

SC16 (CuCl) Structure:

AB_cP16_205_c_c-001

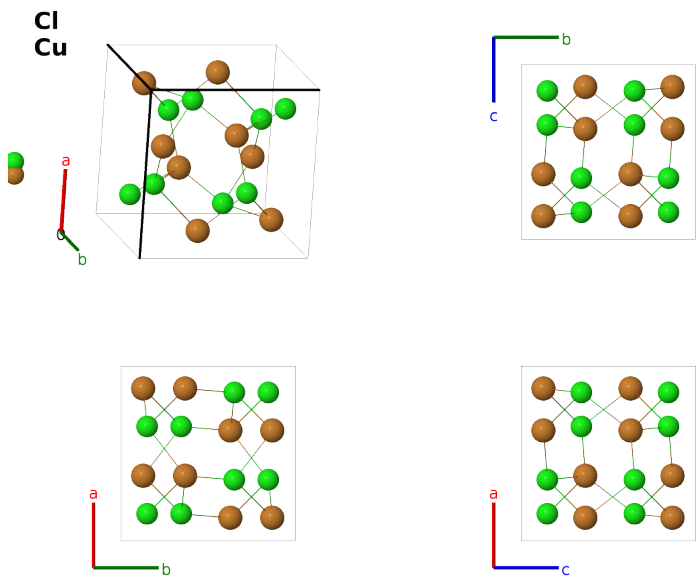
This structure previously used the label(s) **AB_cP16_205_c_c**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/F4G8>

https://aflow.org/prototype-encyclopedia/AB_cP16_205_c_c-001



Prototype	ClCu
AFLOW prototype label	AB_cP16_205_c_c-001
ICSD	78271
CCDC	1638556
Pearson symbol	cP16
Space group number	205
Space group symbol	$Pa\bar{3}$
AFLOW prototype command	<code>aflow --proto=AB_cP16_205_c_c-001</code> <code>--params=a, x_1, x_2</code>

Other compounds with this structure

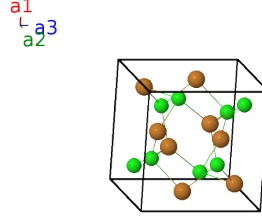
BrCu

- 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

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= a \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(8c)	Cl I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cl I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cl I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(8c)	Cl I
$\mathbf{B}_5$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(8c)	Cl I
$\mathbf{B}_6$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + x_1 \mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cl I
$\mathbf{B}_7$	$= x_1 \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cl I
$\mathbf{B}_8$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(8c)	Cl I
$\mathbf{B}_9$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B}_{10}$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B}_{11}$	$= -x_2 \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B}_{12}$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B}_{13}$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B}_{14}$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + x_2 \mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B}_{15}$	$= x_2 \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B}_{16}$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(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.

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