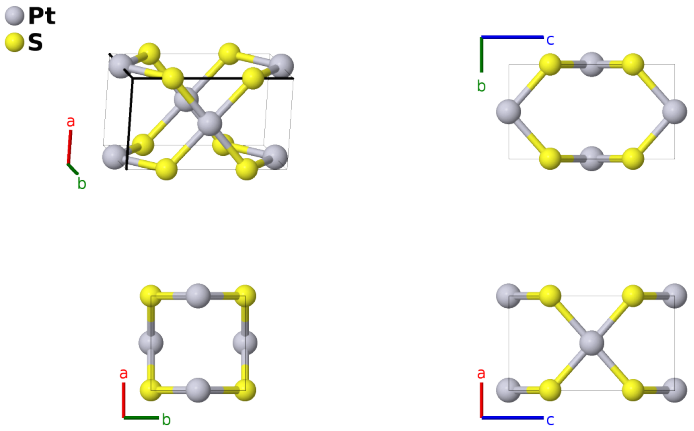
# Cooperite (PtS, $B17$) Structure: AB_tP4_131_c_e-001

This structure originally had the label `AB_tP4_131_c_e`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. 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

https://aflow.org/p/8GEP

https://aflow.org/p/AB_tP4_131_c_e-001



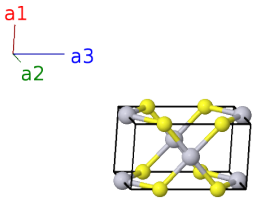

| | |
|---|---|
| **Prototype** | PtS |
| **AFLOW prototype label** | AB_tP4_131_c_e-001 |
| ***Strukturbericht* designation** | $B17$ |
| **Mineral name** | cooperite |
| **ICSD** | 654379 |
| **Pearson symbol** | tP4 |
| **Space group number** | 131 |
| **Space group symbol** | $P4_2/mmc$ |
| **AFLOW prototype command** | `aflow --proto=AB_tP4_131_c_e-001 --params=`$a, c/a$ |

**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 subsitute for sulfur on the (2e) site, and excess sulfur substitutes for platinum on the (2c) site.
- Previous versions of this page incorrectly used a = 4.9073Å. We have changed this to the correct value of 3.47Å. We thank Dr. Frank Hoffmann of the University of Hamburg for point 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.