

LETTER

**Determination of the crystal structure of sanderite,  $\text{MgSO}_4 \cdot 2\text{H}_2\text{O}$ , by X-ray powder diffraction and the charge flipping method**

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ABSTRACT

The crystal structure of sanderite,  $\text{MgSO}_4 \cdot 2\text{H}_2\text{O}$ , was determined from laboratory X-ray powder diffraction data measured from 2–140 °2 $\theta$  using  $\text{CuK}\alpha$  radiation. Sanderite is orthorhombic, space group  $P2_12_12_1$ , with unit-cell parameters  $a = 8.8932(1) \text{ \AA}$ ,  $b = 8.4881(1) \text{ \AA}$ ,  $c = 12.4401(2) \text{ \AA}$ ,  $V = 939.16(3) \text{ \AA}^3$ ,  $Z = 8$ . The crystal structure model was determined using the charge flipping method and was refined using fundamental parameters Rietveld refinement method to  $R_{\text{wp}} = 6.52\%$ ,  $R_{\text{exp}} = 1.89\%$ , and  $\chi^2 = 3.43$ . Bond-valence calculations for the refined model show that the structure is chemically reasonable. In the refined structure,  $\text{Mg}^{2+}$  cations are coordinated by four O atoms from  $[\text{SO}_4]^{2-}$  groups and by two  $\text{H}_2\text{O}$  molecules, forming distorted octahedra. By sharing vertex O atoms,  $[\text{SO}_4]$  tetrahedra and  $[\text{MgO}_4(\text{H}_2\text{O})_2]$  octahedra build up a 3-D framework.

**Keywords:** Sanderite,  $\text{MgSO}_4 \cdot 2\text{H}_2\text{O}$ , crystal structure, charge flipping, structure determination, powder diffraction