

$\text{Ba}_3\text{Sb}_7\text{Se}_3[\text{CO}_3]_{0.75}\text{O}_{9.75}$	<i>hP</i> 68	(176) $P6_3/m - i^3h^4fe$
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**Ba<sub>6</sub>[Sb<sub>12</sub>O<sub>18</sub>](SbSe<sub>3</sub>)<sub>2</sub>(CO<sub>3</sub>)<sub>1.5</sub>O<sub>1.5</sub>** [1], cetineite family

Structural features: :SbO<sub>3</sub>  $\psi$ -tetrahedra share vertices to form infinite tubes with Sb<sub>6</sub>O<sub>6</sub> rings parallel to [001]; single :SbSe<sub>3</sub>  $\psi$ -tetrahedra (orientational disorder up-down) between the tubes, Ba atoms and CO<sub>3</sub> trigonal units (partial disorder) in the tubes.

Wang X., Liebau F. (1999) [1]

Ba<sub>3</sub>C<sub>0.78</sub>O<sub>11.94</sub>Sb<sub>7</sub>Se<sub>3</sub>

$a = 1.4405$ ,  $c = 0.5616$  nm,  $c/a = 0.390$ ,  $V = 1.0092$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.104	0.065	0.107	0.49	single atom C
Se2	12 <i>i</i>	1	0.1655	0.5197	0.207	0.5	
O3	12 <i>i</i>	1	0.3461	0.0584	0.001		non-colinear Sb <sub>2</sub>
Ba4	6 <i>h</i>	<i>m</i> ..	0.0917	0.2498	<sup>1</sup> / <sub>4</sub>		10-vertex polyhedron O <sub>10</sub>
O5	6 <i>h</i>	<i>m</i> ..	0.347	0.22	<sup>1</sup> / <sub>4</sub>		non-colinear Sb <sub>2</sub>
Sb6	6 <i>h</i>	<i>m</i> ..	0.4015	0.3776	<sup>1</sup> / <sub>4</sub>		non-coplanar triangle O <sub>3</sub>
Sb7	6 <i>h</i>	<i>m</i> ..	0.4413	0.1586	<sup>1</sup> / <sub>4</sub>		non-coplanar triangle O <sub>3</sub>
Sb8	4 <i>f</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0991	0.5	single atom Sb
C9	4 <i>e</i>	3..	0	0	0.078	0.39	

Transformation from published data: *y*,*x*,*-z*; origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.063

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Wang X., Liebau F. (1999), Z. Kristallogr. 214, 820-834.