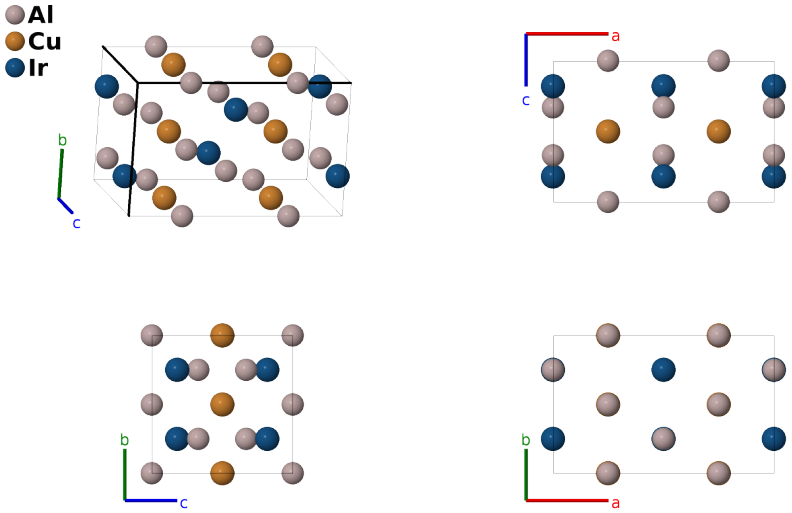
Al_2CuIr Structure: A2BC_oC16_67_ag_b_g-001

This structure originally had the label `A2BC_oC16_67_ag_b_g`. Calls to that address will be redirected here.

Cite this page as: 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

https://aflow.org/p/08UR

https://aflow.org/p/A2BC_oC16_67_ag_b_g-001

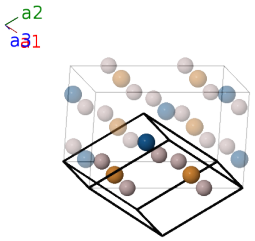


Prototype	Al_2CuIr
AFLOW prototype label	A2BC_oC16_67_ag_b_g-001
ICSD	167666
Pearson symbol	oC16
Space group number	67
Space group symbol	*Cmme*
AFLOW prototype command	`aflow --proto=A2BC_oC16_67_ag_b_g-001 --params=`$a, b/a, c/a, z_3, z_4$

- We have shifted the origin to move the Al-I atoms to the (4a) Wyckoff positions.
- Al_2CuIr (A2BC_oC16_67_ag_b_g) and $CuHoP_2$ (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

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\tfrac{1}{4}\,\mathbf{a}_1 + \tfrac{1}{4}\,\mathbf{a}_2$	=	$\tfrac{1}{4}a\,\hat{\mathbf{x}}$	(4a)	Al I
$\mathbf{B_2}$	=	$\tfrac{3}{4}\,\mathbf{a}_1 + \tfrac{3}{4}\,\mathbf{a}_2$	=	$\tfrac{3}{4}a\,\hat{\mathbf{x}}$	(4a)	Al I
$\mathbf{B_3}$	=	$\tfrac{1}{4}\,\mathbf{a}_1 + \tfrac{1}{4}\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3$	=	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(4b)	Cu I
$\mathbf{B_4}$	=	$\tfrac{3}{4}\,\mathbf{a}_1 + \tfrac{3}{4}\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3$	=	$\tfrac{3}{4}a\,\hat{\mathbf{x}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(4b)	Cu I
$\mathbf{B_5}$	=	$\tfrac{3}{4}\,\mathbf{a}_1 + \tfrac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4g)	Al II
$\mathbf{B_6}$	=	$\tfrac{1}{4}\,\mathbf{a}_1 + \tfrac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4g)	Al II
$\mathbf{B_7}$	=	$\tfrac{3}{4}\,\mathbf{a}_1 + \tfrac{1}{4}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{4}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4g)	Ir I
$\mathbf{B_8}$	=	$\tfrac{1}{4}\,\mathbf{a}_1 + \tfrac{3}{4}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{4}b\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4g)	Ir I

References

[1] L. Meshi, V. Ezersky, D. Kapush, and B. Grushko, *Crystal Structure of the Al_2CuIr 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.