

Structural trends for celestite (SrSO₄), anglesite (PbSO₄), and barite (BaSO₄): Confirmation of expected variations within the SO₄ groups

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ABSTRACT

The crystal structures of the isostructural orthorhombic sulfates celestite (SrSO₄), anglesite (PbSO₄), and barite (BaSO₄) were refined by Rietveld methods using synchrotron high-resolution powder X-ray diffraction (HRPXRD) data. Their structural model was refined in space group *Pbnm*. The unit-cell parameters are $a = 6.87032(3)$, $b = 8.36030(5)$, $c = 5.34732(1)$ Å, and $V = 307.139(3)$ Å³ for SrSO₄; $a = 6.95802(1)$, $b = 8.48024(3)$, $c = 5.39754(1)$ Å, and $V = 318.486(1)$ Å³ for PbSO₄; and $a = 7.15505(1)$, $b = 8.88101(3)$, $c = 5.45447(1)$ Å, and $V = 346.599(1)$ Å³ for BaSO₄. The average <M-O> [12] distances are 2.827(1), 2.865(1), and 2.953(1) Å for SrSO₄, PbSO₄, and BaSO₄, respectively, and their corresponding average <S-O> [4] distances are 1.480(1), 1.477(3), and 1.471(1) Å. The geometrical features of the SO₄ and MO₁₂ polyhedra become more symmetrical from SrSO₄ to BaSO₄. Across the series, the a , b , and c parameters vary non-linearly with increasing V . The radii of the M²⁺ cations, r_M , <M-O> [12], and <S-O> [4] distances vary linearly with V . These structural trends arise from the effective size of the M²⁺ cation (r_M : Sr < Pb < Ba) that is coordinated to 12 O atoms.

Keywords: Celestite, SrSO₄, anglesite, PbSO₄, barite, BaSO₄, Rietveld refinement, synchrotron high-resolution powder X-ray diffraction (HRPXRD), crystal structure