

CsCuCl₃*hP*30(178) *P*6₁22 – *cb*²*a***CsCuCl₃** [2], perovskite 2H

Structural features: Close-packed CsCl₃ layers in h stacking; Cu in octahedral (Cl₆) voids. Infinite twisted chains of vertex-linked CuCl₄ squares (face-linked elongated CuCl₆ octahedra). Deformation derivative of BaNiO₃. See Fig. IV.47.

Christy A.G. et al. (1994) [1]

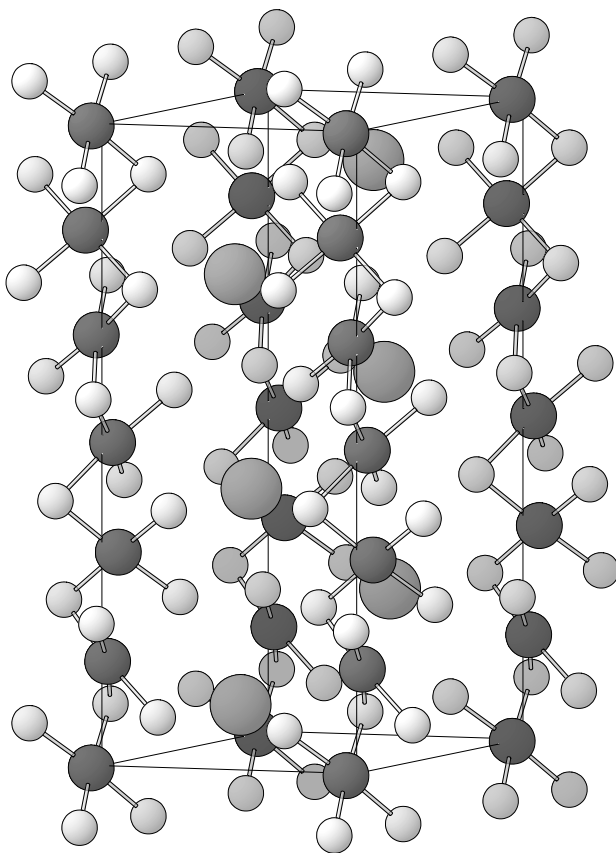
Cl₃CsCu*a* = 0.7218, *c* = 1.8183 nm, *c/a* = 2.519, *V* = 0.8204 nm³, *Z* = 6

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cl1	12 <i>c</i>	1	0.2119	0.3576	0.09093		non-colinear Cu ₂
Cs2	6 <i>b</i>	..2	0.355	0.71	1/4		bicapped square prism Cl ₁₀
Cl3	6 <i>b</i>	..2	0.8896	0.7792	1/4		non-colinear Cu ₂
Cu4	6 <i>a</i>	.2.	0.0644	0	0		coplanar square Cl ₄

Experimental: single crystal, diffractometer, X-rays, *wR* = 0.056

Remarks: In table 4 of [1] the Cl site in general position is misprinted as Cl1 instead of Cl2 (distinguished elsewhere).

References: [1] Christy A.G., Angel R.J., Haines J., Clark S.M. (1994), *J. Phys.: Condens. Matter* 6, 3125-3136. [2] Wells A.F. (1947), *J. Chem. Soc.* 1947, 1662-1670.

Fig. IV.47. **CsCuCl₃**

Arrangement of CuCl₄ squares (Cu atoms dark, Cl atoms light) and Cs atoms (large).