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Hydrogen position and hydrogen bonding in the phase E structure

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Phase E is one of dense hydrous magnesium silicates (DHMS) which play an important role to carry and reserve water in the Earth's interior. Phase E can be stable under PT conditions from the upper mantle to mantle transition zone. Hydrogen bonds are thought of influencing on physical property and stability fields of the DHMS in the Earth's interior.Crystallographically, the crystal structure of phase E is unique in the view of having short-range order but no long-range order with high disorder making vacancy of cations.
Therefore, it is important to understand how hydrogen bond is forming in the phase E. In the previous vibrational spectroscopic studies, hydrogen bond strength exist three or four kinds in the phase E structure. These things can be discussed precisely by being provided hydrogen site of phase E. Aim of this study is to determine a hydrogen position and discus about hydrogen bonding in the phase E structure.

Two samples were prepared to obtain information of hydrogen bond and hydrogen site, and structural changes of phase E. First is sample #1, which is Al, Fe-bearing phase E (Mg1.99Fe0.28 Al0.21Si1.20O6H2.03) synthesized at 9.3GPa, 875℃. The other is sample #2, which is Al-bearing phase E (Mg2.28Al0.12Si1.33O6H1.72) synthesized at 15GPa, 1000℃. Single crystal X-ray diffraction experiments using synchrotron radiation was conducted to obtain structural information and FT-IR observation was conducted to understand hydrogen bonding.

Difference Fourier map of the both samples showed the position of hydrogen site and site-splitting of oxygen. FT-IR spectrum showed that OH stretching peaks were observed at 3577, 3424, 3046 and 2467 cm-1 for sample #1 and 3599, 3406, 3005 and 2455cm-1 for sample#2, respectively. Based on the empirical calculation, O...O bond distances were 3.14-2,56A for sample #1 and 3.50-2.56A for sample #2, respectively. The environment around hydrogen of phase E is similar to that of brucite. Therefore, phase E structure can be featured by brucite-layer included SiO4 tetrahedra and M2O6 octahedra. Average structure is divided to three simple structural units. These three units are contained without long-range order in the phase E structure.
FT-IR spectra showed that phase E structure has a several kinds of hydrogen bonding such as brucite-like and more stronger one. These various hydrogen bonding can be explained by oxygen split model.

Keywords: phase E, Hydrogen bond, single crystal X-ray diffraction, IR spectroscopy