

K₆[Sb₁₂O₁₈](SbSe₃)₂(H₂O)₆ [1], cetinite family

Structural features: :SbO₃ ψ -tetrahedra share vertices to form infinite tubes with Sb₆O₆ rings parallel to [001]; single :SbSe₃ ψ -tetrahedra (orientational disorder up-down) between the tubes, K and H₂O in the tubes. See Fig. IV.75.

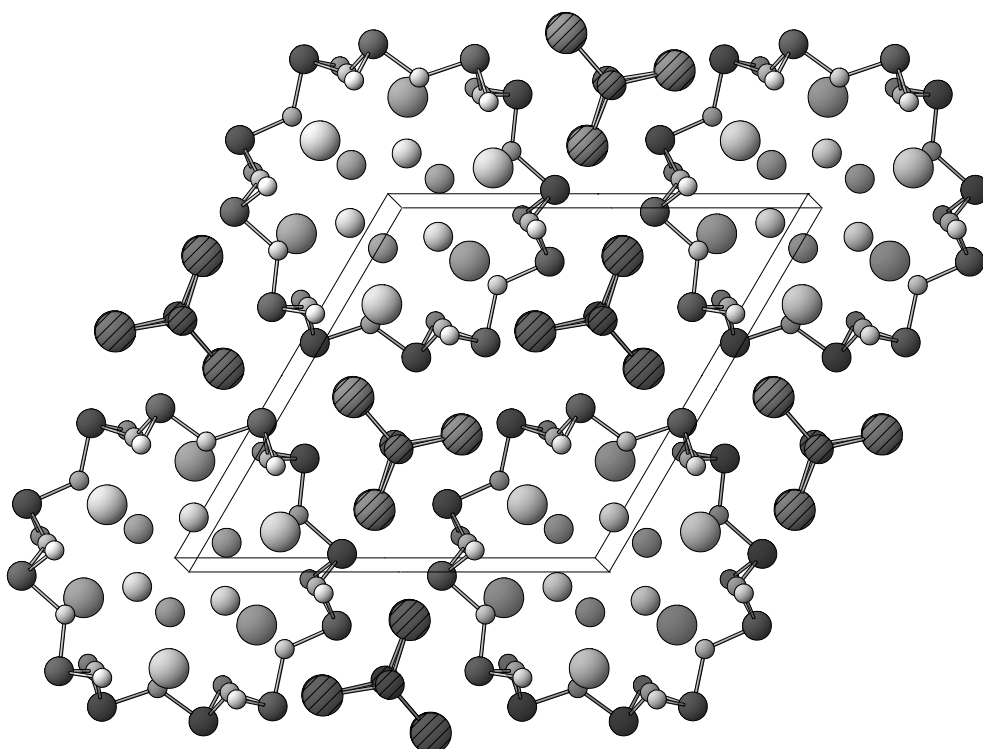


Fig. IV.75. **K₆[Sb₁₂O₁₈](SbSe₃)₂(H₂O)₆**

Arrangement of :SbO₃ ψ -tetrahedra (Sb atoms dark, O atoms light), :SbSe₃ ψ -tetrahedra (Sb atoms medium size hatched, Se atoms large hatched; partly occupied sites), K atoms (large light) and H₂O molecules (O atoms medium size light).

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

H₆K₃O₁₂Sb₇Se₃

$a = 1.463$, $c = 0.56164$ nm, $c/a = 0.384$, $V = 1.0411$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.0591	0.3502	0.001	0.5	non-collinear Sb ₂
Se2	12i	1	0.3682	0.5292	0.22		single atom O
(OH ₂)3	6h	$m..$	0.14	0.051	$\frac{1}{4}$		single atom O
K4	6h	$m..$	0.1749	0.275	$\frac{1}{4}$		single atom O
O5	6h	$m..$	0.3484	0.1267	$\frac{1}{4}$	0.5	non-collinear Sb ₂
Sb6	6h	$m..$	0.3997	0.0205	$\frac{1}{4}$		non-coplanar triangle O ₃
Sb7	6h	$m..$	0.4399	0.2824	$\frac{1}{4}$		non-coplanar triangle O ₃
Sb8	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0927		single atom Sb

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

Experimental: single crystal, diffractometer, X-rays, R = 0.041

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Average structure; the superstructure was refined in space group (173) $P6_3$ (new axes 2a,2b,c; R = 0.139).

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