-ray diffraction