$Cu_2Fe[CN]_6$ Structure: A12B2C_cF60_196_h_ac_b-001

This structure originally had the label `A12B2C_cF60_196_h_bc_a`. Calls to that address will be redirected here.

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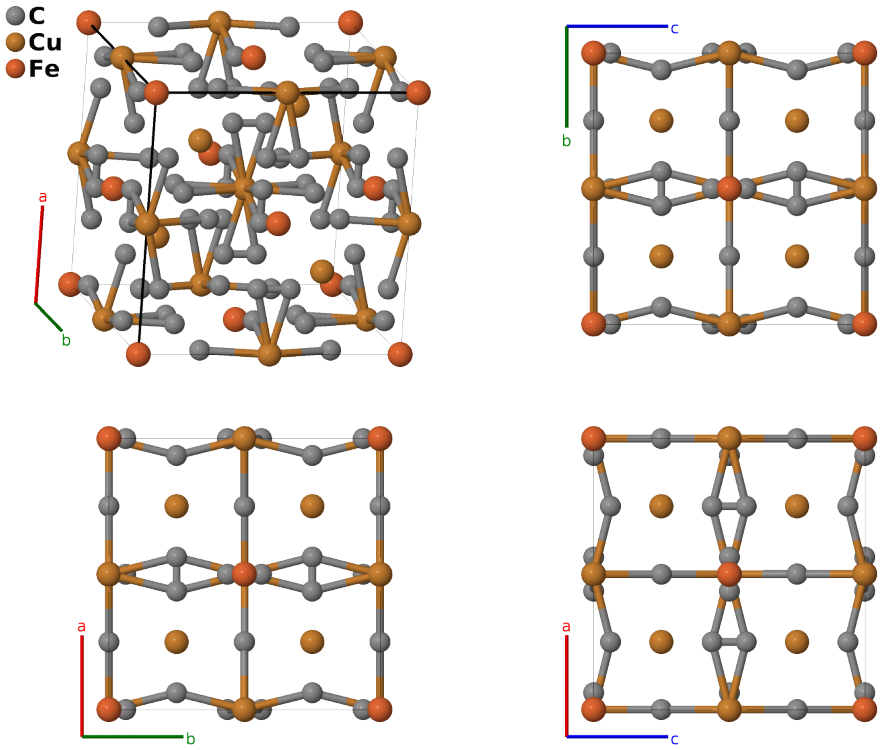
https://aflow.org/p/DJ7F

https://aflow.org/p/A12B2C_cF60_196_h_ac_b-001

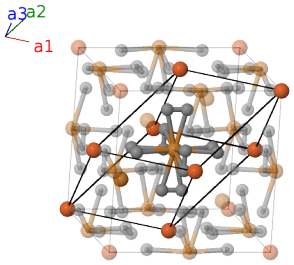


Prototype	$C_6Cu_2FeN_6$
AFLOW prototype label	A12B2C_cF60_196_h_ac_b-001
ICSD	none
Pearson symbol	cF60
Space group number	196
Space group symbol	$F23$
AFLOW prototype command	`aflow --proto=A12B2C_cF60_196_h_ac_b-001 --params=`a, x_4, y_4, z_4

- The sites we have labeled as carbon are actually a 50-50 mixture of carbon and nitrogen.
- This structure is taken from (Villars, 2013), repeated in (Villars, 2023). Our print versions of (Rigamonti, 1937) gives a structure consistent with the K_2PtCl_6 ($J1_1$) prototype.

Face-centered Cubic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(4b)	Fe I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(4c)	Cu II
$\mathbf{B_4}$	=	$(-x_4 + y_4 + z_4)\,\mathbf{a}_1 + (x_4 - y_4 + z_4)\,\mathbf{a}_2 + (x_4 + y_4 - z_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$	(48h)	C I
$\mathbf{B_5}$	=	$(x_4 - y_4 + z_4)\,\mathbf{a}_1 + (-x_4 + y_4 + z_4)\,\mathbf{a}_2 - (x_4 + y_4 + z_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$	(48h)	C I
$\mathbf{B_6}$	=	$(x_4 + y_4 - z_4)\,\mathbf{a}_1 - (x_4 + y_4 + z_4)\,\mathbf{a}_2 + (-x_4 + y_4 + z_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}}$	(48h)	C I
$\mathbf{B_7}$	=	$-(x_4 + y_4 + z_4)\,\mathbf{a}_1 + (x_4 + y_4 - z_4)\,\mathbf{a}_2 + (x_4 - y_4 + z_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}}$	(48h)	C I
$\mathbf{B_8}$	=	$(x_4 + y_4 - z_4)\,\mathbf{a}_1 + (-x_4 + y_4 + z_4)\,\mathbf{a}_2 + (x_4 - y_4 + z_4)\,\mathbf{a}_3$	=	$az_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ay_4\,\hat{\mathbf{z}}$	(48h)	C I
$\mathbf{B_9}$	=	$-(x_4 + y_4 + z_4)\,\mathbf{a}_1 + (x_4 - y_4 + z_4)\,\mathbf{a}_2 + (-x_4 + y_4 + z_4)\,\mathbf{a}_3$	=	$az_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ay_4\,\hat{\mathbf{z}}$	(48h)	C I
$\mathbf{B_{10}}$	=	$(-x_4 + y_4 + z_4)\,\mathbf{a}_1 + (x_4 + y_4 - z_4)\,\mathbf{a}_2 - (x_4 + y_4 + z_4)\,\mathbf{a}_3$	=	$-az_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + ay_4\,\hat{\mathbf{z}}$	(48h)	C I
$\mathbf{B_{11}}$	=	$(x_4 - y_4 + z_4)\,\mathbf{a}_1 - (x_4 + y_4 + z_4)\,\mathbf{a}_2 + (x_4 + y_4 - z_4)\,\mathbf{a}_3$	=	$-az_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - ay_4\,\hat{\mathbf{z}}$	(48h)	C I
$\mathbf{B_{12}}$	=	$(x_4 - y_4 + z_4)\,\mathbf{a}_1 + (x_4 + y_4 - z_4)\,\mathbf{a}_2 + (-x_4 + y_4 + z_4)\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} + az_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(48h)	C I
$\mathbf{B_{13}}$	=	$(-x_4 + y_4 + z_4)\,\mathbf{a}_1 - (x_4 + y_4 + z_4)\,\mathbf{a}_2 + (x_4 - y_4 + z_4)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} + az_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(48h)	C I

$\mathbf{B_{14}}$	$=$	$-(x_4+y_4+z_4)\,\mathbf{a}_1+$ $(-x_4+y_4+z_4)\,\mathbf{a}_2+$ $(x_4+y_4-z_4)\,\mathbf{a}_3$	$=$	$ay_4\,\hat{\mathbf{x}}-az_4\,\hat{\mathbf{y}}-ax_4\,\hat{\mathbf{z}}$	(48h)	C I
$\mathbf{B_{15}}$	$=$	$(x_4+y_4-z_4)\,\mathbf{a}_1+$ $(x_4-y_4+z_4)\,\mathbf{a}_2-$ $(x_4+y_4+z_4)\,\mathbf{a}_3$	$=$	$-ay_4\,\hat{\mathbf{x}}-az_4\,\hat{\mathbf{y}}+ax_4\,\hat{\mathbf{z}}$	(48h)	C I

References

[1] R. Rigamonti, *Structure of Cupriferrocyanides I. Copper Ferrocyanide and Potassium Copper Ferrocyanide*, Gazz. Chim. Ital. **67**, 137–146 (1937).

Found in

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

[2] P. Villars, *PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.)* (2023). Cu2Fe(CN)6 (Cu2Fe[CN]6) Crystal Structure, $sd_1902947$.