

Structural systematics of hydrous ringwoodite and water in Earth's interior

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ABSTRACT

Seven separate samples of hydrous ringwoodite with compositions ranging from Fo₁₀₀ to Fo₈₉ and hydrogen contents from 0.2 to 1.1 wt% were synthesized in the 5000 ton multi-anvil press at the Bayerisches Geoinstitut. Synthesis conditions ranged from 18 to 22 GPa and 1400 to 1500 °C. The crystals were characterized by single-crystal X-ray diffraction, electron microprobe, IR and Mössbauer spectroscopy, and by analytical and high-resolution transmission electron microscopy. The crystals are optically isotropic, and the Fe-bearing samples are deep blue in color. Mössbauer spectroscopy and ELNE spectroscopy applied to the Fe-bearing samples indicates about 10% of the iron is in the ferric state. High-resolution TEM examination of one of the Fe-bearing samples indicates that the crystals are homogeneous and free of significant inclusions or exsolution features. Infrared spectra show a broad absorption band extending from about 2500 to 3600 cm⁻¹ with maxima ranging from 3105 for the pure magnesian samples to 3150 cm⁻¹ for the Fo₈₉ samples. The crystal structures of the seven ringwoodite samples were refined by X-ray single-crystal diffraction. Refinement of cation site occupancies indicates full occupancy of the tetrahedral site for all samples, whereas the occupancy of the octahedral site appears to decrease systematically with H content. The principal hydration mechanism involves octahedral cation vacancies. The IR spectra are consistent with protonation of the short O-O approach on the tetrahedral edge, which would imply partial Mg-Si disorder.