

Chalcopyrite (CuFeS_2 , $E1_1$) Structure: ABC2_tI16_122_a_b_d-001

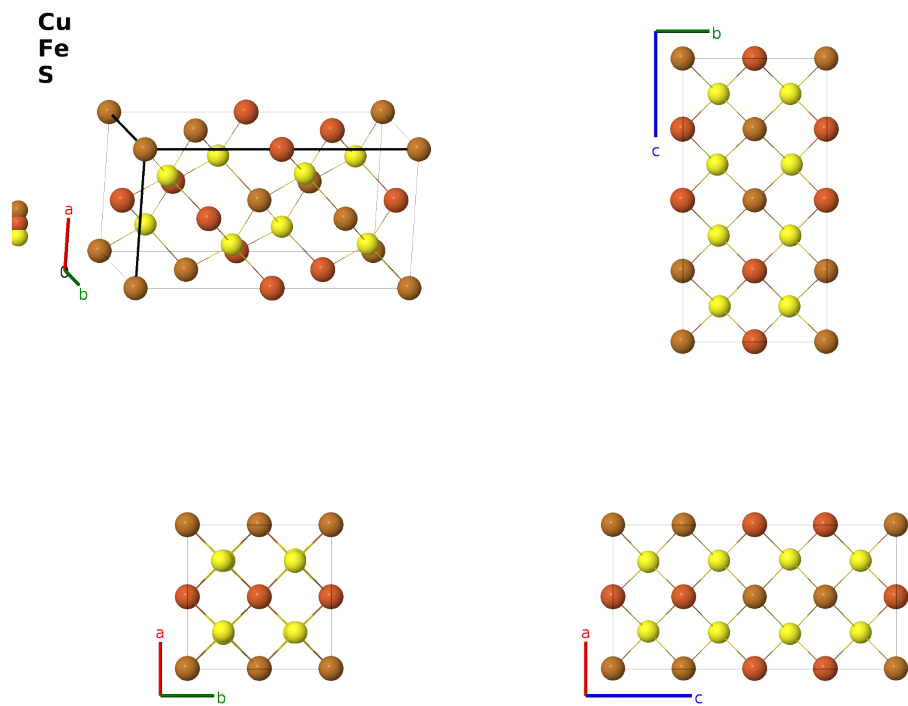
This structure previously used the label(s) **ABC2_tI16_122_a_b_d**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/XWJF>

https://aflow.org/prototype-encyclopedia/ABC2_tI16_122_a_b_d-001



Prototype	CuFeS_2
AFLOW prototype label	ABC2_tI16_122_a_b_d-001
<i>Strukturbericht</i> designation	$E1_1$
Mineral name	chalcopyrite
ICSD	2518
CCDC	1592395
Pearson symbol	tI16
Space group number	122
Space group symbol	$I\bar{4}2d$

AFLOW prototype command `aflow --proto=ABC2_tI16_122_a_b_d-001`
 `--params=a,c/a,x3`

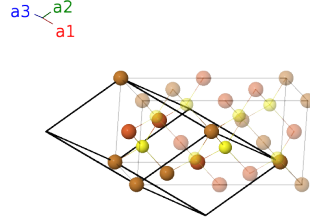
Other compounds with this structure

AgAlS₂, AgAlSe₂, AgAlTe₂, AgFeS₂, AgGaS₂, AgGaSe₂, AgGaTe₂, AgInS₂, AgInSe₂, AgInTe₂, AgTlS₂, AgTlSe₂, AgTlTe₂, BeNSi₂, CdGaSe₂, CdGaTe₂, CdGeAs₂, CdGeP₂, CdGeSb₂, CdSiAs₂, CdSiP₂, CdSiSb₂, CdSnAs₂, CdSnP₂, CdSnSb₂, CuAlS₂, CuAlSe₂, CuAlTe₂, CuGaS₂, CuGaSe₂, CuGaTe₂, CuInS₂, CuInSe₂, CuInTe₂, CuLaS₂, CuTlS₂, CuTlSe₂, CuTlTe₂, GaHgTe₂, GaZnTe₂, GeZnAs₂, GeZnP₂, GeZnSb₂, SiZnAs₂, SiZnP₂, SiZnSb₂, SnZnAs₂, SnZnP₂, SnZnSb₂, SrZnBi₂, SrZnSb₂

- When $c = 2a$ and $x_3 = 1/8$ the atoms are on the sites of the diamond (*A4*) structure. In that case if we replace the Fe atoms by Cu we get the zincblende (*B3*) structure.

Body-centered Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(4a)	Cu I
$\mathbf{B}_2$	$\frac{3}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(4a)	Cu I
$\mathbf{B}_3$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{2}c\hat{\mathbf{z}}$	(4b)	Fe I
$\mathbf{B}_4$	$\frac{1}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}c\hat{\mathbf{z}}$	(4b)	Fe I
$\mathbf{B}_5$	$\frac{3}{8}\mathbf{a}_1 + (x_3 + \frac{1}{8})\mathbf{a}_2 + (x_3 + \frac{1}{4})\mathbf{a}_3$	$=$	$ax_3\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{8}c\hat{\mathbf{z}}$	(8d)	S I
$\mathbf{B}_6$	$\frac{7}{8}\mathbf{a}_1 - (x_3 - \frac{1}{8})\mathbf{a}_2 - (x_3 - \frac{3}{4})\mathbf{a}_3$	$=$	$-ax_3\hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{y}} + \frac{1}{8}c\hat{\mathbf{z}}$	(8d)	S I
$\mathbf{B}_7$	$-(x_3 - \frac{7}{8})\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 - (x_3 - \frac{1}{4})\mathbf{a}_3$	$=$	$-\frac{1}{4}a\hat{\mathbf{x}} - a(x_3 - \frac{1}{2})\hat{\mathbf{y}} + \frac{3}{8}c\hat{\mathbf{z}}$	(8d)	S I
$\mathbf{B}_8$	$(x_3 + \frac{7}{8})\mathbf{a}_1 + \frac{5}{8}\mathbf{a}_2 + (x_3 + \frac{3}{4})\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + a(x_3 + \frac{1}{2})\hat{\mathbf{y}} + \frac{3}{8}c\hat{\mathbf{z}}$	(8d)	S I

References

- [1] S. R. Hall and J. M. Stewart, *The Crystal Structure Refinement of Chalcopyrite, CuFeS₂*, Acta Crystallogr. Sect. B **29**, 579–585 (1973), doi:10.1107/S0567740873002943.

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