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The structures of becquerelite and Sr-exchanged becquerelite

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ABSTRACT

The crystal structures of becquerelite, $Ca[(UO_2)_6O_4(OH)_6](H_2O)_8$, and Sr-exchanged becquerelite obtained by ion exchange, $Sr_{1.27}[(UO_2)_3O_{3.54}(OH)_{1.46}](H_2O)_3$, have been refined using diffraction data collected with Mo$K\alpha$ X-rays and a CCD-based detector. The structure of becquerelite, orthorhombic, space group $Pn2_1a$, a = 13.8527(5), b = 12.3929(4), c = 14.9297(5) Å, V = 2563.2(1) Å^3, has been refined on the basis of F^2 for 4875 unique reflections to $R1$ = 3.39%, calculated using 4581 unique observed reflections ($|F| \geq 4\sigma_F$), and a goodness-of-fit (S) of 1.04. Sr-exchanged becquerelite was obtained by placing single crystals of synthetic becquerelite in 2.5 M $SrCl_2$ solution for 60 h at 160 °C. The structure of Sr-exchanged becquerelite is trigonal, space group $P3$, a = 7.020(4), c = 6.992(6) Å, V = 298.4(3) Å^3, and has been refined on the basis of F^2 for 683 unique reflections to $R1$ = 4.26%, calculated using the 564 unique observed reflections ($|F| \geq 4\sigma_F$), and an S of 1.01. The results for becquerelite confirm the cation polyhedra and structural connectivity reported previously, but collection of data for a high-quality crystal using a CCD-based detector has substantially improved the precision of the atom positions. The structure contains α-U_3O_8-type sheets of uranyl pentagonal bipyramids, with a single symmetrically distinct Ca cation and eight symmetrically distinct H_2O groups located in the interlayer. The structure of Sr-exchanged becquerelite also contains α-U_3O_8-type sheets of uranyl pentagonal bipyramids, although the amount of H in the sheets is lower than for becquerelite. The interlayer contains two symmetrically distinct Sr cations and a single H_2O group. Ion exchange of Sr into the interlayer of becquerelite without destruction of the crystals has potential important implications for the mobility of ^{90}Sr in contaminated areas, and for the geologic disposal of nuclear waste.