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Crystal chemistry of chromian pumpellyite from Osayama, Okayama Prefecture, Japan

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ABSTRACT

The crystal structure and crystal chemistry of chromian pumpellyite from basic schist in the Osayama ultramafic body, Okayama, Japan, were investigated using electron probe microanalysis (EPMA), Fourier transform infrared spectroscopy (FTIR), and single-crystal X-ray diffraction to determine the distribution of chromium between two independent octahedral sites and structural changes caused by ionic substitutions in pumpellyite, ${}^{VII}W_8{}^{VI}X_4{}^{VI}Y_8{}^{IV}Z_{12}O_{56-n}(OH)_n$ ($Z = 1$). Five chromian pumpellyite crystals (ocp1211, ocp0604, ocp1028, ocp1013, and ocp1016) with 0.52, 1.65, 1.26, 1.94, and 1.43 Cr atoms per formula unit (apfu) (EPMA data), respectively, were picked from a hand specimen for X-ray diffraction analysis. The crystal structures (space group $C2/m$) of ocp1211 [a = 19.1129(6), b = 5.8963(5), c = 8.818(1) Å, β = 97.449(2)°], ocp0604 [a = 19.0935(4), b = 5.900(1), c = 8.810(2) Å, β = 97.540(7)°], ocp1028 [a = 19.105(2), b = 5.9021(6), c = 8.8143(7) Å, β = 97.513(3)°], ocp1013 [a = 19.1558(6), b = 5.9125(9), c = 8.844(1) Å, β = 97.448(4)°], and ocp1016 [a = 19.174(3), b = 5.9194(8), c = 8.830(1) Å, β = 97.497(4)°] were refined using 1058, 829, 1070, 1105, and 1095 unique reflections, and calculations converged at R factors of 4.08, 5.02, 6.32, 6.92, and 7.88%, respectively. The resulting site populations at the X and Y sites are $(Mg_{1.88}Al_{1.51}Fe^{2+}_{0.38}Cr_{0.16}Mn^{2+}_{0.05}Ni_{0.02})^X(Al_{7.90}Ti_{0.07}V_{0.03})^Y$ for ocp1211, $(Mg_{1.81}Al_{1.53}Cr_{0.42}Fe^{2+}_{0.18}Mn^{2+}_{0.04}Ni_{0.01})^X(Al_{7.34}Cr_{0.65}V_{0.01})^Y$ for ocp0604, $(Al_{1.62}Mg_{1.60}Cr_{0.61}Fe^{2+}_{0.13}Mn^{2+}_{0.03}Ni_{0.01})^X(Al_{7.36}Cr_{0.61}V_{0.03})^Y$ for ocp1028, $(Mg_{1.79}Al_{1.33}Cr_{0.47}Fe^{2+}_{0.33}Mn^{2+}_{0.08})^X(Al_{6.66}Cr_{1.31}V_{0.03})^Y$ for ocp1013, and $(Mg_{1.94}Al_{1.23}Cr_{0.38}Fe^{2+}_{0.37}Mn^{2+}_{0.08})^X(Al_{6.72}Cr_{1.25}V_{0.03})^Y$ for ocp1016. Cr^{3+} ions in ocp1211 are distributed only in the X site. The distribution coefficient of Cr and Al between the X and Y sites $[(Cr/Al)^X/(Cr/Al)^Y]$ is 1.66, 1.79, 3.09, and 4.54 for ocp1016, ocp1013, ocp0604, and ocp1028, respectively, indicating a stronger preference of Cr for the X site than the Y site. The a and b axes increase with increasing Cr content, whereas the c axis is almost constant. The mean Y-O distances increase linearly with increased Cr^{3+} content in the Y site. However, the mean X-O distances do not depend on the substitution of Cr^{3+} for Al^{3+} at the X site.

The bond valence sums and the difference-Fourier synthesis indicate that hydroxyl groups are located at the O5, O7, O10, and O11 positions. FTIR spectrum shows main absorption bands at ca. 2911, 3220, 3397, and 3512 cm^{-1} of OH-stretching vibrations, indicating the presence of OH···O hydrogen bonds.

Keywords: Pumpellyite, chromium, X-ray structural analysis, crystal chemistry, FTIR