

Ti₂Cu₃ Structure:

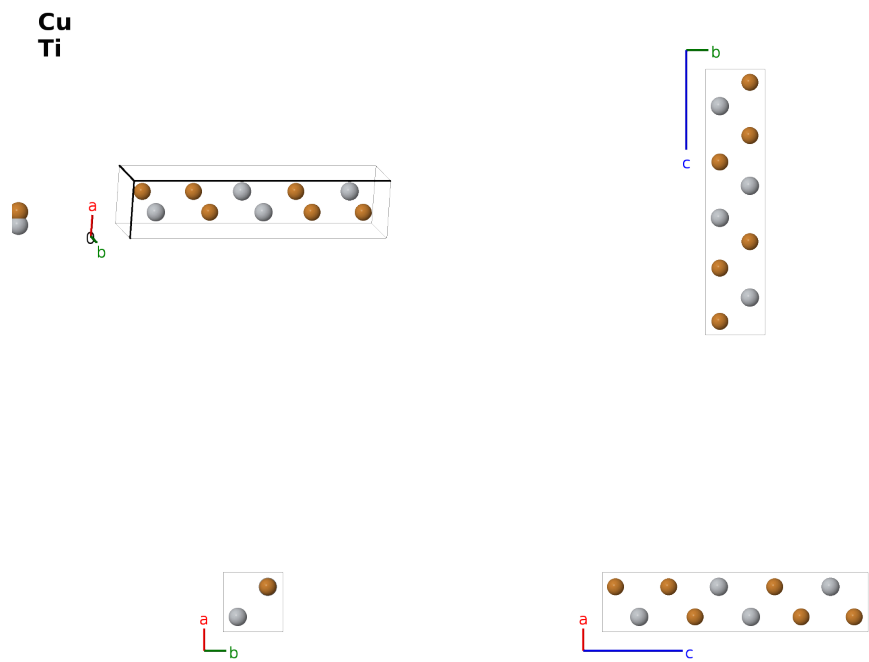
A3B2_tP10_129_3c_2c-001

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<https://aflow.org/prototype-encyclopedia/T7XE>

https://aflow.org/prototype-encyclopedia/A3B2_tP10_129_3c_2c-001



Prototype	Cu ₃ Ti ₂
AFLOW prototype label	A3B2_tP10_129_3c_2c-001
ICSD	103133
CCDC	1661085
Pearson symbol	tP10
Space group number	129
Space group symbol	$P4/nmm$
AFLOW prototype command	<code>aflow --proto=A3B2_tP10_129_3c_2c-001</code> <code>--params=a, c/a, z₁, z₂, z₃, z₄, z₅</code>

Simple Tetragonal primitive vectors



$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(2c)	Cu I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(2c)	Cu I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2c)	Cu II
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(2c)	Cu II
$\mathbf{B}_5$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2c)	Cu III
$\mathbf{B}_6$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(2c)	Cu III
$\mathbf{B}_7$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2c)	Ti I
$\mathbf{B}_8$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(2c)	Ti I
$\mathbf{B}_9$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(2c)	Ti II
$\mathbf{B}_{10}$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(2c)	Ti II

References

- [1] K. Schubert, A. Raman, and W. Rossteutscher, *Einige Strukturdaten metallischer Phasen (11)*, *Naturwissenschaften* **51**, 507 (1964), doi:10.1007/BF00632207.

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