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Ca_2SiO_3OHF—A high-pressure phase with dense calcium polyhedral packing and tetrahedral silicon

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ABSTRACT

The composition and structure of a new phase crystallizing in high-pressure experiments in the system CaO-$Ca(OH)_2$-CaF_2-SiO_2 are described. The composition is on the join $Ca_2SiO_3(OH)_2$-$Ca_2SiO_3F_2$, with the relative amounts of OH and F near 50/50 from electron probe microanalysis, or near the ideal midpoint composition Ca_2SiO_3OHF. The symmetry is monoclinic, space group $P2_1/c$, with a = 5.8111(7), b = 10.6050(13), and c = 6.6968(8) Å, and β = 102.025(3)°, V = 403.65(8) Å^3, Z = 4. In the structure isolated SiO_3OH tetrahedral groups occupy narrow linear channels whose axes lie along **a**. The channels are lined by two types of eight-coordinated CaO_5OHF_2 polyhedra that share edges and faces. The axes of the channels lie on a nearly hexagonal array in the **b**-**c** plane, leading to a c_p/b ratio of 0.618, close to the ideal ratio of 0.577 for a hexagonal array. However, there is no simple packing rule for either the cation or anion array. Although the channels are arranged in a nearly hexagonal fashion, the overall symmetry of the structure is not hexagonal, but instead has 5-rings of calcium polyhedra around the channels. The calcium atoms lie on a 5-3-5-3 net of triangles and pentagons that can be compared to the α-U_3O_8 net.