$CsCuCl_3$ Structure: A3BC_hP30_178_bc_b_a-001

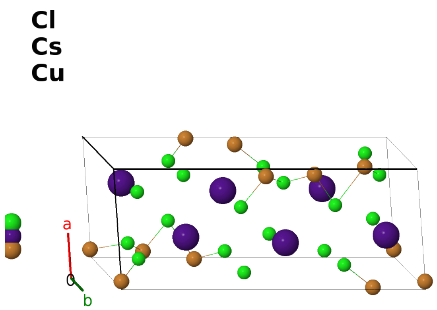
Cite this page as:

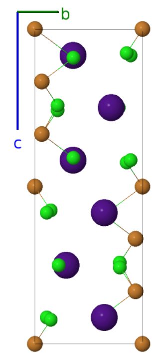
- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

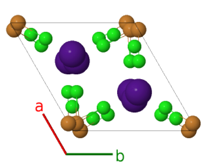
---

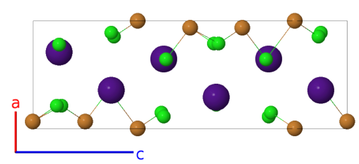
https://aflow.org/prototype-encyclopedia/8791

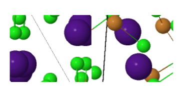
https://aflow.org/prototype-encyclopedia/A3BC_hP30_178_bc_b_a-001











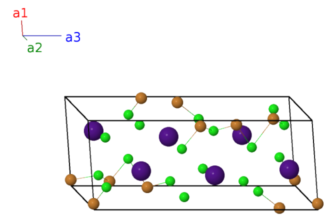
Prototype	Cl_3CsCu
AFLOW prototype label	A3BC_hP30_178_bc_b_a-001
ICSD	78435
CCDC	1638714
Pearson symbol	hP30
Space group number	178
Space group symbol	$P6_122$

AFLOW prototype command `aflow --proto=A3BC_hP30_178_bc_b_a-001`
`--params=`$a, c/a, x_1, x_2, x_3, x_4, y_4, z_4$

- (Christy, 1994) call this a "hexagonal perovskite" structure.
- This chiral structure can also be found in the enantiomorphic space group $P6_522$ #179. (Kousaka, 2014).
- We use the data taken at ambient pressure.

Hexagonal primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\mathbf{\hat{x}} - \tfrac{\sqrt{3}}{2}a\,\mathbf{\hat{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\mathbf{\hat{x}} + \tfrac{\sqrt{3}}{2}a\,\mathbf{\hat{y}} \\
\mathbf{a_3} &= c\,\mathbf{\hat{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1$	=	$\frac{1}{2}ax_1\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_1\,\mathbf{\hat{y}}$	(6a)	Cu I
$\mathbf{B_2}$	=	$x_1\,\mathbf{a}_2 + \frac{1}{3}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_1\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_1\,\mathbf{\hat{y}} + \frac{1}{3}c\,\mathbf{\hat{z}}$	(6a)	Cu I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \frac{2}{3}\,\mathbf{a}_3$	=	$-ax_1\,\mathbf{\hat{x}} + \frac{2}{3}c\,\mathbf{\hat{z}}$	(6a)	Cu I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_1\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_1\,\mathbf{\hat{y}} + \frac{1}{2}c\,\mathbf{\hat{z}}$	(6a)	Cu I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_2 + \frac{5}{6}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_1\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_1\,\mathbf{\hat{y}} + \frac{5}{6}c\,\mathbf{\hat{z}}$	(6a)	Cu I
$\mathbf{B_6}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + \frac{1}{6}\,\mathbf{a}_3$	=	$ax_1\,\mathbf{\hat{x}} + \frac{1}{6}c\,\mathbf{\hat{z}}$	(6a)	Cu I
$\mathbf{B_7}$	=	$x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_2\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_2\,\mathbf{\hat{y}} + \frac{1}{4}c\,\mathbf{\hat{z}}$	(6b)	Cl I
$\mathbf{B_8}$	=	$-2x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{7}{12}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_2\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_2\,\mathbf{\hat{y}} + \frac{7}{12}c\,\mathbf{\hat{z}}$	(6b)	Cl I
$\mathbf{B_9}$	=	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{11}{12}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_2\,\mathbf{\hat{y}} + \frac{11}{12}c\,\mathbf{\hat{z}}$	(6b)	Cl I
$\mathbf{B_{10}}$	=	$-x_2\,\mathbf{a}_1 - 2x_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_2\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_2\,\mathbf{\hat{y}} + \frac{3}{4}c\,\mathbf{\hat{z}}$	(6b)	Cl I
$\mathbf{B_{11}}$	=	$2x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{1}{12}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_2\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_2\,\mathbf{\hat{y}} + \frac{1}{12}c\,\mathbf{\hat{z}}$	(6b)	Cl I
$\mathbf{B_{12}}$	=	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{5}{12}\,\mathbf{a}_3$	=	$\sqrt{3}ax_2\,\mathbf{\hat{y}} + \frac{5}{12}c\,\mathbf{\hat{z}}$	(6b)	Cl I
$\mathbf{B_{13}}$	=	$x_3\,\mathbf{a}_1 + 2x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_3\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_3\,\mathbf{\hat{y}} + \frac{1}{4}c\,\mathbf{\hat{z}}$	(6b)	Cs I
$\mathbf{B_{14}}$	=	$-2x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{7}{12}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_3\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_3\,\mathbf{\hat{y}} + \frac{7}{12}c\,\mathbf{\hat{z}}$	(6b)	Cs I
$\mathbf{B_{15}}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{11}{12}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_3\,\mathbf{\hat{y}} + \frac{11}{12}c\,\mathbf{\hat{z}}$	(6b)	Cs I
$\mathbf{B_{16}}$	=	$-x_3\,\mathbf{a}_1 - 2x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_3\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_3\,\mathbf{\hat{y}} + \frac{3}{4}c\,\mathbf{\hat{z}}$	(6b)	Cs I
$\mathbf{B_{17}}$	=	$2x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{1}{12}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_3\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_3\,\mathbf{\hat{y}} + \frac{1}{12}c\,\mathbf{\hat{z}}$	(6b)	Cs I
$\mathbf{B_{18}}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{5}{12}\,\mathbf{a}_3$	=	$\sqrt{3}ax_3\,\mathbf{\hat{y}} + \frac{5}{12}c\,\mathbf{\hat{z}}$	(6b)	Cs I
$\mathbf{B_{19}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 + y_4)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(12c)	Cl II
$\mathbf{B_{20}}$	=	$-y_4\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - 2y_4)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_4\,\mathbf{\hat{y}} + c\left(z_4 + \frac{1}{3}\right)\,\mathbf{\hat{z}}$	(12c)	Cl II

$\mathbf{B_{21}}$	=	$-\left(x_4-y_4\right)\,\mathbf{a}_1-x_4\,\mathbf{a}_2+\left(z_4+\frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_4-y_4\right)\,\mathbf{\hat{x}}-\frac{\sqrt{3}}{2}ay_4\,\mathbf{\hat{y}}+\frac{1}{3}c\left(3z_4+2\right)\,\mathbf{\hat{z}}$	(12c)	Cl II
$\mathbf{B_{22}}$	=	$-x_4\,\mathbf{a}_1-y_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_4+y_4\right)\,\mathbf{\hat{x}}+\frac{\sqrt{3}}{2}a\left(x_4-y_4\right)\,\mathbf{\hat{y}}+c\left(z_4+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12c)	Cl II
$\mathbf{B_{23}}$	=	$y_4\,\mathbf{a}_1-\left(x_4-y_4\right)\,\mathbf{a}_2+\left(z_4+\frac{5}{6}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_4+2y_4\right)\,\mathbf{\hat{x}}-\frac{\sqrt{3}}{2}ax_4\,\mathbf{\hat{y}}+\frac{1}{6}c\left(6z_4+5\right)\,\mathbf{\hat{z}}$	(12c)	Cl II
$\mathbf{B_{24}}$	=	$\left(x_4-y_4\right)\,\mathbf{a}_1+x_4\,\mathbf{a}_2+\left(z_4+\frac{1}{6}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_4-y_4\right)\,\mathbf{\hat{x}}+\frac{\sqrt{3}}{2}ay_4\,\mathbf{\hat{y}}+c\left(z_4+\frac{1}{6}\right)\,\mathbf{\hat{z}}$	(12c)	Cl II
$\mathbf{B_{25}}$	=	$y_4\,\mathbf{a}_1+x_4\,\mathbf{a}_2-\left(z_4-\frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4+y_4\right)\,\mathbf{\hat{x}}+\frac{\sqrt{3}}{2}a\left(x_4-y_4\right)\,\mathbf{\hat{y}}-c\left(z_4-\frac{1}{3}\right)\,\mathbf{\hat{z}}$	(12c)	Cl II
$\mathbf{B_{26}}$	=	$\left(x_4-y_4\right)\,\mathbf{a}_1-y_4\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4-2y_4\right)\,\mathbf{\hat{x}}-\frac{\sqrt{3}}{2}ax_4\,\mathbf{\hat{y}}-cz_4\,\mathbf{\hat{z}}$	(12c)	Cl II
$\mathbf{B_{27}}$	=	$-x_4\,\mathbf{a}_1-\left(x_4-y_4\right)\,\mathbf{a}_2-\left(z_4-\frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_4-y_4\right)\,\mathbf{\hat{x}}+\frac{\sqrt{3}}{2}ay_4\,\mathbf{\hat{y}}-\frac{1}{3}c\left(3z_4-2\right)\,\mathbf{\hat{z}}$	(12c)	Cl II
$\mathbf{B_{28}}$	=	$-y_4\,\mathbf{a}_1-x_4\,\mathbf{a}_2-\left(z_4-\frac{5}{6}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_4+y_4\right)\,\mathbf{\hat{x}}-\frac{\sqrt{3}}{2}a\left(x_4-y_4\right)\,\mathbf{\hat{y}}-\frac{1}{6}c\left(6z_4-5\right)\,\mathbf{\hat{z}}$	(12c)	Cl II
$\mathbf{B_{29}}$	=	$-\left(x_4-y_4\right)\,\mathbf{a}_1+y_4\,\mathbf{a}_2-\left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_4+2y_4\right)\,\mathbf{\hat{x}}+\frac{\sqrt{3}}{2}ax_4\,\mathbf{\hat{y}}-c\left(z_4-\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12c)	Cl II
$\mathbf{B_{30}}$	=	$x_4\,\mathbf{a}_1+\left(x_4-y_4\right)\,\mathbf{a}_2-\left(z_4-\frac{1}{6}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_4-y_4\right)\,\mathbf{\hat{x}}-\frac{\sqrt{3}}{2}ay_4\,\mathbf{\hat{y}}-c\left(z_4-\frac{1}{6}\right)\,\mathbf{\hat{z}}$	(12c)	Cl II

References

[1] A. G. Christy, R. J. Angel, J. Haines, and S. M. Clark, *Crystal structural variation and phase transition in caesium trichlorocuprate at high pressure*, J. Phys.: Condens. Matter **6**, 3125–3136 (1994), doi:10.1088/0953-8984/6/17/005.

[2] Y. Kousaka, T. Koyama, M. Miyagawa, K. Tanaka, J. Akimitsu, and K. Inoue, *Crystal Growth of Chiral Magnetic Material in $CsCuCl_3$*, J. Phys.: Conf. Ser. **502**, 012019 (2014), doi:10.1088/1742-6596/502/1/012019. 1st Conference on Light and Particle Beams in Materials Science 2013.

Found in

[1] P. Villars, K. Cenzual, J. Daams, R. Gladyshevskii, O. Shcherban, V. Dubenskyy, N. Melnichenko-Koblyuk, O. Pavlyuk, I. Savesyuk, S. Stoiko, and L. Sysa, *Landolt-Börnstein - Group III Condensed Matter 43A4* (Springer-Verlag, Berlin Heidelberg, 2006), chap. Structure Types. Part 4: Space Groups (189)P-62m- (174)P-6 · $CsCuCl_3$, doi:10.1007/10920527_420.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.