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LETTER

Coupled substitution of Fe^{3+} and H^+ 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^{3+} and H^+ 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_2O and Fe/(Mg+Fe) of 0.099(2), respectively. Mössbauer spectra showed 13(4)% $Fe^{3+}/\Sigma Fe$ and Fe^{3+} at the tetrahedral site with 5(3)% $^{IV}Fe^{3+}/\Sigma Fe$. Crystal structure refinement by single-crystal X-ray diffraction indicated that Fe (presumably Fe^{3+}) 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^{-1} while no absorption was observed at the region in spectra with **E**//**b**. The pleochroic behavior of the 3477 cm^{-1} 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^{3+} at the tetrahedral site confirms the coupled substitution of Fe^{3+} and H^+ for Si in Fe-bearing hydrous wadsleyite.

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