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The structure of agrinierite: a Sr-containing uranyl oxide hydrate mineral

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ABSTRACT

The structure of agrinierite, $K_2(Ca_{0.65}Sr_{0.35})[(UO_2)_3O_3(OH)_2]_2 \cdot 5H_2O$, orthorhombic, *F*2*mm*, *Z* = 16, *a* = 14.094(2), *b* = 14.127(2), *c* = 24.106(4) Å, *V* = 4799.6(1) Å^3, was solved by direct methods and refined by full-matrix least-squares techniques to an agreement factor (*R*) of 6.55% and a goodness-of-fit (*S*) of 0.851 using 2710 independent observed reflections collected with Mo*K*α X-radiation and a CCD-based detector. This layered material contains four unique U^{6+} positions, each of which is part of a nearly linear $(UO_2)^{2+}$ uranyl ion. The U^{6+} cations are further coordinated by five anions occupying the equatorial vertices of pentagonal bipyramids that are capped by the uranyl ion O atoms. The uranyl polyhedra are linked by the sharing of equatorial vertices and edges in a fashion topologically identical to the α-U_3O_8 sheet found in billietite, protasite, becquerelite, richetite, compreignacite and masuyite. The arrangement of hydroxyl anions within the sheets varies in these minerals; that of agrinierite is identical to protasite. The cations (Ca, Sr, and K) and H_2O reside in the interlayer region of the structure. The inclusion of Sr in the structure of agrinierite suggests that the release of radioactive ^{90}Sr may be impacted by incorporation into this phase if it forms in a geological repository for nuclear waste.