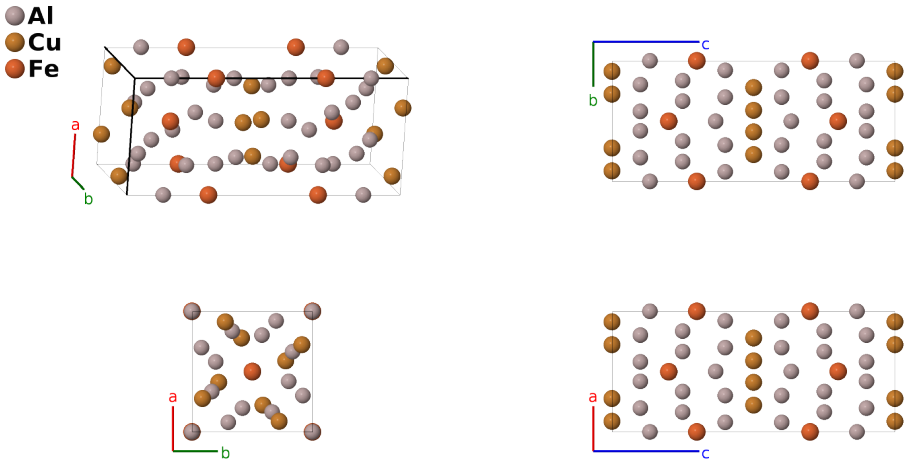
$FeCu_2Al_7$ ($E9_a$) Structure: A7B2C_tP40_128_egi_h_e-001

This structure originally had the label `A7B2C_tP40_128_egi_h_e`. 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/YX16

https://aflow.org/p/A7B2C_tP40_128_egi_h_e-001



Prototype	Al_7Cu_2Fe
AFLOW prototype label	A7B2C_tP40_128_egi_h_e-001
***Strukturbericht* designation**	$E9_a$
ICSD	57677
Pearson symbol	tP40
Space group number	128
Space group symbol	$P4/mnc$
AFLOW prototype command	`aflow --proto=A7B2C_tP40_128_egi_h_e-001 --params=`$a, c/a, z_1, z_2, x_3, x_4, y_4, x_5, y_5, z_5$

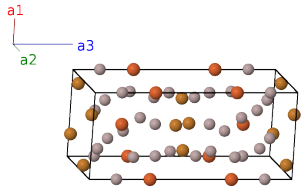
Other compounds with this structure

$CoCu_2Al_7$, $NiCu_3Al_6$, T(CoCuAl) – an alloy with approximate composition $Co_2Cu_{4.9}Al_{17.7}$

- Our original (Hicks, 2019) CIF for this structure has incorrect z-coordinates for the Al I and Fe I atoms. We have corrected the errors with this release.

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
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(4e)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Al I
$\mathbf{B_3}$	=	$-z_1\,\mathbf{a}_3$	=	$-cz_1\,\hat{\mathbf{z}}$	(4e)	Al I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Al I
$\mathbf{B_5}$	=	$z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(4e)	Fe I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Fe I
$\mathbf{B_7}$	=	$-z_2\,\mathbf{a}_3$	=	$-cz_2\,\hat{\mathbf{z}}$	(4e)	Fe I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Fe I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Al II
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Al II
$\mathbf{B_{11}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Al II
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Al II
$\mathbf{B_{13}}$	=	$-x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	Al II
$\mathbf{B_{14}}$	=	$x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	Al II
$\mathbf{B_{15}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	Al II
$\mathbf{B_{16}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	Al II
$\mathbf{B_{17}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}}$	(8h)	Cu I
$\mathbf{B_{18}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}}$	(8h)	Cu I
$\mathbf{B_{19}}$	=	$-y_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2$	=	$-ay_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(8h)	Cu I
$\mathbf{B_{20}}$	=	$y_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$ay_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(8h)	Cu I
$\mathbf{B_{21}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8h)	Cu I
$\mathbf{B_{22}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8h)	Cu I
$\mathbf{B_{23}}$	=	$\left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8h)	Cu I
$\mathbf{B_{24}}$	=	$-\left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8h)	Cu I
$\mathbf{B_{25}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16i)	Al III
$\mathbf{B_{26}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16i)	Al III
$\mathbf{B_{27}}$	=	$-y_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16i)	Al III
$\mathbf{B_{28}}$	=	$y_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16i)	Al III
$\mathbf{B_{29}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	Al III

$$\mathbf{B_{30}} = \left(x_5+\tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_5-\tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_5-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_5+\tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_5-\tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_5-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16i) \quad \text{Al III}$$

$$\mathbf{B_{31}} = \left(y_5+\tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_5+\tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_5-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(y_5+\tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_5+\tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_5-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16i) \quad \text{Al III}$$

$$\mathbf{B_{32}} = -\left(y_5-\tfrac{1}{2}\right)\mathbf{a}_1 - \left(x_5-\tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_5-\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(y_5-\tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_5-\tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_5-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16i) \quad \text{Al III}$$

$$\mathbf{B_{33}} = -x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}} \quad (16i) \quad \text{Al III}$$

$$\mathbf{B_{34}} = x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}} \quad (16i) \quad \text{Al III}$$

$$\mathbf{B_{35}} = y_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3 = ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}} \quad (16i) \quad \text{Al III}$$

$$\mathbf{B_{36}} = -y_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3 = -ay_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}} \quad (16i) \quad \text{Al III}$$

$$\mathbf{B_{37}} = \left(x_5+\tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_5-\tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_5+\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_5+\tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_5-\tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16i) \quad \text{Al III}$$

$$\mathbf{B_{38}} = -\left(x_5-\tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_5+\tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_5+\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_5-\tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_5+\tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16i) \quad \text{Al III}$$

$$\mathbf{B_{39}} = -\left(y_5-\tfrac{1}{2}\right)\mathbf{a}_1 - \left(x_5-\tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_5+\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(y_5-\tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_5-\tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16i) \quad \text{Al III}$$

$$\mathbf{B_{40}} = \left(y_5+\tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_5+\tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_5+\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(y_5+\tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_5+\tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16i) \quad \text{Al III}$$

References

[1] M. G. Bown and P. J. Brown, *The structure of $FeCu_2Al_7$ and T(CoCuAl)*, Acta Cryst. **9**, 911–914 (1956), doi:10.1107/S0365110X56002576.

[2] 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–S1011 (2019), doi:10.1016/j.commatsci.2018.10.043.