

## 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  $\text{Mg}_{1.907(18)}\text{Fe}_{0.127(6)}\text{Al}_{4.01(2)}\text{Si}_{4.96(3)}\text{Na}_{0.026(3)}\text{O}_{18.12(9)}$  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,  $\alpha = 89.963(5)^\circ$ ,  $\beta = 86.252(10)^\circ$ , and  $\gamma = 90.974(8)^\circ$  for cordierite II, and  $a = 8.5191(19)$ ,  $b = 8.2448(3)$ ,  $c = 9.1627(4)$  Å,  $\alpha = 85.672(4)^\circ$ ,  $\beta = 85.986(7)^\circ$ , and  $\gamma = 70.839(10)^\circ$  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