American Mineralogist, Volume 94, pages 1351–1360, 2009

A crystal-chemical investigation of clinozoisite synthesized along the join $Ca_2Al_3Si_3O_{12}(OH)$-$Ca_2Al_2CrSi_3O_{12}(OH)$

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ABSTRACT

Cr^{3+}-bearing clinozoisite along the join $Ca_2Al_3Si_3O_{12}(OH)$-$Ca_2Al_2Cr^{3+}Si_3O_{12}(OH)$ was synthesized using cold-seal pressure vessels at P_{H_2O} = 0.35 to 0.40 GPa and T = 500 °C and a piston-cylinder apparatus at P_{H_2O} = 0.8 to 1.5 GPa and T = 500 to 800 °C. Gel-starting materials of $Ca_2Al_{3-q}Cr^{3+}_qSi_3O_{12.5}$ composition with q = 1.00, 0.75, 0.50, and 0.25 were employed to maximize the yields of clinozoisite. Mass fractions of clinozoisite in the experimental products with q = 0.50, 0.75, and 1 were about 70 to 90% along with lesser amounts of eskolaite, garnet, and quartz. Clinozoisite crystallized from the gel with q = 0.25 was associated only with zoisite. The crystal structures of clinozoisite in four runs, containing 0.28, 0.49, 0.50, and 0.62 Cr apfu were refined using X-ray powder diffraction data and the Rietveld method. The amount of Cr^{3+} at the octahedral M3 and M1 sites ranged from 0.37(1)–0.16(1) to 0.25(1)–0.12(1) apfu, respectively. Corresponding $K_D = (Cr^{3+}/Al)^{M1}/(Cr^{3+}/Al)^{M3}$ values range between 0.57 and 0.73. The M2 site contained only Al. The K_D values, and published results for intracrystalline partitioning in epidote and piemontite, show that the preference of Cr^{3+} for M1 is stronger than that of Fe^{3+} and Mn^{3+} in spite of the fact that most Cr^{3+} is partitioned into M3. Unit-cell parameters of clinozoisite increase with increasing Cr^{3+}. Variations in macroscopic unit-cell parameters can be related to variations in the local M3-O*i* and M1-O*i* distances.

Keywords: Clinozoisite, zoisite, chromium, synthesis, crystal chemistry, Rietveld refinement