$CsCuCl_3$ Structure: A3BC_hP30_178_bc_b_a-001

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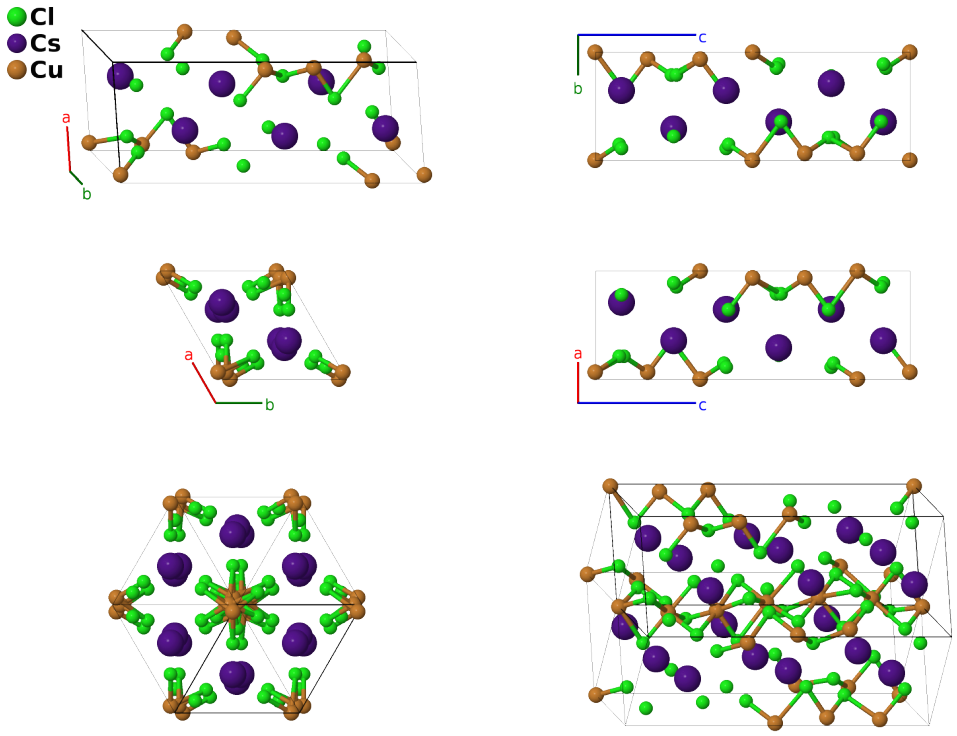
https://aflow.org/p/8791

https://aflow.org/p/A3BC_hP30_178_bc_b_a-001

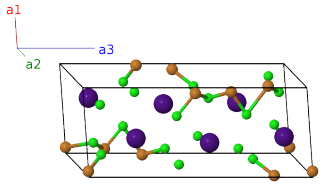


Prototype	Cl_3CsCu
AFLOW prototype label	A3BC_hP30_178_bc_b_a-001
ICSD	78435
Pearson symbol	hP30
Space group number	178
Space group symbol	$P6_122$
AFLOW prototype command	`aflow --proto=A3BC_hP30_178_bc_b_a-001 --params=`$a, c/a, x_1, x_2, x_3, x_4, y_4, z_4$

- (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

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1$	=	$\frac{1}{2}ax_1\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}}$	(6a)	Cu I
$\mathbf{B_2}$	=	$x_1\,\mathbf{a}_2 + \frac{1}{3}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_1\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$	(6a)	Cu I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \frac{2}{3}\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{2}{3}c\,\hat{\mathbf{z}}$	(6a)	Cu I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_1\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6a)	Cu I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_2 + \frac{5}{6}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_1\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \frac{5}{6}c\,\hat{\mathbf{z}}$	(6a)	Cu I
$\mathbf{B_6}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + \frac{1}{6}\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6a)	Cu I
$\mathbf{B_7}$	=	$x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6b)	Cl I
$\mathbf{B_8}$	=	$-2x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{7}{12}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{7}{12}c\,\hat{\mathbf{z}}$	(6b)	Cl I
$\mathbf{B_9}$	=	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{11}{12}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_2\,\hat{\mathbf{y}} + \frac{11}{12}c\,\hat{\mathbf{z}}$	(6b)	Cl I
$\mathbf{B_{10}}$	=	$-x_2\,\mathbf{a}_1 - 2x_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6b)	Cl I
$\mathbf{B_{11}}$	=	$2x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{1}{12}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{1}{12}c\,\hat{\mathbf{z}}$	(6b)	Cl I
$\mathbf{B_{12}}$	=	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{5}{12}\,\mathbf{a}_3$	=	$\sqrt{3}ax_2\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6b)	Cl I
$\mathbf{B_{13}}$	=	$x_3\,\mathbf{a}_1 + 2x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6b)	Cs I
$\mathbf{B_{14}}$	=	$-2x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{7}{12}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{7}{12}c\,\hat{\mathbf{z}}$	(6b)	Cs I
$\mathbf{B_{15}}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{11}{12}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_3\,\hat{\mathbf{y}} + \frac{11}{12}c\,\hat{\mathbf{z}}$	(6b)	Cs I
$\mathbf{B_{16}}$	=	$-x_3\,\mathbf{a}_1 - 2x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6b)	Cs I
$\mathbf{B_{17}}$	=	$2x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{1}{12}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{12}c\,\hat{\mathbf{z}}$	(6b)	Cs I
$\mathbf{B_{18}}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{5}{12}\,\mathbf{a}_3$	=	$\sqrt{3}ax_3\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6b)	Cs I
$\mathbf{B_{19}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12c)	Cl II
$\mathbf{B_{20}}$	=	$-y_4\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - 2y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(12c)	Cl II
$\mathbf{B_{21}}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(z_4 + \frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_4 + 2)\,\hat{\mathbf{z}}$	(12c)	Cl II
$\mathbf{B_{22}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12c)	Cl II
$\mathbf{B_{23}}$	=	$y_4\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{5}{6}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_4 + 2y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{6}c\,(6z_4 + 5)\,\hat{\mathbf{z}}$	(12c)	Cl II
$\mathbf{B_{24}}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{6}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{6}\right)\,\hat{\mathbf{z}}$	(12c)	Cl II
$\mathbf{B_{25}}$	=	$y_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(12c)	Cl II
$\mathbf{B_{26}}$	=	$(x_4 - y_4)\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - 2y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12c)	Cl II
$\mathbf{B_{27}}$	=	$-x_4\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 - \left(z_4 - \frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} - \frac{1}{3}c\,(3z_4 - 2)\,\hat{\mathbf{z}}$	(12c)	Cl II

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

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[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.

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