Stannite (Cu_2FeS_4Sn, $H2_6$) Structure: A2BC4D_tI16_121_d_a_i_b-001

This structure originally had the label `A2BC4D_tI16_121_d_a_i_b`. Calls to that address will be redirected here.

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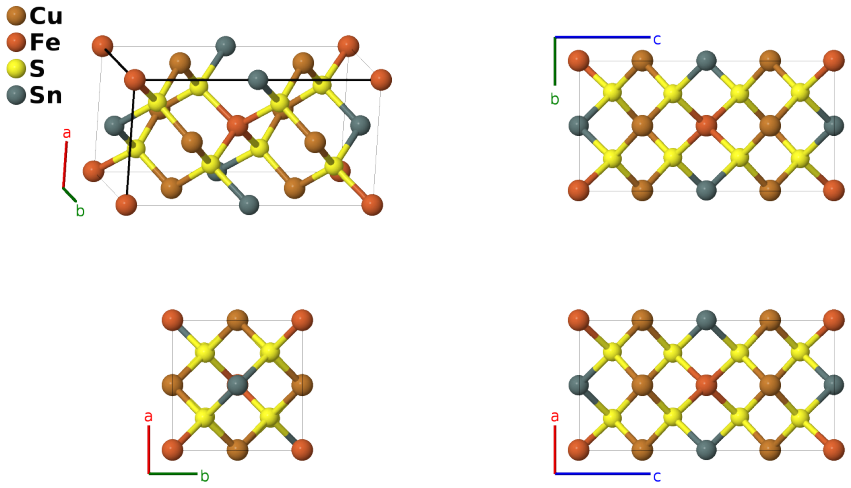
https://aflow.org/p/JRUG

https://aflow.org/p/A2BC4D_tI16_121_d_a_i_b-001



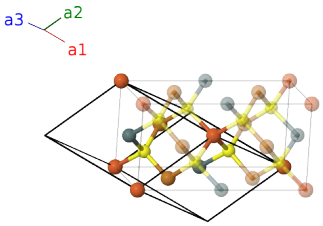
Prototype	Cu_2FeS_4Sn
AFLOW prototype label	A2BC4D_tI16_121_d_a_i_b-001
***Strukturbericht* designation**	$H2_6$
Mineral name	stannite
ICSD	26721
Pearson symbol	tI16
Space group number	121
Space group symbol	$I\bar{4}2m$
AFLOW prototype command	`aflow --proto=A2BC4D_tI16_121_d_a_i_b-001 --params=`$a, c/a, x_4, z_4$

Other compounds with this structure
Cu_2CdSe_4Sn, Cu_2CoS_4Sn, Cu_2GeHgS_4, Cu_2HgS_4Sn, Ag_2FeS_4Sn, Ag_2KS_4Sb

- If $c = 2a$, $x = 1/4$, and $z = 3/8$, the atoms are on the sites of the diamond ($A4$) structure. If, in addition, the Cu, Fe, and Sn atoms are replaced by a single atom type the crystal reduces to 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	(2a)	Fe I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Sn I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Cu I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Cu I
$\mathbf{B_5}$	=	$(x_4 + z_4)\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2 + 2x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8i)	S I
$\mathbf{B_6}$	=	$-(x_4 - z_4)\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - 2x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8i)	S I
$\mathbf{B_7}$	=	$-(x_4 + z_4)\,\mathbf{a}_1 + (x_4 - z_4)\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8i)	S I
$\mathbf{B_8}$	=	$(x_4 - z_4)\,\mathbf{a}_1 - (x_4 + z_4)\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8i)	S I

References

[1] L. O. Brockway, *The Crystal Structure of Stannite, Cu_2FeSnS_4*, Z. Kristallogr. **89**, 434–441 (1934), doi:10.1524/zkri.1934.89.1.434.