

Cu₁₀Sb₃ Structure:

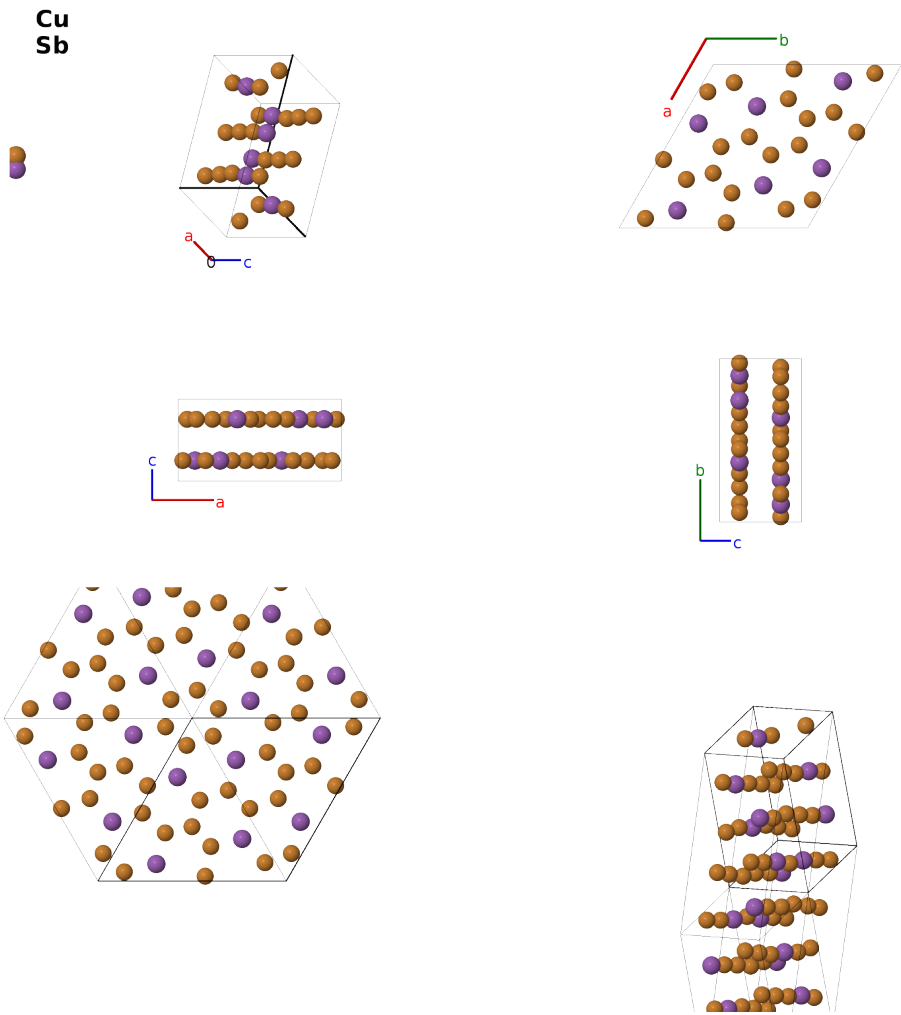
A10B3_hP26_176_c3h_h-001

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<https://aflow.org/prototype-encyclopedia/4QXQ>

https://aflow.org/prototype-encyclopedia/A10B3_hP26_176_c3h_h-001



Prototype	Cu ₁₀ Sb ₃
AFLOW prototype label	A10B3_hP26_176_c3h_h-001
ICSD	44480
CCDC	1613864
Pearson symbol	hP26
Space group number	176

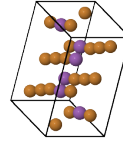
Space group symbol $P6_3/m$

AFLOW prototype command `aflow --proto=A10B3_hP26_176_c3h_h-001`
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- (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
$\mathbf{B}_4$	$= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_2 - 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Cu II
$\mathbf{B}_5$	$= -(x_2 - y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(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
$\mathbf{B}_7$	$= y_2 \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_2 + 2y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Cu II
$\mathbf{B}_8$	$= (x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_2 - y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a y_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(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
$\mathbf{B}_{10}$	$= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Cu III
$\mathbf{B}_{11}$	$= -(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(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
$\mathbf{B}_{13}$	$= y_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_3 + 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Cu III
$\mathbf{B}_{14}$	$= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a y_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(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
$\mathbf{B}_{16}$	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Cu IV
$\mathbf{B}_{17}$	$= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(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
$\mathbf{B}_{19}$	$= y_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_4 + 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Cu IV
$\mathbf{B}_{20}$	$= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a y_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(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

$$\begin{aligned}
\mathbf{B}_{22} &= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}} &(6h) &\text{Sb I} \\
\mathbf{B}_{23} &= -(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= -\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}} &(6h) &\text{Sb I} \\
\mathbf{B}_{24} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= -\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}} &(6h) &\text{Sb I} \\
\mathbf{B}_{25} &= y_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}} &(6h) &\text{Sb I} \\
\mathbf{B}_{26} &= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}} &(6h) &\text{Sb I}
\end{aligned}$$

References

- [1] E. Günzel and K. Schubert, *Strukturuntersuchungen im System Kupfer-Antimon*, Z. Metallkd. **49**, 124–133 (1958).

Found in

- [1] K. Cenzual, L. M. Gelato, M. Penzo, and E. Parthé, *Inorganic structure types with revised space groups. I*, Acta Crystallogr. Sect. B **47**, 433–439 (1991), doi:10.1107/S0108768191000903.

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