

α -CuAlCl₄ Structure: AB4C_tP12_112_b_n_e-001

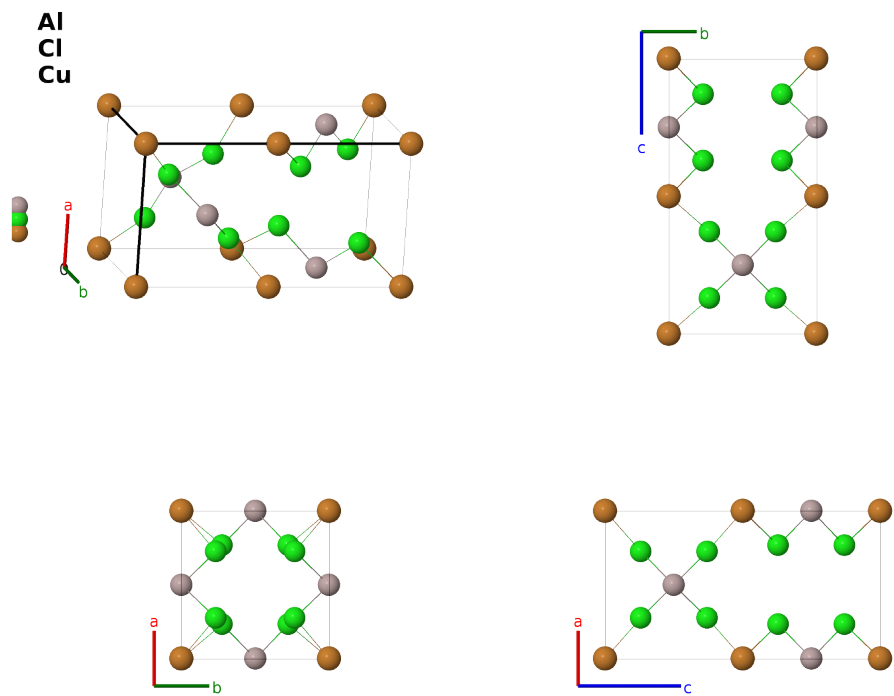
This structure previously used the label(s) **AB4C_tP12_112_b_n_e**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/FV74>

https://aflow.org/prototype-encyclopedia/AB4C_tP12_112_b_n_e-001



Prototype	AlCl ₄ Cu
AFLOW prototype label	AB4C_tP12_112_b_n_e-001
ICSD	165608
CCDC	121550
Pearson symbol	tP12
Space group number	112
Space group symbol	$P\bar{4}2c$
AFLOW prototype command	<code>aflow --proto=AB4C_tP12_112_b_n_e-001</code> <code>--params=a, c/a, x₃, y₃, z₃</code>

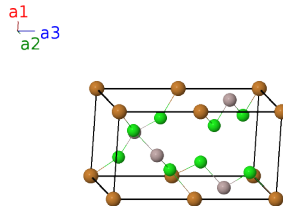
Other compounds with this structure

α -CuAlBr₄, α -CuAlCl₂Br₂, α -CuAlCl₃Br, α -CuAlClBr₃, α -CuGaBr₄, α -CuGaCl₄

- This is the ground state structure of CuAlCl₄. There is also a metastable orthorhombic β -CuAlCl₄ structure.
 - The lattice parameters and coordinates of the Wyckoff positions have been inferred from the distance and angular data in (Martin, 1998).
 - The ICSD entry from (Martin, 1998) refers to the related compound α -CuAlBr₄.
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Simple Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2b)	Al I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2b)	Al I
$\mathbf{B}_3$	$= 0$	$=$	0	(2e)	Cu I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	(2e)	Cu I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8n)	Cl I
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8n)	Cl I
$\mathbf{B}_7$	$= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8n)	Cl I
$\mathbf{B}_8$	$= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8n)	Cl I
$\mathbf{B}_9$	$= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8n)	Cl I
$\mathbf{B}_{10}$	$= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8n)	Cl I
$\mathbf{B}_{11}$	$= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8n)	Cl I
$\mathbf{B}_{12}$	$= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8n)	Cl I

References

- [1] J. D. Martin, B. R. Leafblad, R. M. Sullivan, and P. D. Boyle, α - and β -CuAlCl₄: *Framework Construction Using Corner-Shared Tetrahedral Metal-Halide Building Blocks* **37**, 1341–1346 (1998), doi:10.1021/ic971148v.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043