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LETTER

Determination of the crystal structure of sanderite, $MgSO_4 \cdot 2H_2O$, by X-ray powder diffraction and the charge flipping method

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ABSTRACT

The crystal structure of sanderite, $MgSO_4 \cdot 2H_2O$, was determined from laboratory X-ray powder diffraction data measured from 2–140 °2θ using Cu$K\alpha$ radiation. Sanderite is orthorhombic, space group $P2_12_12_1$, with unit-cell parameters a = 8.8932(1) Å, b = 8.4881(1) Å, c = 12.4401(2) Å, V = 939.16(3) Å^3, Z = 8. The crystal structure model was determined using the charge flipping method and was refined using fundamental parameters Rietveld refinement method to R_{wp} = 6.52%, R_{exp} = 1.89%, and χ^2 = 3.43. Bond-valence calculations for the refined model show that the structure is chemically reasonable. In the refined structure, Mg^{2+} cations are coordinated by four O atoms from $[SO_4]^{2-}$ groups and by two H_2O molecules, forming distorted octahedra. By sharing vertex O atoms, $[SO_4]$ tetrahedra and $[MgO_4(H_2O)_2]$ octahedra build up a 3-D framework.

Keywords: Sanderite, $MgSO_4 \cdot 2H_2O$, crystal structure, charge flipping, structure determination, powder diffraction