β-$TiCu_3$ ($D0_a$) Structure: A3B_oP8_59_ae_b-001

This structure originally had the label `A3B_oP8_59_bf_a`. Calls to that address will be redirected here.

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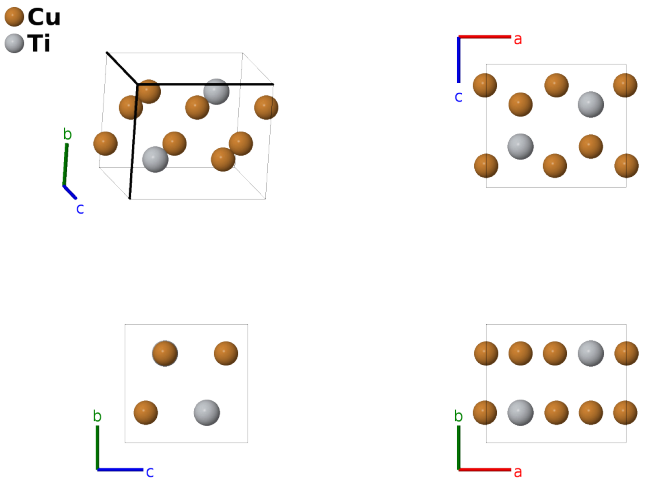
https://aflow.org/p/CJHD

https://aflow.org/p/A3B_oP8_59_ae_b-001



Prototype	Cu_3Ti
AFLOW prototype label	A3B_oP8_59_ae_b-001
***Strukturbericht* designation**	$D0_a$
ICSD	197784
Pearson symbol	oP8
Space group number	59
Space group symbol	$Pmmn$
AFLOW prototype command	`aflow --proto=A3B_oP8_59_ae_b-001 --params=`$a, b/a, c/a, z_1, z_2, y_3, z_3$

Other compounds with this structure

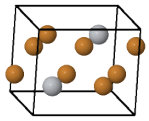
$HfAu_3$, $InAu_3$, $MoNi_3$, $NbNi_3$, α-$NbPt_3$, β-$SbCu_3$ (H.T.), $SbNi_3$ (L.T.), $TaNi_3$ (L.T.), $TaPt_3$, $TiAu_3$, β-$TiCu_3$ (L.T.), $ZrAu_3$

- We have been so far unable to obtain the original reference (Karlsson, 1951), and Pearson does not give the exact atomic coordinates. Wyckoff positions have been deduced from the structure of Cu_3Sb, which Villars (1991) lists as having the $TiCu_3$ structure.
- Atomic positions are set to give the approximate nearest-neighbor distances listed in Pearson.
- (Giessen, 1971) says that the (Karlsson, 1951) structure of β-$TiCu_3$ is mistaken. They do find a metastable β-$TiCu_3$ phase which has the same space group and Wyckoff positions, but substantially different lattice constants than the original determination for β-$TiCu_3$.

- The ICSD entry is from (Karlsson, 1951).

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(2a)	Cu I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(2a)	Cu I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2b)	Ti I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2b)	Ti I
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4e)	Cu II
$\mathbf{B_6}$	=	$\frac{1}{4}\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4e)	Cu II
$\mathbf{B_7}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4e)	Cu II
$\mathbf{B_8}$	=	$\frac{3}{4}\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4e)	Cu II

References

[1] B. C. Giessen and D. Szymanski, *A metastable phase $TiCu_3(m)$*, J. Appl. Crystallogr. **4**, 257–259 (1971), doi:10.1107/S0021889871006824.

[2] N. Karlsson, *An X-ray study of the phases in the copper-titanium system*, J. Inst. Metals **79**, 391 (1951).

Found in

[1] N. Karlsson, , Journal of the Institute of Metals **79**, 391 (1951).