Crystal chemistry of synthetic Ca₂Al₃Si₃O₁₂OH–Sr₂Al₃Si₃O₁₂OH solid-solution series of zoisite and clinozoisite

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ABSTRACT

Coexisting solid-solution series of synthetic zoisite-(Sr) and clinozoisite-(Sr) were synthesized in a 1 *M* (Ca,Sr)Cl₂ solution at 2.0 GPa, 600 °C for 6 days in a piston cylinder press. Solid solutions were synthesized from $X_{Sr}^{Qe} = Sr/(Ca + Sr) = 0.06$ to 1 and $X_{Sr}^{Cao} = 0.08$ to 0.5 in zoisite and clinozoisite, respectively. The products were characterized with SEM, EMP, and powder-XRD. Zoisites form crystals up to 30 µm in size. Lattice parameters of zoisite increase linearly with increasing Sr content. For synthetic zoisite-(Sr) lattice parameters are a = 16.3567(5) Å, b = 5.5992(2) Å, c = 10.2612(5) Å, and V = 939.78(7) Å³ in space group *Pnma*. Volume of clinozoisite (*P*2₁/*m*) increases with increasing X_{Sr}^{Cao} , but the lattice parameter *a* collapses, and *b*, *c*, and β have a discontinuity at $X_{Sr}^{Czo} \approx 0.25$. The decrease in angle β of clinozoisite results in compression of M3 and T3 polyhedra and increase of the A2 polyhedron. A1-O7 distance of 2.12 Å in clinozoisite is extremely short at $X_{Sr}^{Czo} \approx 0.25$, but with further Sr incorporation on A2 this distance relaxes quickly to 2.24 Å, combined with a torsion of T3. In zoisite, Sr incorporation leads to an opposite movement of neighboring octahedral chains parallel *a* and causes changes in the linked T3, and angle O5-T3-O6 increases with X_{Sr} from 96.3 to 101°. The intra-crystalline distribution of Sr shows that A2 is the favored position and continuous incorporation on A1-position starts above $X_{Sr}^{Zo} \approx 0.35$ for zoisite and above $X_{Sr}^{Zo} \approx 0.45$ for clinozoisite.

Keywords: Zoisite, clinozoisite, strontium, synthesis, solid-solution series, hydrothermal, EMP data, XRD data