ζ-$Cu_{10}Sn_3$ Structure: A10B3_hP26_176_bcfi_h-001

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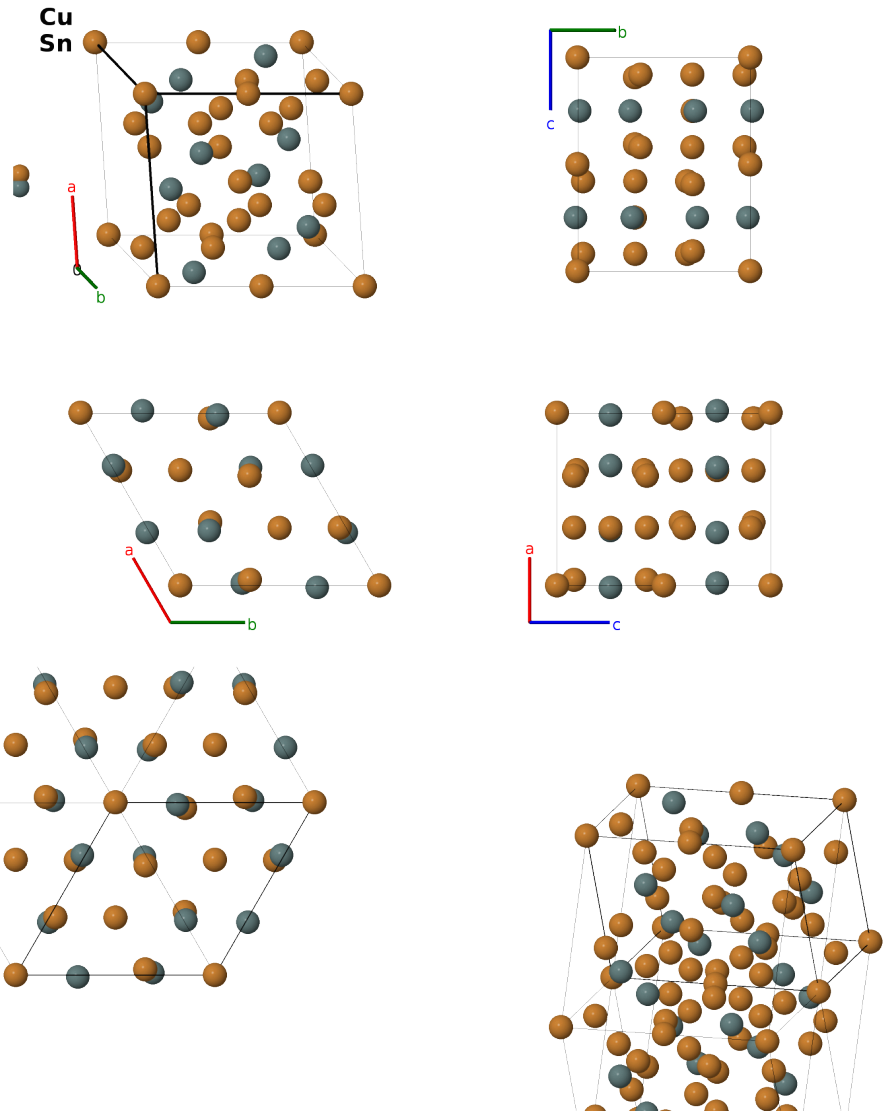
https://aflow.org/prototype-encyclopedia/YGNT

https://aflow.org/prototype-encyclopedia/A10B3_hP26_176_bcfi_h-001



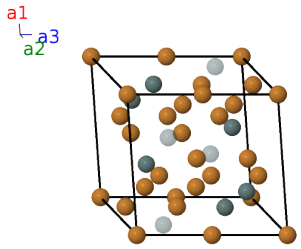
Prototype	$Cu_{10}Sn_3$
AFLOW prototype label	A10B3_hP26_176_bcfi_h-001
ICSD	103105
CCDC	1661061

Pearson symbol	hP26
Space group number	176
Space group symbol	$P6_3/m$
AFLOW prototype command	`aflow --proto=A10B3_hP26_176_bcfi_h-001 --params=`$a, c/a, z_3, x_4, y_4, x_5, y_5, z_5$

- We have shifted the origin by $1/2c\hat{z}$ from that used by (Lenz, 1971).
- This is designated as the ζ phase in the Cu-Sn system. (Massalski, 1990)

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a_1} &= \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_2} &= \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_3} &= c\,\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2b)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Cu I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Cu II
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	Cu II
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4f)	Cu III
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Cu III
$\mathbf{B_7}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4f)	Cu III
$\mathbf{B_8}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Cu III
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Sn I
$\mathbf{B_{10}}$	=	$-y_4\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - 2y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Sn I
$\mathbf{B_{11}}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Sn I
$\mathbf{B_{12}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Sn I
$\mathbf{B_{13}}$	=	$y_4\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_4 + 2y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Sn I
$\mathbf{B_{14}}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Sn I
$\mathbf{B_{15}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12i)	Cu IV
$\mathbf{B_{16}}$	=	$-y_5\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - 2y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12i)	Cu IV
$\mathbf{B_{17}}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12i)	Cu IV
$\mathbf{B_{18}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	Cu IV

$\mathbf{B_{19}}$	=	$y_5\,\mathbf{a}_1-(x_5-y_5)\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_5+2y_5)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	Cu IV
$\mathbf{B_{20}}$	=	$(x_5-y_5)\,\mathbf{a}_1+x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_5-y_5)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	Cu IV
$\mathbf{B_{21}}$	=	$-x_5\,\mathbf{a}_1-y_5\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5+y_5)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_5-y_5)\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(12i)	Cu IV
$\mathbf{B_{22}}$	=	$y_5\,\mathbf{a}_1-(x_5-y_5)\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_5+2y_5)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(12i)	Cu IV
$\mathbf{B_{23}}$	=	$(x_5-y_5)\,\mathbf{a}_1+x_5\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_5-y_5)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(12i)	Cu IV
$\mathbf{B_{24}}$	=	$x_5\,\mathbf{a}_1+y_5\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5+y_5)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_5-y_5)\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	Cu IV
$\mathbf{B_{25}}$	=	$-y_5\,\mathbf{a}_1+(x_5-y_5)\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5-2y_5)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	Cu IV
$\mathbf{B_{26}}$	=	$-(x_5-y_5)\,\mathbf{a}_1-x_5\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_5-y_5)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	Cu IV

References

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[2] T. B. Massalski, H. Okamoto, P. R. S., and L. Kacprzak, eds., *Binary Alloy Phase Diagrams* (ASM International, Materials Park, Ohio, USA, 1990), vol. 2, chap. Cu-Sn (Copper-Tin), pp. 1481–1483, 2^{nd} edn.

First cited in

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