

γ -CuTi (*B*11) Structure: AB_tP4_129_c_c-001

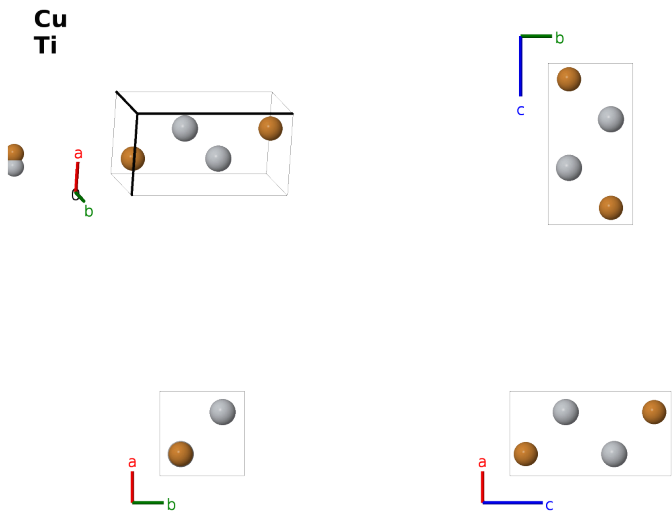
This structure previously used the label(s) **AB_tP4_129_c_c**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/EKF2>

https://aflow.org/prototype-encyclopedia/AB_tP4_129_c_c-001



Prototype	CuTi
AFLOW prototype label	AB_tP4_129_c_c-001
<i>Strukturbericht</i> designation	<i>B</i> 11
ICSD	629389
CCDC	1753366
Pearson symbol	tP4
Space group number	129
Space group symbol	<i>P</i> 4/ <i>nmm</i>
AFLOW prototype command	<code>aflow --proto=AB_tP4_129_c_c-001</code> <code>--params=<i>a</i>,<i>c/a</i>,<i>z</i>₁,<i>z</i>₂</code>

Other compounds with this structure

AgZr, AlRe, AuCu, AuHf, AuMn, AuTi, HgPd, PdTa, SZr, TiF-I (high-temperature)

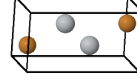
- When $c = 2a$, $z_1 = 1/8$, and $z_2 = 5/8$, the atoms are on the sites of a body-centered cubic lattice. If, on the other hand, $c = 2\sqrt{2}a$, with the same z_i , the atoms are on the site of a face-centered cubic lattice. This is the phase that (Lu, 1991) refer to as “Z2”.

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)	Ti I
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(2c)	Ti I

References

- [1] V. N. Eremenko, Y. I. Buyanov, and S. B. Prima, *Phase diagram of the system titanium-copper*, Soviet Powder Metallurgy and Metal Ceramics **5**, 494–502 (1966), doi:10.1007/BF00775543.
- [2] Z. W. Lu, S.-H. Wei, and A. Zunger, *Long-Range Order in Binary Late-Transition-Metal Alloys*, Phys. Rev. Lett. **66**, 1753–1756 (1991), doi:10.1103/PhysRevLett.66.1753.

Found in

- [1] P. Villars and L. Calvert, *Pearson’s Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017