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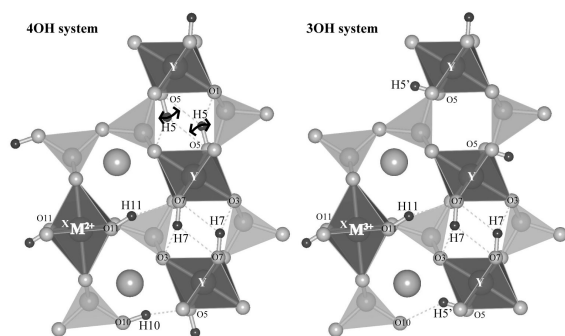
## Close relationship between oxidation state of transition elements and hydrogen-bonding system

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The behavior of hydrogen in minerals is one of the prominent topics in Earth Science. The numbers of hydroxyl groups in minerals are not necessarily fixed. In some cases, the exact number of hydroxyl groups depends on the concentration of divalent and trivalent cations in the octahedral sites. In pumpellyite-group minerals with the simplified formula of  $^{VII}W2^{VI}X^{VI}Y_2^{IV}Si_3O_{14-n}(OH)_n$  ( $Z = 4$ ), the Y site is generally only occupied by trivalent cations, and the X site is occupied by both divalent and trivalent cation. The  $M^{2+}/(M^{2+} + M^{3+})$  at X varies in a range of ca. 0.4-0.6. Thus, the number of OH, n in the formula, is 3-4. It means that pumpellyite with only divalent cations at the X site has four hydroxyl groups in the formula unit, but the number of hydroxyl groups will be three if only trivalent cations occupy the X site, as suggested by the substitutional scheme of  $M^{2+} + 4OH^- \leftrightarrow M^{3+} + 3OH^- + O^{2-}$ . It has been known that, in pumpellyite structure, hydroxyl groups are located at four oxygen positions, O5, O7, O10 and O11, and the hydrogen-bonding system in pumpellyite structure has been realized based on those hydroxyl groups. However, Nagashima et al. (2009, 2010) recently found two different hydrogen-bonding systems in pumpellyite and sursassite. Such situation that OH-bearing minerals have two or more different hydrogen-bonding systems can be also expected in other hydrous minerals containing transition elements.

In this presentation, I review and summarize the close relationship between oxidation state of transition elements and hydrogen-bonding systems in hydrous silicate minerals, and clarify the importance of further studies using neutron diffraction.



Hydrogen-bonding systems in pumpellyite (Nagashima et al. 2010)

Keywords: Hydrogen bond, Hydrous mineral, Transition element