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Structure and stability of the high-pressure phase, $Ca_3TiSi_2(Al,Ti,Si)_3O_{14}$

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ABSTRACT

The pressure and compositional dependence of element partitioning were examined in the pseudo-ternary section anorthite-titanite-perovskite of the system CaO-Al_2O_3-TiO_2-SiO_2. Preliminary phase relations in that section were experimentally determined at pressures from 1 atm to 1.5 GPa and at temperatures from 1300 to 1500 °C, using a double-ellipsoid mirror furnace and a piston cylinder apparatus. Further experiments were carried out with trace element extended compositions. All run products represent near-equilibrium parageneses consisting of crystals with their coexisting melt; the pairing is desired for element partitioning studies. At pressures above 1.0 GPa a new Ti-rich compound, having the ideal formula $Ca_3TiSi_2(Al,Ti,Si)_3O_{14}$, appears as the dominant phase in this paragenesis.

The composition and homogeneity of the phases were checked with electron microprobe and scanning electron microscopy. Determination of the structure of this compound was performed with a conventional four circle diffractometer on a single crystal, cut from a larger specimen of the equilibrium paragenesis. The compound crystallizes in space group *P*321 with cell dimensions $a = 7.943(1)$ Å and $c = 4.930(1)$ Å. Its structure consists of layers stacked parallel to (001) such that sheets of two types of corner-linked tetrahedra (T1 = Si; T2 = Al, Ti, Si) at $z = 1/2$ alternate with sheets centered at $z = 0$ containing $^{[6]}$Ti- and irregular eightfold-coordinated Ca-sites. A statistical distribution for Al, Si, and Ti atoms at one of the two tetrahedral sites in the crystal structure was confirmed by X-ray diffraction data. The Ti-octahedron is distorted, with Ti-O = 1.952(3) Å and O-Ti-O bond angles between 85.5° and 102.4°, which results in an angle bend of the vertex O atoms of 167.6°.