

LETTER

**Coupled substitution of Fe<sup>3+</sup> and H<sup>+</sup> for Si in wadsleyite: A study by polarized infrared and Mössbauer spectroscopies and single-crystal X-ray diffraction**

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ABSTRACT

Coupled substitution of Fe<sup>3+</sup> and H<sup>+</sup> for Si in wadsleyite was studied by polarized infrared and Mössbauer spectroscopies and single-crystal X-ray diffraction. Single crystals of Fe-bearing hydrous wadsleyite were synthesized at 16 GPa and 1870 K using a Kawai-type multi-anvil apparatus. Water and Fe contents of the sample were 0.19–0.26 wt% H<sub>2</sub>O and Fe/(Mg+Fe) of 0.099(2), respectively. Mössbauer spectra showed 13(4)% Fe<sup>3+</sup>/ΣFe and Fe<sup>3+</sup> at the tetrahedral site with 5(3)% <sup>14</sup>Fe<sup>3+</sup>/ΣFe. Crystal structure refinement by single-crystal X-ray diffraction indicated that Fe (presumably Fe<sup>3+</sup>) occupied 4.9(5)% of the tetrahedral site. Infrared light polarized with the electric vector **E**//**a** and **c** was absorbed at 3477(2) cm<sup>-1</sup> while no absorption was observed at the region in spectra with **E**//**b**. The pleochroic behavior of the 3477 cm<sup>-1</sup> band can be interpreted as protonation of silicate oxygen O3 in Fe-bearing hydrous wadsleyite. The protonation of O3 together with the presence of Fe<sup>3+</sup> at the tetrahedral site confirms the coupled substitution of Fe<sup>3+</sup> and H<sup>+</sup> for Si in Fe-bearing hydrous wadsleyite.

**Keywords:** Wadsleyite, hydrogen, ferric iron, polarized infrared spectroscopy, single-crystal X-ray diffraction, Mössbauer spectroscopy