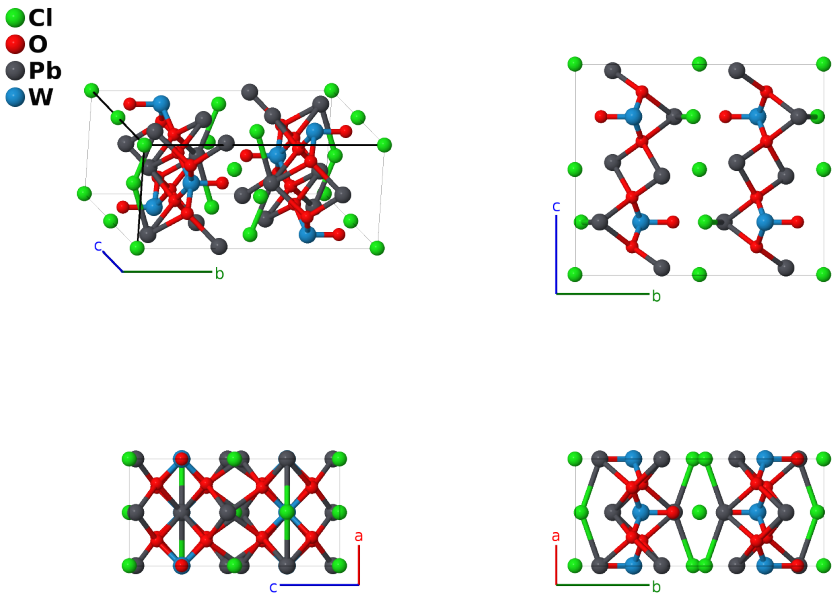
# Pinalite ($Pb_3WO_5Cl_2$) Structure: A2B5C3D_oC44_63_ac_ch_cf_c-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/S4ZE

https://aflow.org/p/A2B5C3D_oC44_63_ac_ch_cf_c-001



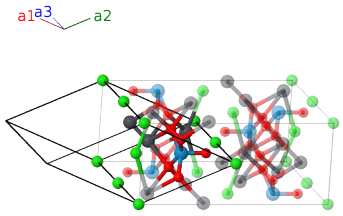

| | |
|---|---|
| **Prototype** | $Cl_2O_5Pb_3W$ |
| **AFLOW prototype label** | A2B5C3D_oC44_63_ac_ch_cf_c-001 |
| **Mineral name** | pinalite |
| **ICSD** | 89833 |
| **Pearson symbol** | oC44 |
| **Space group number** | 63 |
| **Space group symbol** | $Cmcm$ |
| **AFLOW prototype command** | `aflow --proto=A2B5C3D_oC44_63_ac_ch_cf_c-001 --params=`$a, b/a, c/a, y_2, y_3, y_4, y_5, y_6, z_6, x_7, y_7, z_7$ |

**Other compounds with this structure**
$Ba_3ReO_5Cl_2$, $Sr_3ReO_5Cl_2$

- (Grice, 2000) give the structure of pinalite in the *Amam* setting of space group #63. We used FINDSYM to transform this to the standard *Cmcm* setting.

## Base-centered Orthorhombic primitive vectors

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




## Basis vectors

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (4a) | Cl I |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}c\,\hat{\mathbf{z}}$ | (4a) | Cl I |
| $\mathbf{B_3}$ | = | $-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (4c) | Cl II |
| $\mathbf{B_4}$ | = | $y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $-by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (4c) | Cl II |
| $\mathbf{B_5}$ | = | $-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (4c) | O I |
| $\mathbf{B_6}$ | = | $y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $-by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (4c) | O I |
| $\mathbf{B_7}$ | = | $-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $by_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (4c) | Pb I |
| $\mathbf{B_8}$ | = | $y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $-by_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (4c) | Pb I |
| $\mathbf{B_9}$ | = | $-y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $by_5\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (4c) | W I |
| $\mathbf{B_{10}}$ | = | $y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $-by_5\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (4c) | W I |
| $\mathbf{B_{11}}$ | = | $-y_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$ | = | $by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (8f) | Pb II |
| $\mathbf{B_{12}}$ | = | $y_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (8f) | Pb II |
| $\mathbf{B_{13}}$ | = | $-y_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $by_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (8f) | Pb II |
| $\mathbf{B_{14}}$ | = | $y_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$ | = | $-by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$ | (8f) | Pb II |
| $\mathbf{B_{15}}$ | = | $(x_7 - y_7)\,\mathbf{a}_1 + (x_7 + y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$ | = | $ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$ | (16h) | O II |
| $\mathbf{B_{16}}$ | = | $-(x_7 - y_7)\,\mathbf{a}_1 - (x_7 + y_7)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (16h) | O II |
| $\mathbf{B_{17}}$ | = | $-(x_7 + y_7)\,\mathbf{a}_1 - (x_7 - y_7)\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (16h) | O II |
| $\mathbf{B_{18}}$ | = | $(x_7 + y_7)\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$ | = | $ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$ | (16h) | O II |
| $\mathbf{B_{19}}$ | = | $-(x_7 - y_7)\,\mathbf{a}_1 - (x_7 + y_7)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$ | = | $-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$ | (16h) | O II |
| $\mathbf{B_{20}}$ | = | $(x_7 - y_7)\,\mathbf{a}_1 + (x_7 + y_7)\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (16h) | O II |
| $\mathbf{B_{21}}$ | = | $(x_7 + y_7)\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (16h) | O II |
| $\mathbf{B_{22}}$ | = | $-(x_7 + y_7)\,\mathbf{a}_1 - (x_7 - y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$ | = | $-ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$ | (16h) | O II |

## References

[1] J. D. Grice and P. J. Dunn, *Crystal-structure determination of pinalite*, Am. Mineral. **85**, 806–809 (2000).