American Mineralogist, Volume 85, pages 1492–1496, 2000

High-pressure $Ca_4Al_6O_{13}$: An example of a calcium aluminate with three different types of coordination polyhedra for aluminum

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ABSTRACT

The crystal structure of tetracalcium trialuminate ($Ca_4Al_6O_{13}$), synthesized at 1250 °C and 2.5 GPa, has been determined from single-crystal X-ray data by direct methods [space group *Pcan*, Z = 8, a = 5.3002(2) Å, b = 17.7610(5), c = 21.0887(9) Å] and refined to $R1$ = 6.42%. The unit cell parameters of $Ca_4Al_6O_{13}$ exhibit a relationship to those of perovskite: $a \approx \sqrt{2}\ a_{Pv}$, $b \approx 5\ a_{Pv.}$ and $c \approx 4\sqrt{2}\ a_{Pv.}$. The diffraction data showed the typical features of a pseudotranslational symmetry: all reflections (*hkl*) with l equal 4n (n is an integer) had significantly higher intensity than the reflections with $l \neq 4n$. Furthermore, diffuse streaks parallel to b^* were observed. The new compound exhibits Al^{3+} in three different kinds of coordination polyhedra: octahedra, tetrahedra, and trigonal bipyramids. One of the two main building units is slightly corrugated sheets of perovskite-type corner sharing AlO_6 octahedra perpendicular to [010]. The octahedral sheets are connected by layers containing tetrahedral zweier single chains. Within these layers the tetrahedral chains are linked by two different kinds of rods containing distorted trigonal bipyramids sharing common corners and edges, respectively. The tetrahedral chains and the bipyramidal rods are parallel to [100]. Charge compensation is achieved by the Ca ions, which are coordinated by 9 or 10 oxygen cations.