

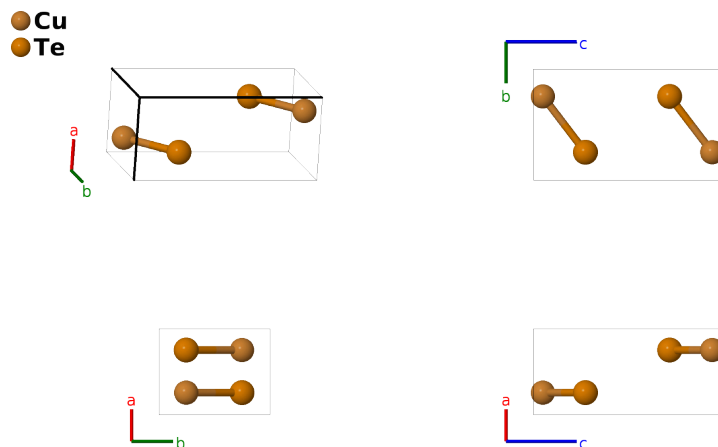
Vulcanite (CuTe) Structure: AB_oP4_59_a_b-001

This structure originally had the label AB_oP4_59_a_b. Calls to that address will be redirected here.

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<https://aflow.org/p/9JE2>

https://aflow.org/p/AB_oP4_59_a_b-001

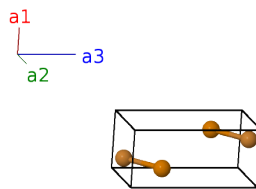


Prototype	CuTe
AFLOW prototype label	AB_oP4_59_a_b-001
Mineral name	vulcanite
ICSD	42591
Pearson symbol	oP4
Space group number	59
Space group symbol	<i>Pmnm</i>
AFLOW prototype command	aflow --proto=AB_oP4_59_a_b-001 --params=a, b/a, c/a, z ₁ , z ₂

- Our data is from (Cameron, 1961), but the ICSD is from (Baranova, 1964).

Simple Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{x} \\ \mathbf{a}_2 &= b \hat{y} \\ \mathbf{a}_3 &= c \hat{z} \end{aligned}$$



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) Te 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) Te I

References

- [1] E. N. Cameron and I. M. Threadgold, *Vulcanite, a new copper telluride from Colorado, with notes on certain associated materials*, Am. Mineral. **46**, 258–268 (1961).
- [2] R. V. Baranova and Z. G. Pinsker, *Study of the copper-tellurium system in thin films*, Kristallografiya **9**, 104–106 (1964).

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).