

STRUCTURAL AND RAMAN-SPECTROSCOPIC INVESTIGATIONS OF SYNTHETIC HEXAGONAL AND ORTHORHOMBIC Fe-CORDIERITE

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Crystal structures of synthetic hexagonal and orthorhombic Fe-cordierite polymorphs with space groups P6/mcc and Cccm were refined from single-crystal X-ray diffraction data to $R_w = 3.14\%$ and $R_{1, \text{ortho}} = 4.48\%$. The substitution of the larger Fe^{2+} for Mg leads to multiple structural changes and an increase of the unit cell volumes, with a , c (hex) = 11.16(1) Å, 9.2852(5) Å and a , b , c (ortho) = 17.2306(2) Å, 9.8239(1) Å, 9.2892(1) Å. Fe incorporation leads to an increase of the octahedral volumes, although the octahedral diameter reduction of the c -axis decreases in both polymorphs. X-ray powder diffraction analysis indicates a high degree of Al/Si ordering in the orthorhombic polymorph with a distortion of ~ 0.24 (MIYASHIRO, 1957). Estimations of site occupancies based on the refined tetrahedral volumes result in the following values for hexagonal Fe-cordierite: $\sim 10\%$ Al for T_1 and $\sim 28\%$ Al for T_2 . Raman spectra of the hexagonal polymorph were recorded at ambient conditions and at $-190\text{ }^\circ\text{C}$ using laser-light with 633 and 532 nm wavelength for excitation.

MIYASHIRO, A. (1957): American Journal of Science, 255, 43-62.