Effect of Fe on the possible hydrogen atom positions in hydrous forsterite

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The result of the structural refinement of synthetic Fe-bearing hydrous forsterite (Kudoh et al., 2007) revealed that the cation vacancies at the octahedral M sites predominantly occur at the M2 site, in contrast to the case of Fe-free hydrous forsterite (Kudoh et al., 2006) in which the cation vacancies at the octahedral M sites predominantly occur at the M1 site.

In the case of Fe-free hydrous forsterite, the strain of M1-site may be larger than that of M2-site from the size expected for the ideal size of edge shared SiO4 tetrahedron. To minimize the strain, two H atoms may replace the Mg atom at the M1-site.

In the case of Fe-bearing hydrous forsterite, the Fe atoms occupy both M1 and M2 sites, leading the combinations of Mg-Mg, Fe-Fe, Mg-Fe and Fe-Mg for M1-M2 sites. Among these, the combination of Fe-Mg for M1-M2 sites may have maximum strain. To minimize the strain, two H atoms may replace the Mg atom at the M2-site.