$Cu_3[Fe(CN)_6]_2 \cdot xH_2O$ ($J2_5$) Structure: A6B9CD2E6_cF96_225_e_af_b_c_e-001

This structure originally had the label `A6B9CD2E6_cF96_225_e_bf_a_c_e`. Calls to that address will be redirected here.

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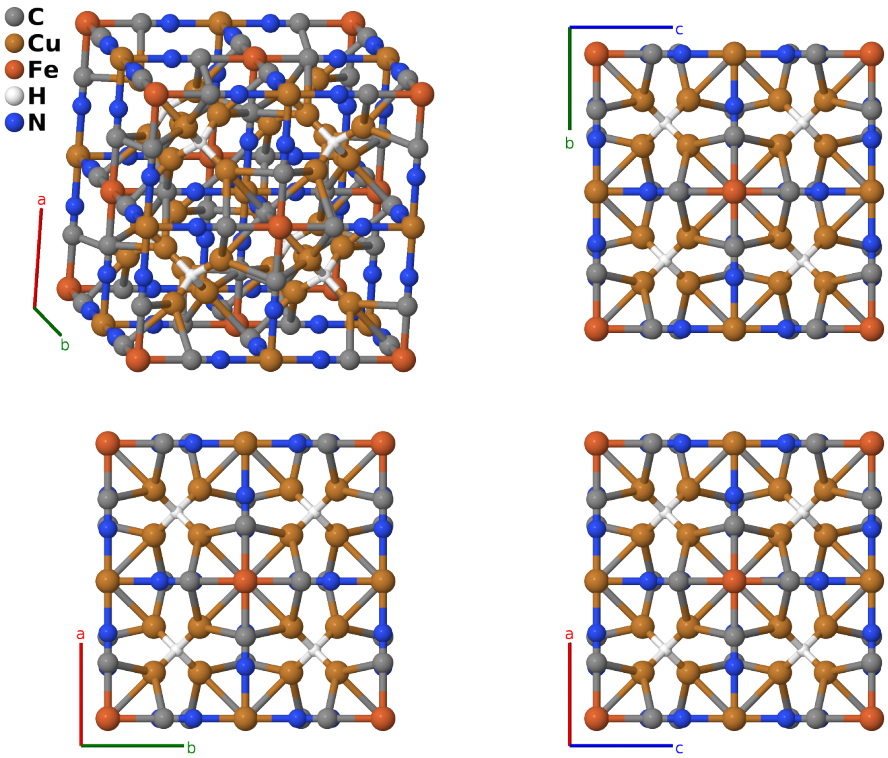
https://aflow.org/p/N4GS

https://aflow.org/p/A6B9CD2E6_cF96_225_e_af_b_c_e-001



Prototype	$C_{12}Cu_3Fe_2(H_2O)_xN_{12}$
AFLOW prototype label	A6B9CD2E6_cF96_225_e_af_b_c_e-001
***Strukturbericht* designation**	$J2_5$
Mineral name	prussian blue analog
ICSD	77916
Pearson symbol	cF96
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	`aflow --proto=A6B9CD2E6_cF96_225_e_af_b_c_e-001 --params=`a, x_4, x_5, x_6

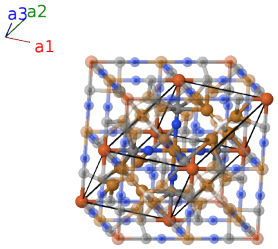
Other compounds with this structure

$Cd_3[Co(CN)_6]_2$, $Co_3[Co(CN)_6]_2$, $Cu_3[Fe(CN)_6]_2$, $Fe_3[Fe(CN)_6]_2$, $Td_3[Fe(CN)_6]_2$, $Zn_3[Fe(CN)_6]_2$

- These compounds form a class called "Prussian Blue Analogs," where Prussian Blue is $Fe_3[Fe(CN)_6]_2$.
- (van Bever, 1938) studied what he believed to be the hydrated form of this structure, with $x \approx 3$. In that case the water molecules occupy the (8c) sites, but each site is only occupied 75% of the time. The water sites are surrounded by a tetrahedron of copper (32e) sites, but only 6.25% of these sites are occupied.
- (Weiser, 1942) studied the anhydrous form. They found that copper atoms partially occupying the (32e) sites move to the (8c) site and replace the water molecules. This site is now fully occupied with copper.
- To convert from the hydrated to anhydrous structure, remove the copper (32e) molecules from the (32e) sites in the CIF or POSCAR file, and relabel the (8c) site as copper.
- For a picture of the resulting structure see (Jiao, 2017).
- The AFLOW label models the structure as if the sites were fully occupied.

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
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	H I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(8c)	H I
$\mathbf{B_5}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}$	(24e)	C I
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}$	(24e)	C I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{y}}$	(24e)	C I
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{y}}$	(24e)	C I
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{z}}$	(24e)	C I
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{z}}$	(24e)	C I
$\mathbf{B_{11}}$	=	$-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}$	(24e)	N I
$\mathbf{B_{12}}$	=	$x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}$	(24e)	N I
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{y}}$	(24e)	N I
$\mathbf{B_{14}}$	=	$-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{y}}$	(24e)	N I
$\mathbf{B_{15}}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{z}}$	(24e)	N I
$\mathbf{B_{16}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{z}}$	(24e)	N I
$\mathbf{B_{17}}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(32f)	Cu II
$\mathbf{B_{18}}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - 3x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(32f)	Cu II
$\mathbf{B_{19}}$	=	$x_6\,\mathbf{a}_1 - 3x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(32f)	Cu II

$\mathbf{B_{20}}$	=	$-3x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(32f)	Cu II
$\mathbf{B_{21}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + 3x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(32f)	Cu II
$\mathbf{B_{22}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(32f)	Cu II
$\mathbf{B_{23}}$	=	$-x_6\,\mathbf{a}_1 + 3x_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(32f)	Cu II
$\mathbf{B_{24}}$	=	$3x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(32f)	Cu II

References

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[3] S. Jiao, J. Tu, H. Xie, Z. Cai, S. Wang, and J. Zhu, *The electrochemical performance of $Cu_3[Fe(CN)_6]_2$ as a cathode material for sodium-ion batteries*, Mater. Res. Bull. **86**, 194–200 (2017), doi:10.1016/j.materresbull.2016.10.019.