

Pb(Pb<sub>0.3</sub>Sb<sub>0.7</sub>)<sub>2</sub>Sb<sub>2</sub>S<sub>7</sub>

*hP*72

(176)  $P6_3/m - h^{12}$

**Pb<sub>6</sub>Sb<sub>14</sub>S<sub>27</sub>** [1], zinckenite

Structural features: SbS<sub>6</sub> octahedra, (Sb,Pb)S<sub>5</sub> square pyramids and :SbS<sub>3</sub>  $\psi$ -tetrahedra (SbS<sub>8</sub> square antiprisms) share edges and vertices to form a 3D-framework; additional Pb in square antiprismatic voids.

Lebas G., Le Bihan M.T. (1976) [1]

Pb<sub>1.60</sub>S<sub>7</sub>Sb<sub>3.40</sub>

$a = 2.212$ ,  $c = 0.432$  nm,  $c/a = 0.195$ ,  $V = 1.8306$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	6 <i>h</i>	<i>m</i> ..	0.0	0.115	<sup>1</sup> / <sub>4</sub>		non-collinear Sb <sub>2</sub>
Sb2	6 <i>h</i>	<i>m</i> ..	0.104	0.348	<sup>1</sup> / <sub>4</sub>		octahedron S <sub>6</sub>
M3	6 <i>h</i>	<i>m</i> ..	0.108	0.518	<sup>1</sup> / <sub>4</sub>		square pyramid S <sub>5</sub>
Sb4	6 <i>h</i>	<i>m</i> ..	0.161	0.2	<sup>1</sup> / <sub>4</sub>		square antiprism S <sub>8</sub>
S5	6 <i>h</i>	<i>m</i> ..	0.232	0.598	<sup>1</sup> / <sub>4</sub>		single atom Sb
S6	6 <i>h</i>	<i>m</i> ..	0.255	0.435	<sup>1</sup> / <sub>4</sub>		tetrahedron Sb <sub>2</sub> Pb <sub>2</sub>
S7	6 <i>h</i>	<i>m</i> ..	0.277	0.172	<sup>1</sup> / <sub>4</sub>		non-coplanar triangle Sb <sub>3</sub>
S8	6 <i>h</i>	<i>m</i> ..	0.315	0.033	<sup>1</sup> / <sub>4</sub>		non-coplanar triangle Sb <sub>3</sub>
M9	6 <i>h</i>	<i>m</i> ..	0.344	0.4	<sup>1</sup> / <sub>4</sub>		square pyramid S <sub>5</sub>
S10	6 <i>h</i>	<i>m</i> ..	0.44	0.321	<sup>1</sup> / <sub>4</sub>		non-coplanar square Sb <sub>4</sub>
S11	6 <i>h</i>	<i>m</i> ..	0.497	0.081	<sup>1</sup> / <sub>4</sub>		non-coplanar square Sb <sub>4</sub>
Pb12	6 <i>h</i>	<i>m</i> ..	0.536	0.244	<sup>1</sup> / <sub>4</sub>		square antiprism S <sub>8</sub>

M3 = 0.6Sb + 0.4Pb; M9 = 0.8Sb + 0.2Pb

Transformation from published data ( $P6_3/m$  \*):  $y, x, -z$ ; origin shift 0 0 <sup>3</sup>/<sub>4</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.090

Remarks: Natural specimen from Oruro, Bolivia. Pb:Sb ratio 0.460 from chemical analysis. In [1] the origin of the cell is shifted by 0 0 <sup>1</sup>/<sub>4</sub> from the description in the International Tables for Crystallography. Average structure; additional reflections could be indexed with an 8-fold supercell (new axes 2a,2b,2c).

References: [1] Lebas G., Le Bihan M.T. (1976), Bull. Soc. Fr. Mineral. Cristallogr. 99, 351-360.