ζ-Cu$_{10}$Sn$_3$ Structure:
A10B3_hP26_176_bcfi_h-001

https://aflow.org/p/YGNT

https://aflow.org/p/A10B3_hP26_176_bcfi_h-001
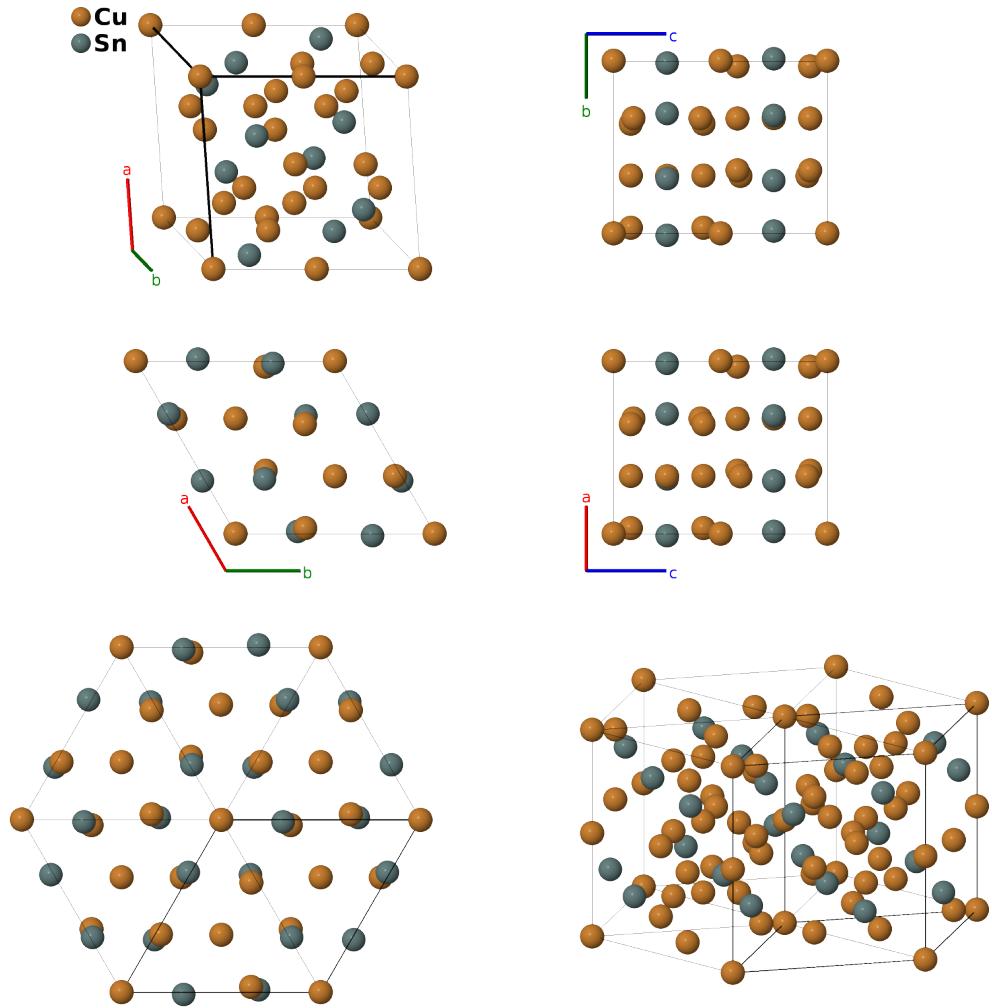
Prototype	Cu$_{10}$Sn$_3$
AFLOW prototype label	A10B3_hP26_176_bcfi_h-001
ICSD	103105
Pearson symbol	hP26
Space group number	176
Space group symbol	$P6_3/m$
AFLOW prototype command	aflow --proto=A10B3_hP26_176_bcfi_h-001 --params=$a, c/a, z_3, x_4, y_4, x_5, y_5, z_5$

- 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

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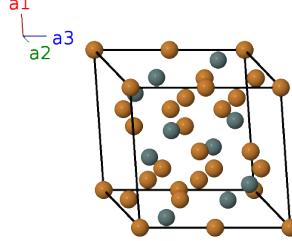
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	0	$=$	0	(2b)	Cu I
$\mathbf{B_2}$	$=$	$\tfrac{1}{2}\mathbf{a_3}$	$=$	$\tfrac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Cu I
$\mathbf{B_3}$	$=$	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Cu II
$\mathbf{B_4}$	$=$	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	Cu II
$\mathbf{B_5}$	$=$	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} + z_3\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4f)	Cu III
$\mathbf{B_6}$	$=$	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} + \left(z_3 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4f)	Cu III
$\mathbf{B_7}$	$=$	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} - z_3\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4f)	Cu III
$\mathbf{B_8}$	$=$	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} - \left(z_3 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_3 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4f)	Cu III
$\mathbf{B_9}$	$=$	$x_4\mathbf{a_1} + y_4\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_4 + y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Sn I
$\mathbf{B_{10}}$	$=$	$-y_4\mathbf{a_1} + \left(x_4 - y_4\right)\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_4 - 2y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Sn I
$\mathbf{B_{11}}$	$=$	$-\left(x_4 - y_4\right)\mathbf{a_1} - x_4\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(2x_4 - y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Sn I
$\mathbf{B_{12}}$	$=$	$-x_4\mathbf{a_1} - y_4\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_4 + y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Sn I
$\mathbf{B_{13}}$	$=$	$y_4\mathbf{a_1} - \left(x_4 - y_4\right)\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(-x_4 + 2y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Sn I
$\mathbf{B_{14}}$	$=$	$\left(x_4 - y_4\right)\mathbf{a_1} + x_4\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(2x_4 - y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Sn I
$\mathbf{B_{15}}$	$=$	$x_5\mathbf{a_1} + y_5\mathbf{a_2} + z_5\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_5 + y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12i)	Cu IV
$\mathbf{B_{16}}$	$=$	$-y_5\mathbf{a_1} + \left(x_5 - y_5\right)\mathbf{a_2} + z_5\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_5 - 2y_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12i)	Cu IV
$\mathbf{B_{17}}$	$=$	$-\left(x_5 - y_5\right)\mathbf{a_1} - x_5\mathbf{a_2} + z_5\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(2x_5 - y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12i)	Cu IV
$\mathbf{B_{18}}$	$=$	$-x_5\mathbf{a_1} - y_5\mathbf{a_2} + \left(z_5 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_5 + y_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	Cu IV
$\mathbf{B_{19}}$	$=$	$y_5\mathbf{a_1} - \left(x_5 - y_5\right)\mathbf{a_2} + \left(z_5 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(-x_5 + 2y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	Cu IV
$\mathbf{B_{20}}$	$=$	$\left(x_5 - y_5\right)\mathbf{a_1} + x_5\mathbf{a_2} + \left(z_5 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(2x_5 - y_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	Cu IV
$\mathbf{B_{21}}$	$=$	$-x_5\mathbf{a_1} - y_5\mathbf{a_2} - z_5\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_5 + y_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(12i)	Cu IV
$\mathbf{B_{22}}$	$=$	$y_5\mathbf{a_1} - \left(x_5 - y_5\right)\mathbf{a_2} - z_5\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(-x_5 + 2y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(12i)	Cu IV
$\mathbf{B_{23}}$	$=$	$\left(x_5 - y_5\right)\mathbf{a_1} + x_5\mathbf{a_2} - z_5\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(2x_5 - y_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(12i)	Cu IV
$\mathbf{B_{24}}$	$=$	$x_5\mathbf{a_1} + y_5\mathbf{a_2} - \left(z_5 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_5 + y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\hat{\mathbf{y}} - c\left(z_5 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	Cu IV

$$\mathbf{B_{25}} = \quad -y_5\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 - \left(z_5 - \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad \tfrac{1}{2}a\left(x_5 - 2y_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} - c\left(z_5 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(12i)} \qquad \text{Cu IV}$$

$$\mathbf{B_{26}} = \quad -(x_5 - y_5)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - \left(z_5 - \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad -\tfrac{1}{2}a\left(2x_5 - y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} - c\left(z_5 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(12i)} \qquad \text{Cu IV}$$

References

[1] J. Lenz and K. Schubert, *Kristallstrukture von $Cu_{10}Sn_3$ (m)*, Monatsh. Chem. **102**, 1689–1698 (1971), doi:10.1007/BF00905642.

[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, 2nd edn.