Crystal structure of Fe-bearing hydrous forsterite and its possible hydrogen positions

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Crystal structure of Fe-bearing hydrous forsterite synthesized at 13.5 GPa and 1400 C was analized. The chemical formula is Mg1.85Fe0.14Si0.99H0.06O4 from the chemical composition by EPMA and H2O contents by FTIR using Bell (2003) and Patterson (1982) calibrations. X-ray diffraction data were measured using a single crystal with dimensions of 70 x 70 x 30 micron3. The unit cell parameters were determined with a four-circle diffractometer MXC3K of MAC Science Corporation(radiation = MoKa voltage = 50 kV, current = 20 mA), employing 25 reflections in the 2theta range 8 to 28. No undesirable features, such as peak broadening or streaks, were present in the XRD patterns. The space group and the unit cell parameters are: Pbnm, a=4.7621(24) A, b=10.2163(17)A, c=5.9899(21) A, V=291.41(18) A3.The single crystal X-ray diffraction intensities data were measured using synchrotron radiation (lambda=0.7006 A) at the beam line BL-10A, Photon Factory, High Energy Accelerator Reasearch Organization, Tukuba, Japan. From the 2314 reflections measured in the 1/4 sphere of sin(theta)/lambda = 1.03 A-1, 1,487 symmetry-independent reflections were obtained by averaging the symmetry equivalent intensities in the Laue group mmm (Rint = 0.026). No absorption correction was applied, because the value of mu∗r (0.09) was considered to be negligible. The refined structure (R=0.024, Rw=0.031 for 1214 reflections stronger than 3sigma(Io) yields the possibility of existing small amount of Fe at the Si site in addition to the existence of Fe at the Mg sites. Calculated bond distances indicate that the O2 and the O3 are the possible oxygen sites for hydrogen.