

## **Structural properties of ferromagnesian cordierites**

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### **ABSTRACT**

A set of natural and heat-treated cordierite crystals has been analyzed using single-crystal X-ray diffraction, EMPA, SIMS, and <sup>57</sup>Fe Mössbauer-spectroscopy. Structure determination of natural cordierite shows that the average size of the tetrahedrally coordinated T<sub>1</sub>1 cation increases systematically by about 0.01 Å as the Fe content of the solid solution decreases toward the Mg end-member. For Fe-rich compositions, the mean tetrahedral bond length T<sub>1</sub>1-O is close to 1.749 Å, a value expected for an AlO<sub>4</sub> tetrahedron in an aluminosilicate framework structure. It is suggested that the structural dilation of the tetrahedral sites, which is driven by the decreasing average size of the octahedral cation, is sustained by substitution of the large cations Mg and Fe<sup>2+</sup> for Al. Mössbauer spectroscopy shows that up to 11% of Fe<sup>2+</sup> can be attributed to tetrahedral coordination in Mg-rich cordierite. Charge balance for the substitutions is either provided by introduction of Na<sup>+</sup> into vacant Ch2(0,0,0) channel sites or by substitution of an additional Al<sup>3+</sup> by Si<sup>4+</sup>. Tetrahedral site occupancies and corresponding Al,Si order parameters are calculated on the basis of a simple hard sphere model, based on refined cation-oxygen mean bond length, chemical composition, and Fe site-occupancy refinements. Almost complete Al,Si ordering among ring sites T<sub>2</sub> is encountered for most natural cordierite samples. Al,Si ordering among the T<sub>1</sub> tetrahedra is less pronounced for Fe-rich compositions. Partial disorder is attributable to Al/Si ratios in excess of 4/5. Orthorhombic shear strain is shown to correlate with the derived average order parameter, if corrections for strain contributions from size effects of the octahedral cation and from channel constituents are employed. Crystal-chemical similarities to other compounds and the implications of the minor cation substitutions for the properties of structural phase transitions in cordierite are discussed.