

CuTl[CO₃][OH]*hP42*(176) *P6₃/m – ih⁴g***TlCu(CO₃)(OH)** [1]

Structural features: Cu(O₂[OH]₂) squares and CO₃ trigonal units share vertices to form infinite chains parallel to [001].

Adam A., Zheng Y.Q. (1994) [1]

CCuHO₄Tl*a* = 1.0849, *c* = 0.6118 nm, *c/a* = 0.564, *V* = 0.6236 nm³, *Z* = 6

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.4471	0.1459	0.0658		single atom C
O2	6 <i>h</i>	<i>m</i> ..	0.1111	0.5073	¹ / ₄		non-colinear Cu ₂
Tl3	6 <i>h</i>	<i>m</i> ..	0.13185	0.28251	¹ / ₄		4-vertex polyhedron O ₄
O4	6 <i>h</i>	<i>m</i> ..	0.396	0.2906	¹ / ₄		single atom C
C5	6 <i>h</i>	<i>m</i> ..	0.4301	0.1948	¹ / ₄		coplanar triangle O ₃
Cu6	6 <i>g</i>	-1	¹ / ₂	0	0		coplanar square O ₄
H7	6 <i>h</i>	<i>m</i> ..	0.177	0.568	¹ / ₄		

Transformation from published data: origin shift 0 0 ¹/₂

Experimental: single crystal, diffractometer, X-rays, wR = 0.020

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Adam A., Zheng Y.Q. (1994), *Z. Anorg. Allg. Chem.* 620, 1707-1713.