

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

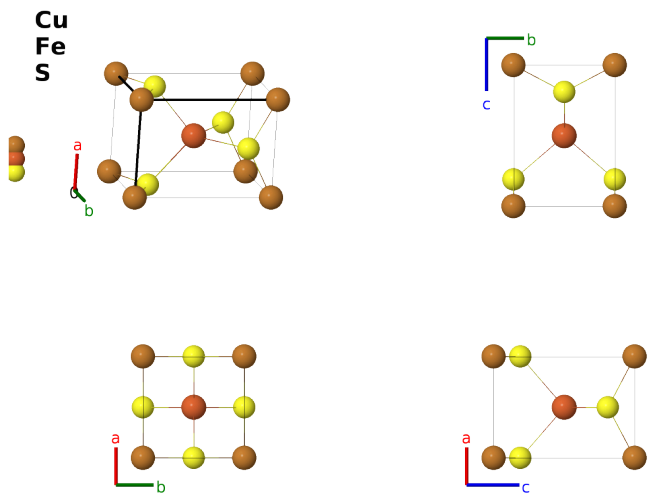
This structure previously used the label(s) **ABC2_tP4_115_a_c_g**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/88N3>

https://aflow.org/prototype-encyclopedia/ABC2_tP4_115_a_c_g-001



Prototype	CuFeS_2
AFLOW prototype label	ABC2_tP4_115_a_c_g-001
<i>Strukturbericht</i> designation	$F6_1$
Mineral name	chalcopyrite
ICSD	27653
CCDC	1602866
Pearson symbol	tP4
Space group number	115
Space group symbol	$P\bar{4}m2$
AFLOW prototype command	<code>aflow --proto=ABC2_tP4_115_a_c_g-001 --params=a, c/a, z₃</code>

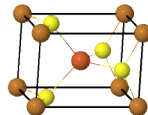
- This structure was presented as the Chalcopyrite structure and given the *Strukturbericht* designation $F6_1$ in (Ewald, 1931). It was subsequently replaced with the $E1_1$ (ABC2_tI16_122_a_b_d) structure, which is now the accepted structure for chalcopyrite and similar compounds. We include the $F6_1$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

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