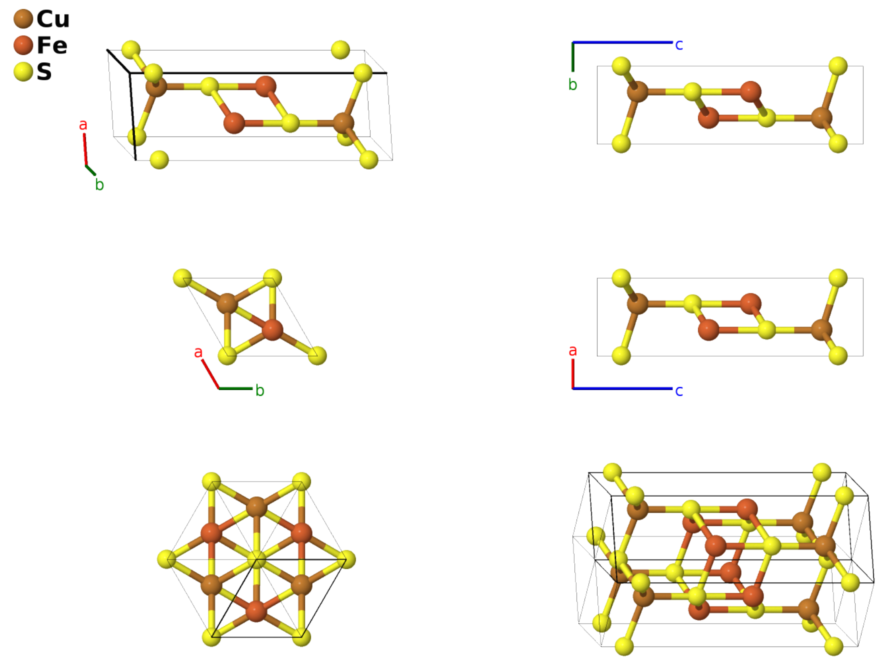
Nukundamite [$(Cu_{1-x}Fe_x)_4S_4$] Structure: ABC2_hP8_164_d_d_cd-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

---

https://aflow.org/p/CG4B

https://aflow.org/p/ABC2_hP8_164_d_d_cd-001

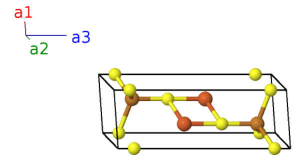


Prototype	$Cu_{1-x}Fe_xS_4$
AFLOW prototype label	ABC2_hP8_164_d_d_cd-001
Mineral name	nukundamite
ICSD	100727
Pearson symbol	hP8
Space group number	164
Space group symbol	$P\bar{3}m1$
AFLOW prototype command	`aflow --proto=ABC2_hP8_164_d_d_cd-001` `--params=`$a, c/a, z_1, z_2, z_3, z_4$

- The sample studied here has x = 0.1525. Presumably the copper and iron atoms are evenly distributed on each site, but for illustrative purposes we label the first (2d) site "Cu" and the second "Fe." In reality both sites have the approximate composition $Cu_{0.8475}Fe_{0.1525}$.

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \frac{1}{2} a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2} a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2c)	S I
$\mathbf{B_2}$	=	$-z_1\,\mathbf{a}_3$	=	$-cz_1\,\hat{\mathbf{z}}$	(2c)	S I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2d)	Cu I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2d)	Cu I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2d)	Fe I
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2d)	Fe I
$\mathbf{B_7}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2d)	S II
$\mathbf{B_8}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(2d)	S II

References

[1] A. Sugaki, H. Shima, A. Kitakaze, and T. Mizota, *Hydrothermal synthesis of nukundamite and its crystal structure*, Am. Mineral. **66**, 398–402 (1981).

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).