δ-CuTi ($L2_a$) Structure: AB_tP2_123_a_d-002

This structure originally had the label `AB_tP2_123_a_d.CuTi`. Calls to that address will be redirected here.

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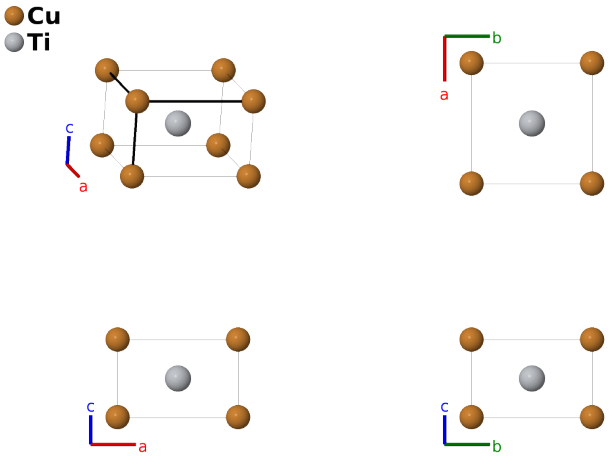
https://aflow.org/p/C9G2

https://aflow.org/p/AB_tP2_123_a_d-002



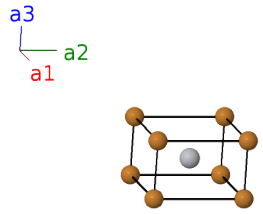
Prototype	CuTi
AFLOW prototype label	AB_tP2_123_a_d-002
***Strukturbericht* designation**	$L2_a$
ICSD	103127
Pearson symbol	tP2
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	`aflow --proto=AB_tP2_123_a_d-002 --params=`$a, c/a$

Other compounds with this structure
HgMn

- As we have been unable to find a copy of (Karlsson, 1951), we obtained the value a = 4.44Å from (Pearson, 1958). The ICSD entry uses a = 3.14Å, referencing the original publication. For now we will continue to use the value from (Pearson, 1958).
- This structure has the same AFLOW designation, AB_tP2_123_a_d, as CuAu ($L1_0$). The only difference in the structures is the c/a ratio. $L1_0$ has $c/a \approx \sqrt{2}$, characteristic of face-centered cubic ordering, while $L2_a$ has $c/a \approx 1$, a body-centered cubic-like system.

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
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(1d)	Ti I

References

[1] N. Karlsson, *An X-Ray Study of the Phases in the Copper-Titanium System*, J. Inst. Met. **79**, 391–405 (1951).

Found in

[1] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys*, *International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 4 (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfort, 1958), 1964 reprint with corrections edn.