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LETTER

Structure determination of the 2.5 hydrate $MgSO_4$ phase by simulated annealing

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ABSTRACT

The crystal structure of the 2.5 hydrate $MgSO_4$ phase was determined by simulated annealing from laboratory X-ray powder diffraction data measured from 2–140 °2θ using Cu$K\alpha$ radiation. The 2.5 hydrate is monoclinic, space group $C2/c$, with unit-cell parameters a = 18.8636(4) Å, b = 12.3391(2) Å, c = 8.9957(2) Å, β = 94.568(2)°, V = 2087.1(6) Å^3, and Z = 16. The model was refined using fundamental-parameters Rietveld refinement, converging to R_{wp} = 8.89%, R_p = 6.61%, R_{exp} = 3.33%, R_{Bragg} = 3.95%, and χ^2 = 2.67. The refined structure is consistent with a formula of 2.5 H_2O. Bond-valence calculations for the refined model show that the structure is chemically sensible. In the refined structure, $[Mg(O,H_2O)_6]$ octahedra and $[SO_4]$ tetrahedra build up 2-D double-sheet slabs by sharing vertex O atoms, which are held together by inter-slab H-bonds involving $(SO_4)^{2-}$ groups and H_2O molecules coordinated with Mg^{2+} cations to form the layer structure of the 2.5 hydrate phase.

Keywords: $MgSO_4 \cdot 2.5H_2O$, $MgSO_4 \cdot 2.4H_2O$, crystal structure, simulated annealing, structure determination, powder diffraction, Rietveld refinement