

$K_3Sb_{7.06}S_3O_9([OH]_{0.06}[H_2O]_{0.94})_3$	<i>hP60</i>	(176) $P6_3/m - i^2h^5fb$
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**$K_6[Sb_{12}O_{18}](SbS_3)_2Sb_{0.12}(OH)_{0.36}(H_2O)_{5.64}$**  [1], cetineite

Structural features:  $:SbO_3$   $\psi$ -tetrahedra share vertices to form infinite tubes with  $Sb_6O_6$  rings parallel to [001]; single  $:SbS_3$   $\psi$ -tetrahedra (orientational disorder up-down) between the tubes, K, additional Sb and  $(OH_2, OH)$  in the tubes.

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

$H_{5.82}K_3O_{12}S_3Sb_{7.06}$

$a = 1.4318$ ,  $c = 0.5633$  nm,  $c/a = 0.393$ ,  $V = 1.0001$  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	0.065	0.3599	0.0		non-colinear Sb <sub>2</sub>
S2	12 <i>i</i>	1	0.3653	0.5324	0.1942	0.5	
M3	6 <i>h</i>	<i>m..</i>	0.1417	0.0497	$\frac{1}{4}$		non-colinear Sb <sub>2</sub>
K4	6 <i>h</i>	<i>m..</i>	0.1826	0.2807	$\frac{1}{4}$		
O5	6 <i>h</i>	<i>m..</i>	0.3532	0.1232	$\frac{1}{4}$		non-colinear Sb <sub>2</sub>
Sb6	6 <i>h</i>	<i>m..</i>	0.40368	0.01413	$\frac{1}{4}$		non-coplanar triangle O <sub>3</sub>
Sb7	6 <i>h</i>	<i>m..</i>	0.45061	0.28261	$\frac{1}{4}$		non-coplanar triangle O <sub>3</sub>
Sb8	4 <i>f</i>	3.. $\frac{1}{3}$	$\frac{1}{3}$	$\frac{2}{3}$	0.1316	0.5	
Sb9	2 <i>b</i>	-3.. $\frac{1}{3}$	0	0	0	0.062	octahedron (OH <sub>2</sub> ) <sub>6</sub>

$M3 = 0.94OH_2 + 0.06OH$

Transformation from published data: origin shift 0 0  $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.060

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

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