

Sb[CNO]Cl<sub>4</sub>*hP48*(176) *P6<sub>3</sub>/m – ih*<sup>6</sup>**[SbCl<sub>4</sub>NCO]<sub>3</sub>** [1]

Structural features: C<sub>3</sub>N<sub>3</sub>O<sub>3</sub>Sb<sub>3</sub>Cl<sub>12</sub> units (a (C<sub>3</sub>N<sub>3</sub>) hexagon with an O bonded to each C, sharing atoms with three surrounding Sb(NOCl<sub>4</sub>) octahedra) in a Mg-type (h.c.p.) arrangement.

Müller U. (1976) [1]

CCl<sub>4</sub>NOSb*a* = 1.167, *c* = 0.995 nm, *c/a* = 0.853, *V* = 1.1735 nm<sup>3</sup>, *Z* = 6

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cl1	12 <i>i</i>	1	0.0642	0.3761	0.0185		single atom Sb
Sb2	6 <i>h</i>	<i>m</i> ..	0.04351	0.36195	<sup>1</sup> / <sub>4</sub>		octahedron ONCl <sub>4</sub>
Cl3	6 <i>h</i>	<i>m</i> ..	0.1845	0.0465	<sup>1</sup> / <sub>4</sub>		single atom Sb
N4	6 <i>h</i>	<i>m</i> ..	0.202	0.574	<sup>1</sup> / <sub>4</sub>		non-colinear C <sub>2</sub>
O5	6 <i>h</i>	<i>m</i> ..	0.25	0.414	<sup>1</sup> / <sub>4</sub>		single atom C
C6	6 <i>h</i>	<i>m</i> ..	0.297	0.537	<sup>1</sup> / <sub>4</sub>		coplanar triangle ON <sub>2</sub>
Cl7	6 <i>h</i>	<i>m</i> ..	0.5277	0.1364	<sup>1</sup> / <sub>4</sub>		single atom Sb

Transformation from published data: *y*,*x*,*-z*Experimental: single crystal, diffractometer, X-rays, *R* = 0.036References: [1] Müller U. (1976), *Z. Anorg. Allg. Chem.* 422, 141-148.