Stannite (Cu_2FeSnS_4, $H2_6$) Structure: A2BC4D_tI16_121_d_a_i_b-001

This structure previously used the label(s) `A2BC4D_tI16_121_d_a_i_b`. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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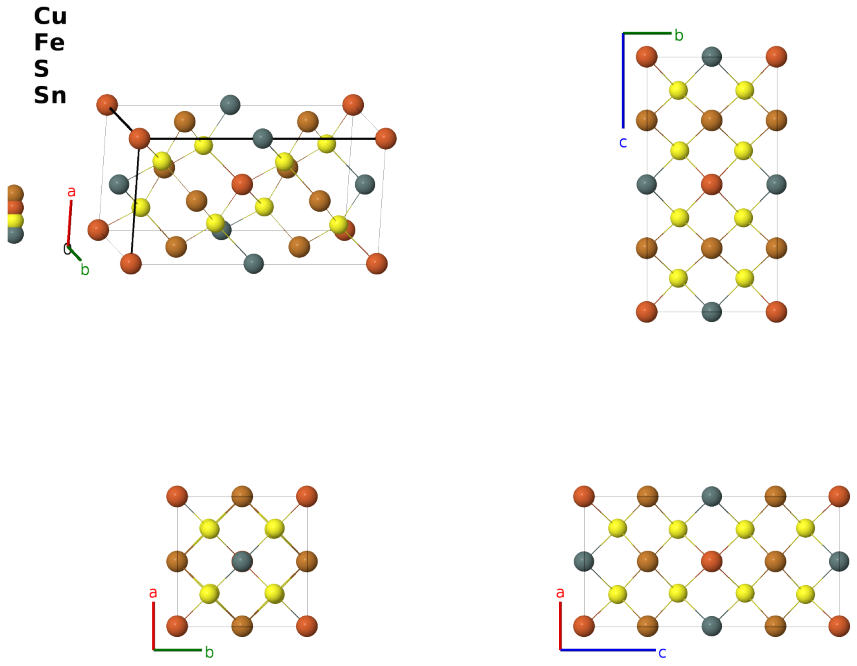
https://aflow.org/prototype-encyclopedia/JRUG

https://aflow.org/prototype-encyclopedia/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
CCDC	1602107
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=`$a, c/a, x_4, z_4$

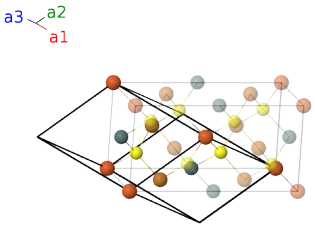
Other compounds with this structure

Ag_2FeGeS_4, Ag_2FeS_4Sn, Ag_2FeSnS_4, Ag_2GeZnS_4, Ag_2KS_4Sb, Ag_2SnZnS_4, $Co_2CuInTe_4$, $Cu_2CdGeSe_4$, $Cu_2CdGeTe_4$, Cu_2CdSe_4Sn, $Cu_2CdSiTe_4$, Cu_2CdSnS_4, $Cu_2CdSnSe_4$, $Cu_2CdSnTe_4$, Cu_2CoGeS_4, Cu_2CoS_4Sn, Cu_2CoSiS_4, Cu_2CoSnS_4, $Cu_2CoSnSe_4$, Cu_2FeGeS_4, $Cu_2FeGeSe_4$, $Cu_2FeSiSe_4$, Cu_2FeSnS_4, $Cu_2FeSnSe_4$, Cu_2GeHgS_4, $Cu_2GeHgSe_4$, $Cu_2GeHgTe_4$, Cu_2GeMnS_4, Cu_2GeZnS_4, $Cu_2GeZnSe_4$, $Cu_2GeZnTe_4$, Cu_2HgS_4Sn, $Cu_2HgSiTe_4$, Cu_2HgSnS_4, $Cu_2HgSnSe_4$, $Cu_2HgSnTe_4$, $Cu_2MgSnSe_4$, $Cu_2MgSnTe_4$, Cu_2MnSnS_4, $Cu_2MnSnSe_4$, Cu_2SbZnS_4, $Cu_2SiZnTe_4$, Cu_2SnZnS_4, $Cu_2SnZnSe_4$, $Cu_2SnZnTe_4$, $Fe_2AgGaTe_4$, Fe_2AlCuS_4, $Fe_2AlCuSe_4$, $Fe_2AlCuTe_4$, Fe_2CuGaS_4, $Fe_2CuGaSe_4$, $Fe_2CuGaTe_4$, Fe_2CuInS_4, $Fe_2CuInSe_4$, $Fe_2CuInTe_4$, In_2CuNaS_4, Li_2BaSnS_4, $Mn_2CuInSe_4$, $Ta_2CuInTe_4$, Zn_2CuGaS_4

- Luzonite (Cu_3AsS_4) is the ternary form of this structure. The ICSD uses stannite for the structure type for both structures.
- 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

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



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.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017