

# **(C<sub>6</sub>N<sub>2</sub>H<sub>18</sub>)Sb<sub>4</sub>S<sub>7</sub> a Thioantimonate(III) with a Layered [Sb<sub>4</sub>S<sub>7</sub>]<sup>2-</sup> Anion in the Presence of a Diprotonated Amine as Structure Director**

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*Dedicated to Professor Wolfgang Jeitschko on the occasion of his 70<sup>th</sup> birthday*

The new thioantimonate(III) (C<sub>6</sub>N<sub>2</sub>H<sub>18</sub>)Sb<sub>4</sub>S<sub>7</sub> (C<sub>6</sub>N<sub>2</sub>H<sub>16</sub> = 1,6-diaminohexane) was synthesized under solvothermal conditions using Sb, S and 1,6-diaminohexane (1,6-DAH). The compound crystallizes as orange needles in the triclinic space group  $P\bar{1}$  with lattice parameters  $a = 6.9834(5)$ ,  $b = 11.8748(10)$ ,  $c = 13.6588(12)$  Å,  $\alpha = 115.248(9)$ ,  $\beta = 100.165(9)$  and  $\gamma = 92.568(9)^\circ$ . A central SbS<sub>4</sub> group shares edges with two other SbS<sub>4</sub> moieties forming Sb<sub>3</sub>S<sub>8</sub> units which are joined by SbS<sub>3</sub> pyramids sharing vertices to form a chain of alternating Sb<sub>3</sub>S<sub>8</sub> and SbS<sub>3</sub> units. One S atom of the SbS<sub>3</sub> pyramid connects neighboring chains into sheets which contain large Sb<sub>10</sub>S<sub>10</sub> heterorings. The sheets are then further connected into four atoms thick double sheets. Six edge-linked SbS<sub>4</sub> units are condensed yielding a complex Sb<sub>6</sub>S<sub>14</sub> building block. Layers of diprotonated amines and thioantimonate(III) layers are stacked along [001] in a sandwich-like fashion with an interlayer distance of 8.46 Å. The amine layer is two molecules thick with the amines being oriented parallel to the anionic layers. The title compound represents the first example for a layered [Sb<sub>4</sub>S<sub>7</sub>]<sup>2-</sup> anion with a diamine as structure director. The compound is an optical semiconductor with a band-gap of about 1.9 eV.

**Key words:** Thioantimonate(III), Solvothermal Synthesis, Crystal Structure, Optical Properties