

Vulcanite (CuTe) Structure:

AB_oP4_59_a_b-001

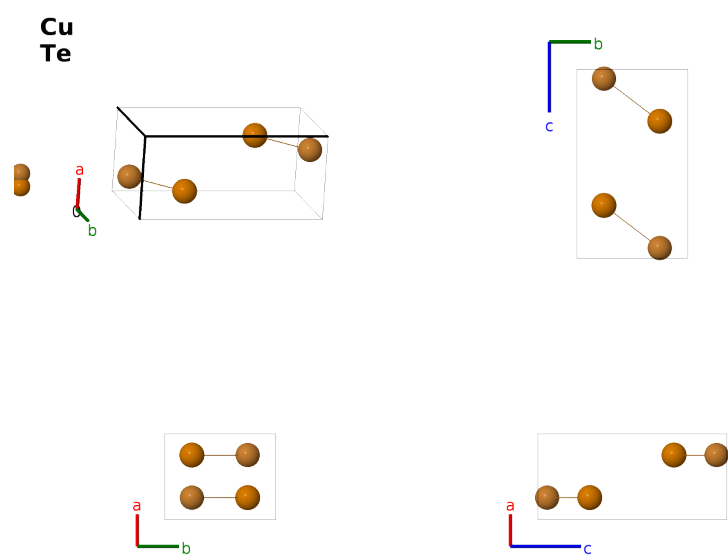
This structure previously used the label(s) **AB_oP4_59_a_b**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/9JE2>

https://aflow.org/prototype-encyclopedia/AB_oP4_59_a_b-001

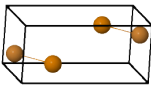


Prototype	CuTe
AFLOW prototype label	AB_oP4_59_a_b-001
Mineral name	vulcanite
ICSD	42591
CCDC	1612243
Pearson symbol	oP4
Space group number	59
Space group symbol	$Pm\bar{m}n$
AFLOW prototype command	<code>aflow --proto=AB_oP4_59_a_b-001 --params=a,b/a,c/a,z₁,z₂</code>

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

Simple Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(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).

First cited in

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