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Structure and crystallization behavior of the (Ba,Sr)$HAsO_4 \cdot H_2O$ solid-solution in aqueous environments

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Abstract

Crystals of different members of the (Ba,Sr)$HAsO_4 \cdot H_2O$ solid solution have been synthesized, and the first structural studies indicate that they crystallize in the same space group, *Pbca*, with $Z = 8$. The unit-cell parameters are $a = 7.436(2)$, $b = 8.481(1)$, $c = 14.348(6)$ Å, and $a = 7.752(1)$, $b = 8.759(1)$, $c = 14.668(3)$ Å for the strontium and barium end-members, respectively. Both end-members have a layered structure with slices parallel to (001) linked by hydrogen bonds from the water molecules. These features are consistent with both the perfect cleavage on {001} and the morphological importance of this form in the crystals obtained. However, the two end-members are not isostructural and show differences in both the anionic hydrogen positions and number of hydrogen bonds. Complementary powder-diffraction measurements indicate that the cell parameters increase in a non-linear way with the barium content indicating that the solid solution is complete but could be non-ideal. Preliminary data suggest that barium partitions preferentially into the solid phase when crystallizing this solid solution from aqueous solutions.