

CRYSTAL STRUCTURE OF MONOCLINIC $\text{Sr}_{2.4}\text{Ca}_{0.6}\text{Al}_2\text{O}_6$

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Although the Portland cement related phases $\text{Sr}_x\text{Ca}_{3-x}\text{Al}_2\text{O}_6$ have been reported to crystallize in the cubic space group $Pa\bar{3}$ for the whole solid solution range, a monoclinic form of $\text{Sr}_{2.4}\text{Ca}_{0.6}\text{Al}_2\text{O}_6$ was prepared at 1300°C . Indexing the powder pattern was challenging; the strong split peaks could be indexing on a small orthorhombic cell, and the supercell tools in the old program NBS*LATTICE were used to identify a $32\times$ monoclinic supercell which accounted for all of the peaks. The space group was identified as $P2_1/c$ by examining possible distortions of the $Pa\bar{3}$ structure using ISODISTORT. $\text{Sr}_{2.4}\text{Ca}_{0.6}\text{Al}_2\text{O}_6$ crystallizes in $P2_1/c$, with $a = 15.7244(8)$, $b = 15.7361(2)$, $c = 15.7265(8)$ Å, $\beta = 90.6235(11)^\circ$, and $V = 3891.13(28)$ Å³. The lowering of the symmetry results in the presence of two independent 6-rings of corner-sharing AlO_4 tetrahedra; one 6-ring is more distorted than the other. The Sr/Ca are mostly ordered; at only one of the 20 alkaline earth sites is the occupation $\sim 50/50$. The Ca are not clustered in the unit cell. Symmetry mode analysis shows that the distortion from the cubic structure is complex, but concentrated in oxygen displacements in a few modes. The as-prepared sample contains some amorphous material, which hydrates to $\text{Sr}_3\text{Al}_2(\text{OH})_{12}$ on storage. Even in a combined synchrotron/laboratory Rietveld refinement (with extensive use of bonded and non-bonded distance restraints) it was difficult to obtain a precise structure. The final coordinates were determined by a density functional geometry optimization using the fixed experimental unit cell.