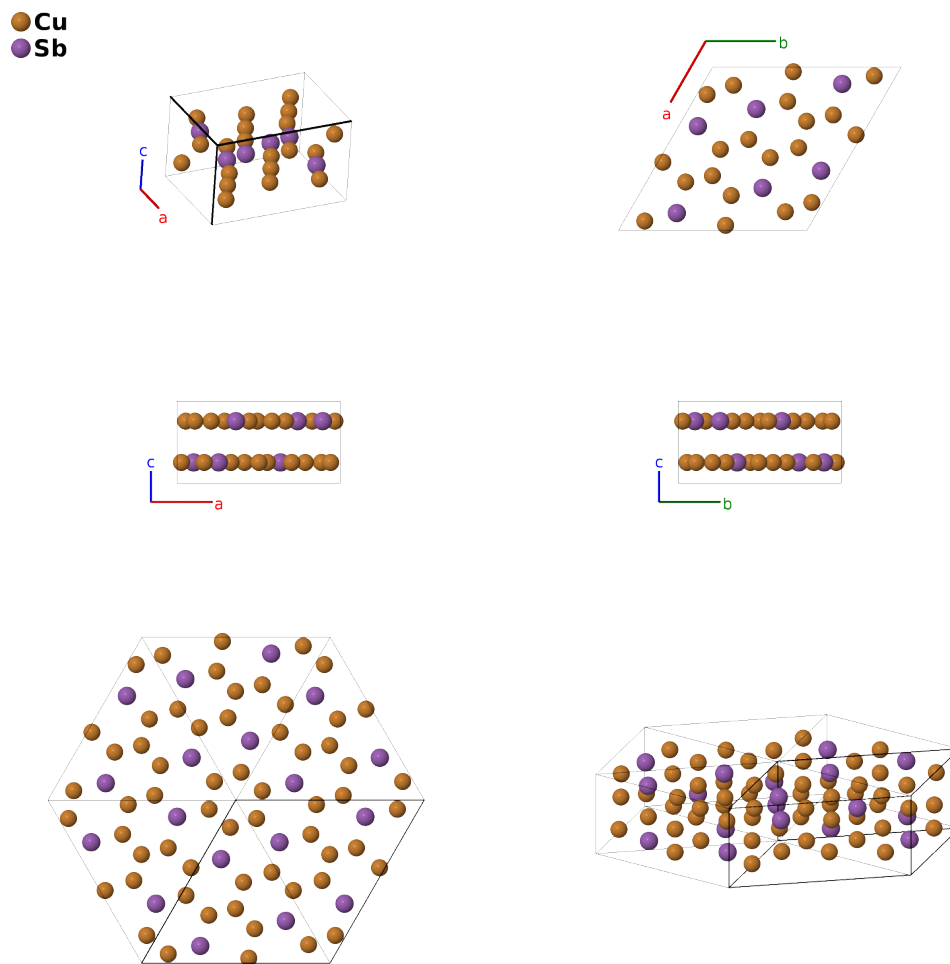


Cu₁₀Sb₃ Structure: A10B3_hP26_176_c3h_h-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

<https://aflow.org/p/4QXQ>

https://aflow.org/p/A10B3_hP26_176_c3h_h-001

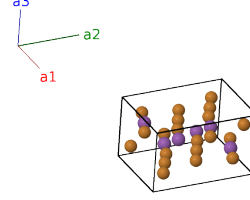


Prototype	Cu ₁₀ Sb ₃
AFLOW prototype label	A10B3_hP26_176_c3h_h-001
ICSD	44480
Pearson symbol	hP26
Space group number	176
Space group symbol	$P6_3/m$
AFLOW prototype command	<code>aflow --proto=A10B3_hP26_176_c3h_h-001 --params=a, c/a, x₂, y₂, x₃, y₃, x₄, y₄, x₅, y₅</code>

- (Günzel, 1958) place this structure in space group $P\bar{3}$ #147 but (Cenzual, 1991) showed that all the atoms have z coordinates which are either $1/4$ or $3/4$. In that case there is a six-fold rotation axis, making the space group $P6_3/m$ #176.
- (Cenzual, 1991) also note that (Günzel, 1958) list the z coordinate of the (3d) copper atoms as $1/4$, but as seen from the figures it must be $3/4$ in their paper, and $1/4$ here.

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	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c)	Cu I
\mathbf{B}_2	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c)	Cu I
\mathbf{B}_3	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_2 + y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_2 - y_2) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Cu II
\mathbf{B}_4	$= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_2 - 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Cu II
\mathbf{B}_5	$= -(x_2 - y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Cu II
\mathbf{B}_6	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_2 + y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_2 - y_2) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Cu II
\mathbf{B}_7	$= y_2 \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_2 + 2y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Cu II
\mathbf{B}_8	$= (x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_2 - y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Cu II
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_3 - y_3) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Cu III
\mathbf{B}_{10}	$= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Cu III
\mathbf{B}_{11}	$= -(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Cu III
\mathbf{B}_{12}	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_3 - y_3) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Cu III
\mathbf{B}_{13}	$= y_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_3 + 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Cu III
\mathbf{B}_{14}	$= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Cu III
\mathbf{B}_{15}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_4 - y_4) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Cu IV
\mathbf{B}_{16}	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Cu IV
\mathbf{B}_{17}	$= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Cu IV
\mathbf{B}_{18}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_4 - y_4) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Cu IV
\mathbf{B}_{19}	$= y_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_4 + 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Cu IV
\mathbf{B}_{20}	$= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Cu IV
\mathbf{B}_{21}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_5 - y_5) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Sb I
\mathbf{B}_{22}	$= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Sb I
\mathbf{B}_{23}	$= -(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Sb I
\mathbf{B}_{24}	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_5 - y_5) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Sb I
\mathbf{B}_{25}	$= y_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_5 + 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Sb I
\mathbf{B}_{26}	$= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Sb I

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