$CuTi_3$ ($L6_0$) Structure: AB3_tP4_123_a_ce-001

This structure originally had the label `AB3_tP4_123_a_ce`. Calls to that address will be redirected here.

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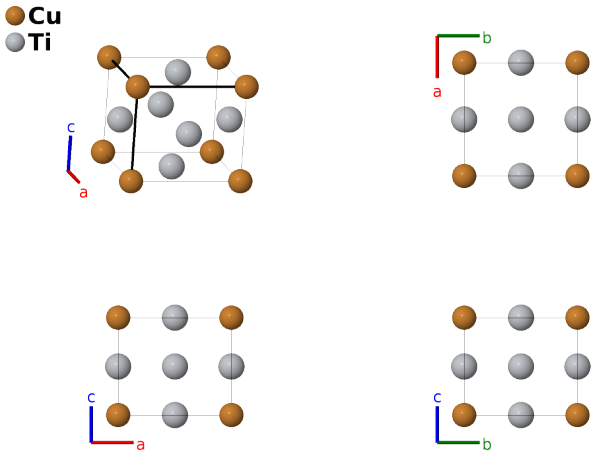
https://aflow.org/p/B4JD

https://aflow.org/p/AB3_tP4_123_a_ce-001



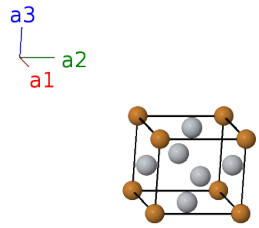
Prototype	$CuTi_3$
AFLOW prototype label	AB3_tP4_123_a_ce-001
***Strukturbericht* designation**	$L6_0$
ICSD	103130
Pearson symbol	tP4
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	`aflow --proto=AB3_tP4_123_a_ce-001 --params=`$a, c/a$

Other compounds with this structure
$AgZr_3$, $AlPu_3$, $BaBi_3$, $\alpha'CdAu_3$, $CuZr_3$, $DyIn_3$, $GaPu_3$, $InPt_3$, $MnAu_3$, $SrPb_3$, $TlPd_3$

- This is a tetragonal distortion of the $L1_2$ (Cu_3Au) structure. When $c = a$ the atoms are at the positions of a face-centered cubic lattice. If we replace the Ti-I atom by Cu, then the system reduces to the $L1_0$ (CuAu) structure. Interestingly, (Massalski, 1986) lists no stable or metastable structures with composition $CuTi_3$. (Byström, 1947) do find a phase of $CdAu_3$ which they say has this structure.

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
$\mathbf{B_1}$	=	0	=	0	(1a)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(1c)	Ti I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2e)	Ti II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2e)	Ti II

References

[1] N. Karlsson, *An X–ray study of the phases in the copper–titanium system*, J. Inst. Met. **79**, 391–405 (1951).

[2] T. B. Massalski, H. Okamoto, P. R. Subramanian, and L. Kacprzak, eds., *Binary Alloy Phase Diagrams* (American Society for Metals, Materials Park, OH, 1990).

[3] A. Byström and K. E. Almin, *X-ray Investigation of Gold-Cadmium Alloys Rich in Gold*, Acta Chem. Scand. **1**, 76–89 (1947), doi:10.3891/acta.chem.scand.01-0076.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.