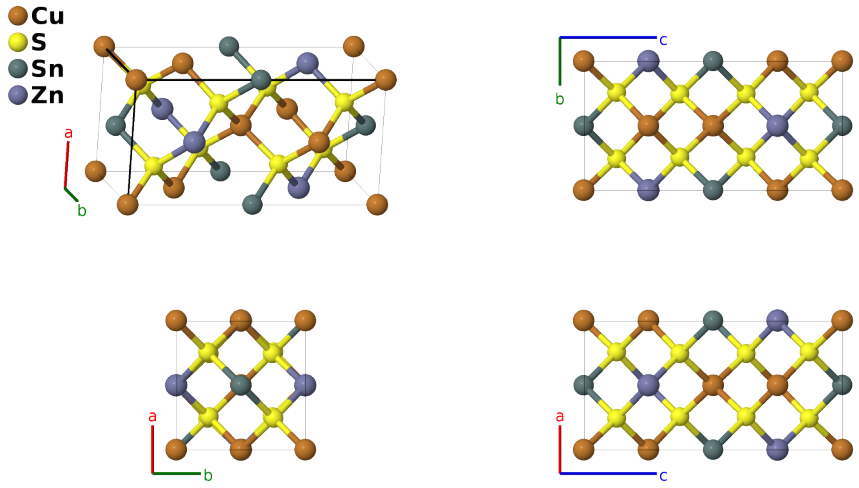
Kesterite [$Cu_2(Zn,Fe)SnS_4$] Structure: A2B4CD_tI16_82_ac_g_b_d-001

This structure originally had the label `A2BCD4_tI16_82_ac_b_d_g`. Calls to that address will be redirected here.

Cite this page as: 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.

https://aflow.org/p/92JU

https://aflow.org/p/A2B4CD_tI16_82_ac_g_b_d-001



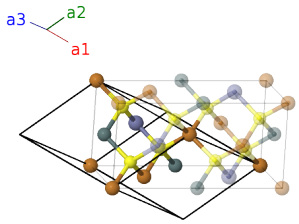
Prototype	Cu_2S_4SnZn
AFLOW prototype label	A2B4CD_tI16_82_ac_g_b_d-001
Mineral name	kesterite
ICSD	5096
Pearson symbol	tI16
Space group number	82
Space group symbol	$I\bar{4}$
AFLOW prototype command	`aflow --proto=A2B4CD_tI16_82_ac_g_b_d-001 --params=`$a, c/a, x_5, y_5, z_5$

Other compounds with this structure
Cu_2ZnSnS_4

- The kesterite structure is related to the stannite structure, with differences occurring due to the positioning of the Cu atoms (Hall, 1978). The (2b) Wyckoff position is partially occupied with iron and zinc. We label this site Zn.

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)	Cu 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
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Cu II
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2d)	Zn I
$\mathbf{B_5}$	=	$(y_5 + z_5)\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + (x_5 + y_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8g)	S I
$\mathbf{B_6}$	=	$-(y_5 - z_5)\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - (x_5 + y_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8g)	S I
$\mathbf{B_7}$	=	$-(x_5 + z_5)\,\mathbf{a}_1 + (y_5 - z_5)\,\mathbf{a}_2 - (x_5 - y_5)\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8g)	S I
$\mathbf{B_8}$	=	$(x_5 - z_5)\,\mathbf{a}_1 - (y_5 + z_5)\,\mathbf{a}_2 + (x_5 - y_5)\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8g)	S I

References

[1] S. R. Hall, J. T. Szymański, and J. M. Stewart, *Kesterite, $Cu_2(Zn,Fe)SnS_4$, and stannite, $Cu_2(Fe,Zn)SnS_4$, structurally similar but distinct minerals*, Can. Mineral. **16**, 131–173 (1978).

[2] S. Schorr, H.-J. Hoebler, and M. Tovar, *A neutron diffraction study of the stannite-kesterite solid solution series*, Euro. J. Mineral. **19**, 65–73 (2007), doi:10.1127/0935-1221/2007/0019-0065.

[3] S. Schoor, *The crystal structure of kesterite type compounds: A neutron and X-ray diffraction study*, Sol. Energy Mater. Sol. Cells **95**, 1482–1488 (2011), doi:10.1016/j.solmat.2011.01.002.