SC16 (CuCl) Structure: AB_cP16_205_c_c-001

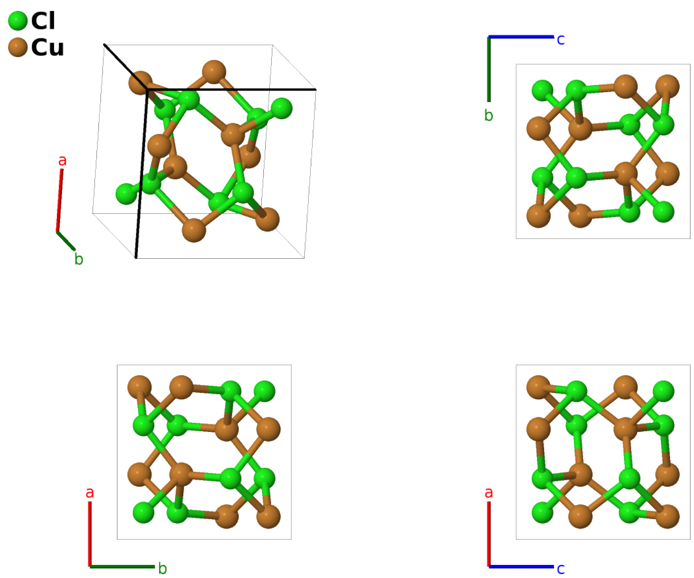
This structure originally had the label `AB_cP16_205_c_c`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

---

https://aflow.org/p/F4G8

https://aflow.org/p/AB_cP16_205_c_c-001



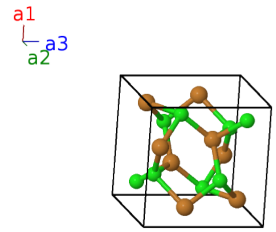
Prototype	ClCu
AFLOW prototype label	AB_cP16_205_c_c-001
ICSD	78271
Pearson symbol	cP16
Space group number	205
Space group symbol	$Pa\overline{3}$
AFLOW prototype command	`aflow --proto=AB_cP16_205_c_c-001` `--params=`a, x_1, x_2

Other compounds with this structure
BrCu

- This is a tetragonally bonded structure which packs more efficiently than diamond.
- This structure is related to BC8 in the same way that zincblende ($B3$) is related to diamond ($A4$): we replace half of the atoms by another species, such that the four nearest neighbors of each atom are of the other species. See (Crain, 1995) and references therein.
- The reference compound chosen here, found in (Hull, 1994), is stable at about 5 GPa.

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\mathbf{\hat{x}}$$
$$\mathbf{a_2} = a\,\mathbf{\hat{y}}$$
$$\mathbf{a_3} = a\,\mathbf{\hat{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\mathbf{\hat{x}} + ax_1\,\mathbf{\hat{y}} + ax_1\,\mathbf{\hat{z}}$	(8c)	Cl I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\mathbf{\hat{x}} - ax_1\,\mathbf{\hat{y}} + a\left(x_1 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8c)	Cl I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\mathbf{\hat{x}} + a\left(x_1 + \frac{1}{2}\right)\,\mathbf{\hat{y}} - a\left(x_1 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8c)	Cl I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\mathbf{\hat{x}} - a\left(x_1 - \frac{1}{2}\right)\,\mathbf{\hat{y}} - ax_1\,\mathbf{\hat{z}}$	(8c)	Cl I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\mathbf{\hat{x}} - ax_1\,\mathbf{\hat{y}} - ax_1\,\mathbf{\hat{z}}$	(8c)	Cl I
$\mathbf{B_6}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\mathbf{\hat{x}} + ax_1\,\mathbf{\hat{y}} - a\left(x_1 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8c)	Cl I
$\mathbf{B_7}$	=	$x_1\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_1\,\mathbf{\hat{x}} - a\left(x_1 - \frac{1}{2}\right)\,\mathbf{\hat{y}} + a\left(x_1 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8c)	Cl I
$\mathbf{B_8}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + a\left(x_1 + \frac{1}{2}\right)\,\mathbf{\hat{y}} + ax_1\,\mathbf{\hat{z}}$	(8c)	Cl I
$\mathbf{B_9}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\mathbf{\hat{x}} + ax_2\,\mathbf{\hat{y}} + ax_2\,\mathbf{\hat{z}}$	(8c)	Cu I
$\mathbf{B_{10}}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\mathbf{\hat{x}} - ax_2\,\mathbf{\hat{y}} + a\left(x_2 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8c)	Cu I
$\mathbf{B_{11}}$	=	$-x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\mathbf{\hat{x}} + a\left(x_2 + \frac{1}{2}\right)\,\mathbf{\hat{y}} - a\left(x_2 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8c)	Cu I
$\mathbf{B_{12}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\mathbf{\hat{x}} - a\left(x_2 - \frac{1}{2}\right)\,\mathbf{\hat{y}} - ax_2\,\mathbf{\hat{z}}$	(8c)	Cu I
$\mathbf{B_{13}}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\mathbf{\hat{x}} - ax_2\,\mathbf{\hat{y}} - ax_2\,\mathbf{\hat{z}}$	(8c)	Cu I
$\mathbf{B_{14}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\mathbf{\hat{x}} + ax_2\,\mathbf{\hat{y}} - a\left(x_2 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8c)	Cu I
$\mathbf{B_{15}}$	=	$x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\mathbf{\hat{x}} - a\left(x_2 - \frac{1}{2}\right)\,\mathbf{\hat{y}} + a\left(x_2 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8c)	Cu I
$\mathbf{B_{16}}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + a\left(x_2 + \frac{1}{2}\right)\,\mathbf{\hat{y}} + ax_2\,\mathbf{\hat{z}}$	(8c)	Cu I

References

[1] S. Hull and D. A. Keen, *High-pressure polymorphism of the copper(I) halides: A neutron-diffraction study to 10 GPa*, Phys. Rev. B **50**, 5868–5885 (1994), doi:10.1103/PhysRevB.50.5868.

[2] J. Crain, G. J. Ackland, and S. J. Clark, *Exotic structures of tetrahedral semiconductors*, Rep. Prog. Phys. **58**, 705–755 (1995), doi:10.1088/0034-4885/58/7/001.