

Cooperite (PtS, *B17*) Structure: AB_tP4_131_c-e-001

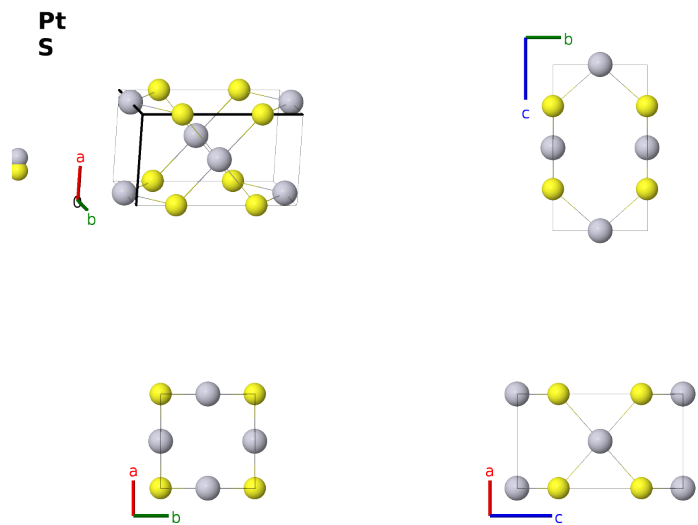
This structure previously used the label(s) **AB_tP4_131_c-e**. Calls to these addresses will be redirected here.

Cite this page as:

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- 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/8GEP>

https://aflow.org/prototype-encyclopedia/AB_tP4_131_c-e-001



Prototype	PtS
AFLOW prototype label	AB.tP4.131.c-e-001
<i>Strukturbericht</i> designation	<i>B17</i>
Mineral name	cooperite
ICSD	654379
CCDC	1765748
Pearson symbol	tP4
Space group number	131
Space group symbol	$P4_2/mmc$
AFLOW prototype command	<code>aflow --proto=AB_tP4_131_c-e-001 --params=a,c/a</code>

Other compounds with this structure

PdO (palladinite)

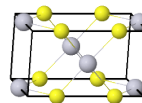
- Actual samples of cooperite have the chemical formula PtS_x , with $0.9 < x < 1.1$. If there is an excess of platinum, these atoms substitute for sulfur on the (2e) site, and excess sulfur substitutes for platinum on the (2c) site.
- Previous versions of this page incorrectly used $a = 4.9073\text{\AA}$. We have changed this to the correct value of $3.47\text{\AA}$. We thank Dr. Frank Hoffmann of the University of Hamburg for pointing out this error.

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
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{y}}$	(2c)	Pt I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2c)	Pt I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} c \hat{\mathbf{z}}$	(2e)	S I
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} c \hat{\mathbf{z}}$	(2e)	S I

References

- [1] F. Gronvold, H. Haraldsen, and A. Kjekshus, *On the Sulfides, Selenides and Tellurides of Platinum*, Acta Chem. Scand. **14**, 1879–1893 (1960), doi:10.3891/acta.chem.scand.14-1879.

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