α-$CuAlCl_4$ Structure: AB4C_tP12_112_b_n_e-001

This structure originally had the label `AB4C_tP12_112_b_n_e`. Calls to that address will be redirected here.

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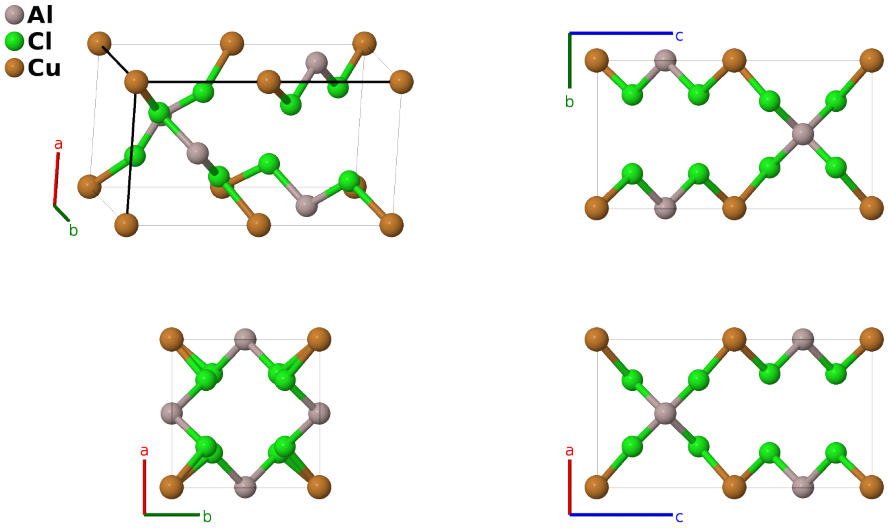
https://aflow.org/p/FV74

https://aflow.org/p/AB4C_tP12_112_b_n_e-001



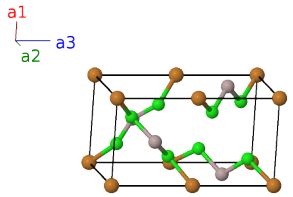
Prototype	$AlCl_4Cu$
AFLOW prototype label	AB4C_tP12_112_b_n_e-001
ICSD	165608
Pearson symbol	tP12
Space group number	112
Space group symbol	$P\bar{4}2c$
AFLOW prototype command	`aflow --proto=AB4C_tP12_112_b_n_e-001 --params=`$a, c/a, x_3, y_3, z_3$

Other compounds with this structure
α-$CuAlBr_4$, α-$CuAlCl_2Br_2$, α-$CuAlCl_3Br$, α-$CuAlClBr_3$, α-$CuGaBr_4$, α-$CuGaCl_4$

- This is the ground state structure of $CuAlCl_4$. There is also a metastable orthorhombic β-$CuAlCl_4$ 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-$CuAlBr_4$.

Simple Tetragonal primitive vectors

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



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-$CuAlCl_4$: 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.