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# Tetrahedral ferric iron in oxidized hydrous wadsleyite

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## Abstract

Crystals of ferrous and ferric iron-bearing hydrous wadsleyite have been synthesized at 1400 °C and 12–13.5 GPa in a multi-anvil press. Crystal structures (atom positions, occupancies, and cell parameters) have been refined by single-crystal X-ray diffraction at ambient conditions. Assuming cation vacancies to be in the M3 site only, their concentration has been estimated from the unit-cell parameter *b*/*a* ratio. Total refined site Fe contents are consistent with microprobe chemical analysis. There appears to be up to 11% iron (presumably ferric) in the tetrahedral site, consistent with reduced silica content (<1 Si per 4 O atoms) in the chemical analysis. Also the volume of the tetrahedron increases with increasing ferric iron content. Strong ordering of Fe in the octahedral sites is apparent in the order FeM3 ≥ FeM1 >> FeM2. The presence of ferric iron in the mantle transition zone is expected to partition preferentially into wadsleyite and may expand the stability region of wadsleyite relative to olivine and ringwoodite. Also, the observation of tetrahedral ferric iron in these samples increases the likelihood that there is compositional continuity between wadsleyite and the spinelloid III phase field observed in the Mg-free system fayalite-magnetite.

**Keywords:** Wadsleyite, crystal structure, ferric iron, crystal chemistry, transition zone