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

This structure originally had the label `ABC2_tI16_122_a_b_d`. Calls to that address will be redirected here.

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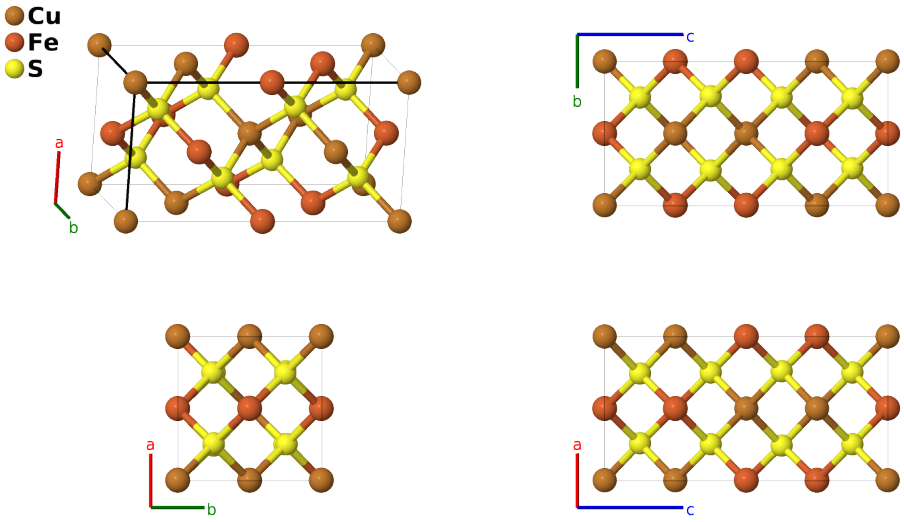
https://aflow.org/p/XWJF

https://aflow.org/p/ABC2_tI16_122_a_b_d-001



Prototype	$CuFeS_2$
AFLOW prototype label	ABC2_tI16_122_a_b_d-001
***Strukturbericht* designation**	$E1_1$
Mineral name	chalcopyrite
ICSD	2518
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=`$a, c/a, x_3$

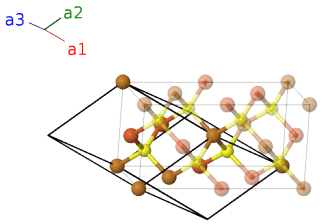
Other compounds with this structure

$AgAlS_2$, $AgAlSe_2$, $AgAlTe_2$, $AgFeS_2$, $AgGaS_2$, $AgGaSe_2$, $AgGaTe_2$, $AgInS_2$, $AgInSe_2$, $AgInTe_2$, $AgTlS_2$, $AgTlSe_2$, $AgTlTe_2$, $BeNSi_2$, $CdGaSe_2$, $CdGaTe_2$, $CdGeAs_2$, $CdGeP_2$, $CdGeSb_2$, $CdSiAs_2$, $CdSiP_2$, $CdSiSb_2$, $CdSnAs_2$, $CdSnP_2$, $CdSnSb_2$, $CuAlS_2$, $CuAlSe_2$, $CuAlTe_2$, $CuGaS_2$, $CuGaSe_2$, $CuGaTe_2$, $CuInS_2$, $CuInSe_2$, $CuInTe_2$, $CuLaS_2$, $CuTlS_2$, $CuTlSe_2$, $CuTlTe_2$, $GaHgTe_2$, $GaZnTe_2$, $GeZnAs_2$, $GeZnP_2$, $GeZnSb_2$, $SiZnAs_2$, $SiZnP_2$, $SiZnSb_2$, $SnZnAs_2$, $SnZnP_2$, $SnZnSb_2$, $SrZnBi_2$, $SrZnSb_2$

- 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

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



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
$\mathbf{B_5}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \left(x_3 + \frac{1}{8}\right)\,\mathbf{a}_2 + \left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(8d)	S I
$\mathbf{B_6}$	=	$\frac{7}{8}\,\mathbf{a}_1 - \left(x_3 - \frac{1}{8}\right)\,\mathbf{a}_2 - \left(x_3 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(8d)	S I
$\mathbf{B_7}$	=	$-\left(x_3 - \frac{7}{8}\right)\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(8d)	S I
$\mathbf{B_8}$	=	$\left(x_3 + \frac{7}{8}\right)\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(8d)	S I

References

[1] S. R. Hall and J. M. Stewart, *The Crystal Structure Refinement of Chalcopyrite, $CuFeS_2$*, Acta Crystallogr. Sect. B **29**, 579–585 (1973), doi:10.1107/S0567740873002943.