Ti_3Cu_4 Structure: A4B3_tI14_139_2e_ae-001

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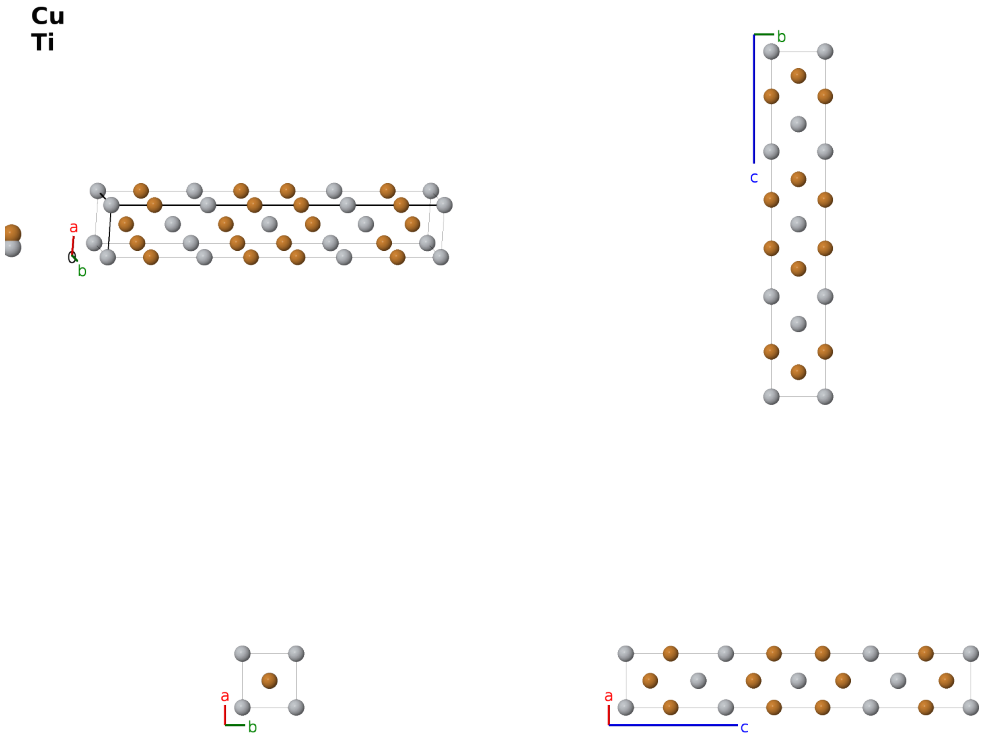
https://aflow.org/prototype-encyclopedia/N44F

https://aflow.org/prototype-encyclopedia/A4B3_tI14_139_2e_ae-001

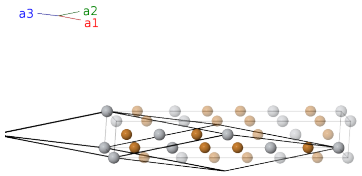


Prototype	Cu_4Ti_3
AFLOW prototype label	A4B3_tI14_139_2e_ae-001
ICSD	103134
CCDC	1661086
Pearson symbol	tI14
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=A4B3_tI14_139_2e_ae-001 --params=`$a, c/a, z_2, z_3, z_4$

- When c = 7 a, $z_2 = 1/7$, $z_3 = 3/7$, and $z_4 = 2/7$ the atoms are on the sites of the bcc lattice.

Body-centered Tetragonal primitive vectors

$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ti I
$\mathbf{B_2}$	=	$z_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2$	=	$cz_2\,\hat{\mathbf{z}}$	(4e)	Cu I
$\mathbf{B_3}$	=	$-z_2\,\mathbf{a}_1 - z_2\,\mathbf{a}_2$	=	$-cz_2\,\hat{\mathbf{z}}$	(4e)	Cu I
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$	=	$cz_3\,\hat{\mathbf{z}}$	(4e)	Cu II
$\mathbf{B_5}$	=	$-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$	=	$-cz_3\,\hat{\mathbf{z}}$	(4e)	Cu II
$\mathbf{B_6}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$	=	$cz_4\,\hat{\mathbf{z}}$	(4e)	Ti II
$\mathbf{B_7}$	=	$-z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2$	=	$-cz_4\,\hat{\mathbf{z}}$	(4e)	Ti II

References

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Found in

[1] J. M. Moya, A. M. Hallas, V. Loganathan, C.-L. Huang, L. Kish, A. A. Aczel, J. Beare, Y. Cai, G. M. Luke, F. Weickert, A. H. Nevidomskyy, C. D. Malliakas, M. G. Kanatzidis, K. Bayliff, and E. Morosan, *Field-induced quantum critical point in the new itinerant antiferromagnet Ti_3Cu_4*, Comm. Phys. **5**, 136 (2022), doi:10.1038/s42005-022-00901-7.

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