

# RIGID-BODY CHARACTER OF THE SO<sub>4</sub> GROUPS IN CELESTINE, ANGLESITE AND BARITE

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## ABSTRACT

The crystal structures of natural celestine (Sr<sub>1.00</sub>)SO<sub>4</sub>, anglesite (Pb<sub>0.99</sub>Sr<sub>0.01</sub>)SO<sub>4</sub>, and barite (Ba<sub>0.99</sub>Sr<sub>0.01</sub>)SO<sub>4</sub> have been refined in space group *Pbnm* utilizing rotating anode, Mo X-ray diffraction data from single crystals. Unit-cell parameters for celestine are *a* 6.8671(7), *b* 8.3545(8), and *c* 5.3458(6) Å, for anglesite, *a* 6.9549(9), *b* 8.472(1), and *c* 5.3973(8) Å, and for barite, *a* 7.154(1), *b* 8.879(2), and *c* 5.454(1) Å. Structural data are presented for these sulfates with greatly improved precision over previous studies due to high peak to background intensity ratios and precise analytical absorption corrections. The final model *R*(*F*) values are 0.025, 0.041, and 0.019, for celestine, anglesite, and barite, respectively. The average bond-distance from divalent cation to the nearest twelve oxygen atoms is 2.827(1) Å in celestine, 2.864(5) Å in anglesite, and 2.951(2) Å in barite. The average sulfur-to-oxygen bond distance is 1.475(2) Å in celestine, 1.476(6) Å in anglesite, and 1.476(2) Å in barite. The sulfate tetrahedra in each structure show very similar distortions that are attributed to the bonding of the various oxygen atoms to the divalent cations, which is similar in each structure. Thus, the different metal cations do not seem to affect the size or shape of the sulfate tetrahedra. An analysis of the displacement parameters suggests that the SO<sub>4</sub> groups behave as rigid molecular units, with an apparent shortening of the S–O bonds of 0.008–0.010 Å.

*Keywords:* sulfates, celestine, anglesite, barite, X-ray diffraction data, rigid-body motion.