$F6_1$ Chalcopyrite ($CuFeS_2$) Structure (*Obsolete*): ABC2_tP4_115_a_c_g-001

This structure originally had the label `ABC2_tP4_115_a_c_g`. Calls to that address will be redirected here.

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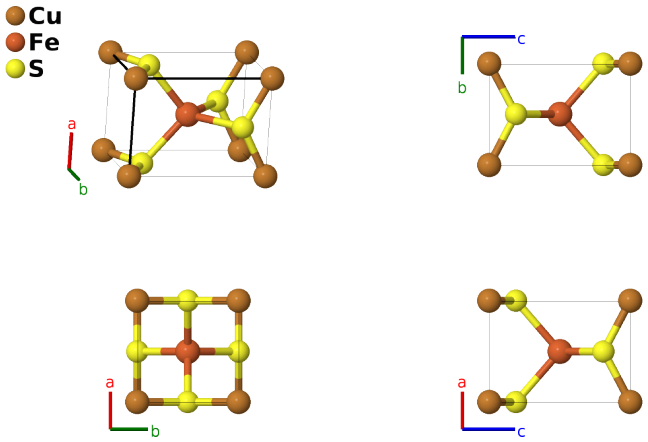
https://aflow.org/p/88N3

https://aflow.org/p/ABC2_tP4_115_a_c_g-001

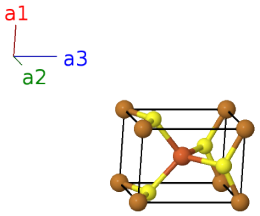


Prototype	$CuFeS_2$
AFLOW prototype label	ABC2_tP4_115_a_c_g-001
***Strukturbericht* designation**	$F6_1$
Mineral name	chalcopyrite
ICSD	27653
Pearson symbol	tP4
Space group number	115
Space group symbol	$P\bar{4}m2$
AFLOW prototype command	`aflow --proto=ABC2_tP4_115_a_c_g-001 --params=`$a, c/a, z_3$

- This structure was presented as the Chalcopyrite structure and given the *Strukturbericht* designatiion $F6_1$ in (Ewald, 1931). It was subsequently replaced with the $E1_1$ (ABC2_tI16_122_a_b_d) structure, which is now the accepted structure for chalcopyrite and similar compounds. We include the $F6_1$ structure as part of this historical record.

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
$\mathbf{B_1}$	=	0	=	0	(1a)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(1c)	Fe I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2g)	S I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_3\,\hat{\mathbf{z}}$	(2g)	S I

References

[1] R. Großand N. Groß, *Die Atomanordnung des Kupferkieses und die Struktur der Beruehrungsflaechen gesetzmaessig verwachsener Kristalle*, Neues Jahrb. f. Min. Beil. **48**, 113–135 (1923).

Found in

[1] P. P. Ewald and C. Hermann, eds., *Strukturbericht 1913-1928* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1931).