

Al₂CuIr Structure:

A2BC_oC16_67_ag_b_g-001

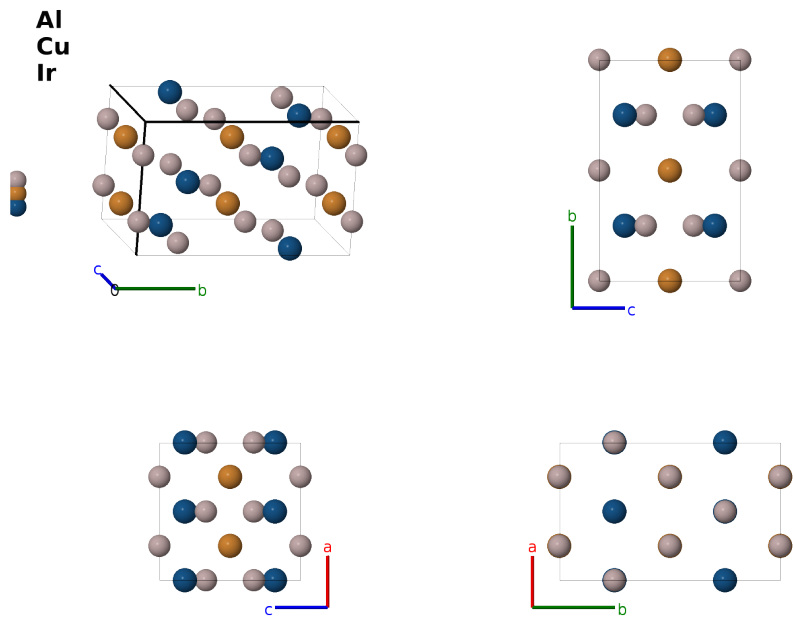
This structure previously used the label(s) **A2BC_oC16_67_ag_b_g**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/08UR>

https://aflow.org/prototype-encyclopedia/A2BC_oC16_67_ag_b_g-001



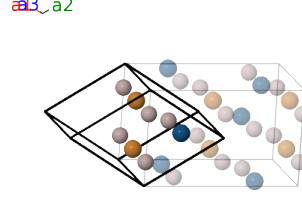
Prototype	Al ₂ CuIr
AFLOW prototype label	A2BC_oC16_67_ag_b_g-001
ICSD	167666
CCDC	1683559
Pearson symbol	oC16
Space group number	67
Space group symbol	<i>Cmme</i>
AFLOW prototype command	<code>aflow --proto=A2BC_oC16_67_ag_b_g-001 --params=a,b/a,c/a,z₃,z₄</code>

- We have shifted the origin to move the Al-I atoms to the (4a) Wyckoff positions.

- Al₂CuIr (A2BC_oC16_67_ag_b_g) and CuHoP₂ (ABC2_oC16_67_b_g_ag) have similar AFLOW prototype labels (i.e., same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Base-centered Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}}$	(4a)	Al I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{3}{4}a \hat{\mathbf{x}}$	(4a)	Al I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4b)	Cu I
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4b)	Cu I
$\mathbf{B}_5$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4g)	Al II
$\mathbf{B}_6$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4g)	Al II
$\mathbf{B}_7$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4g)	Ir I
$\mathbf{B}_8$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4g)	Ir I

References

- [1] L. Meshi, V. Ezersky, D. Kapush, and B. Grushko, *Crystal Structure of the Al₂CuIr Phase*, J. Alloys Compd. **496**, 208–211 (2010), doi:10.1016/j.jallcom.2010.02.129.

Found in

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

First cited in

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