Cu$_2$Te (C_h) Structure: A2B_hP6_191_h_e-001
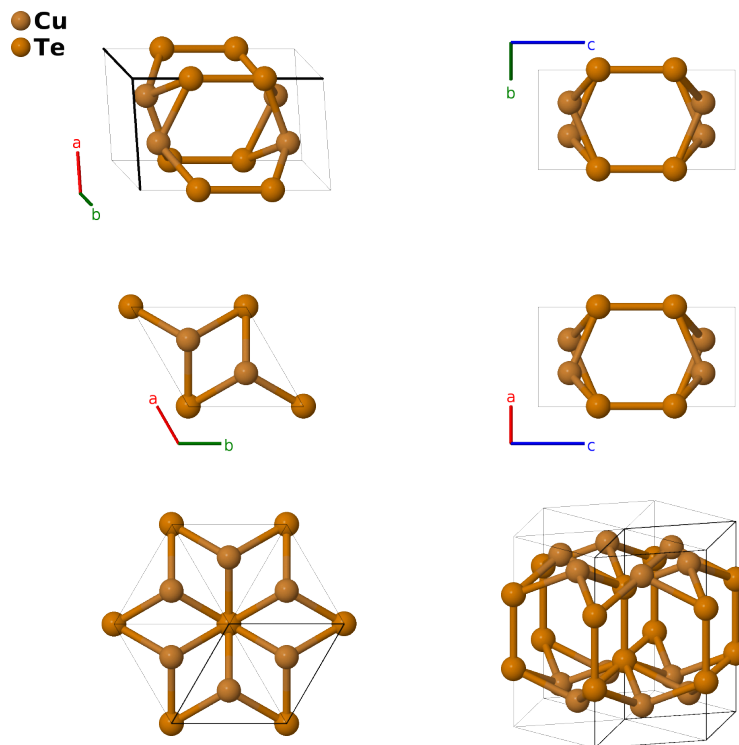
This structure originally had the label `A2B_hP6_191_h_e`. Calls to that address will be redirected here.

https://aflow.org/p/X9YK

https://aflow.org/p/A2B_hP6_191_h_e-001

Prototype	Cu$_2$Te
AFLOW prototype label	A2B_hP6_191_h_e-001
***Strukturbericht* designation**	C_h
ICSD	655706
Pearson symbol	hP6
Space group number	191
Space group symbol	$P6/mmm$
AFLOW prototype command	aflow --proto=A2B_hP6_191_h_e-001
	--params=$a, c/a, z_1, z_2$

Hexagonal primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}
$$
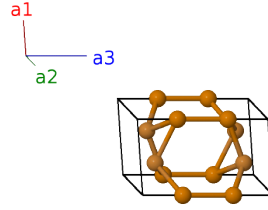
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a_3}$	=	$cz_1\,\hat{\mathbf{z}}$	(2e)	Te I
$\mathbf{B_2}$	=	$-z_1\,\mathbf{a_3}$	=	$-cz_1\,\hat{\mathbf{z}}$	(2e)	Te I
$\mathbf{B_3}$	=	$\frac{1}{3}\mathbf{a_1} + \frac{2}{3}\mathbf{a_2} + z_2\,\mathbf{a_3}$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4h)	Cu I
$\mathbf{B_4}$	=	$\frac{2}{3}\mathbf{a_1} + \frac{1}{3}\mathbf{a_2} + z_2\,\mathbf{a_3}$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4h)	Cu I
$\mathbf{B_5}$	=	$\frac{2}{3}\mathbf{a_1} + \frac{1}{3}\mathbf{a_2} - z_2\,\mathbf{a_3}$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4h)	Cu I
$\mathbf{B_6}$	=	$\frac{1}{3}\mathbf{a_1} + \frac{2}{3}\mathbf{a_2} - z_2\,\mathbf{a_3}$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4h)	Cu I

References

[1] H. Nowotny, *Die Kristallstruktur von Cu₂Te*, Z. Metallkd. **37**, 40–42 (1946), doi:10.1515/ijmr-1946-371-208.

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.