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Effect of iron on the compressibility of hydrous ringwoodite

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Abstract

Single crystals of hydrous ferroan ringwoodites with compositions $(Mg_{0.97}Fe_{1.00})_{1.97}Si_{0.98}H_{0.13}O_4$ and $(Mg_{1.21}Fe^{2+}_{0.66}Fe^{3+}_{0.1})_{1.97}Si_{0.97}H_{0.06}O_4$ have been synthesized. Their lattice parameters at ambient conditions are a = 8.1597(6) Å and V = 543.28(13) Å^3 and a = 8.1384(3) Å and V = 539.03(7) Å^3, respectively. The unit-cell lattice parameters were measured at different pressures up to about 9 GPa by means of X-ray single-crystal diffraction. The P-V data were fitted with a second-order Birch-Murnaghan equation of state (K' fixed to the value of 4) refining to the following equation of state parameters: V_0 = 543.32(7) Å^3 and K_{T0} = 186.5(9) GPa for $(Mg_{0.97}Fe_{1.00})_{1.97}Si_{0.98}H_{0.13}O_4$ and V_0 = 539.01(5) Å^3 and K_{T0} = 184.1(7) GPa for $(Mg_{1.21}Fe^{2+}_{0.66}Fe^{3+}_{0.1})_{1.97}Si_{0.97}H_{0.06}O_4$. Structural refinements indicate the presence of significant octahedral vacancies in sample $(Mg_{1.21}Fe^{2+}_{0.66}Fe^{3+}_{0.1})_{1.97}Si_{0.97}H_{0.06}O_4$ due to the oxidation of 0.1 apfu of ferric iron. Correlation between the O-O distances of the octahedral edges and the shift of the OH-stretching frequency suggest that the H incorporation occurs at the octahedral site.

Keywords: Compressibility, hydrous ringwoodite, single crystal, IR spectrum