

## Structural variations in the stibnite - bismuthinite solid solution series (Sb,Bi)<sub>2</sub>S<sub>3</sub>

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The structural variations in the stibnite (Sb<sub>2</sub>S<sub>3</sub>) - bismuthinite (Bi<sub>2</sub>S<sub>3</sub>) solid solution series have been determined through structural refinements of single crystal X-ray diffraction data for synthetic compounds of (Sb,Bi)<sub>2</sub>S<sub>3</sub>. The substitution of the Bi<sup>3+</sup> for Sb<sup>3+</sup> in the solid solution causes the expansion of the basic building block, which is responsible for the linear increase of the b lattice parameter. The increase of Bi content leads to not only expansion of the basic building block but also contraction of the intervals between their blocks, which contributes to the non-linear increase of both a and c lattice parameters. The coordination environments of the M cations form the (3 + 4) -fold at M1 site and the (5 + 2) -fold at M2 site in the solid solution series. For both M1 and M2 polyhedra, the short M-S bond lengths constantly increase with the increasing Bi concentration whereas the long M-S bond lengths continuously decrease in the polyhedra. The geometrical distributions of ligand atoms around the M cation come to form spherical coordinations because the higher Bi concentration the lower stereochemical activity of lone pair electrons. The M1S<sub>7</sub> polyhedra are usually larger than the M2S<sub>7</sub> polyhedra. Since the large Bi cation is forced to occupy into the small M2 site, the small M2 polyhedra are more expanded than the M1 polyhedra with increasing Bi content. Consequently, the Pnma (stibnite) --- P-1 (intermediate) --- Pnma (bismuthinite) phase transition is attributed to the difference in the magnitudes of stereoactive lone pair electrons.