

# Sb<sub>2</sub>PbO<sub>4</sub> Structure:

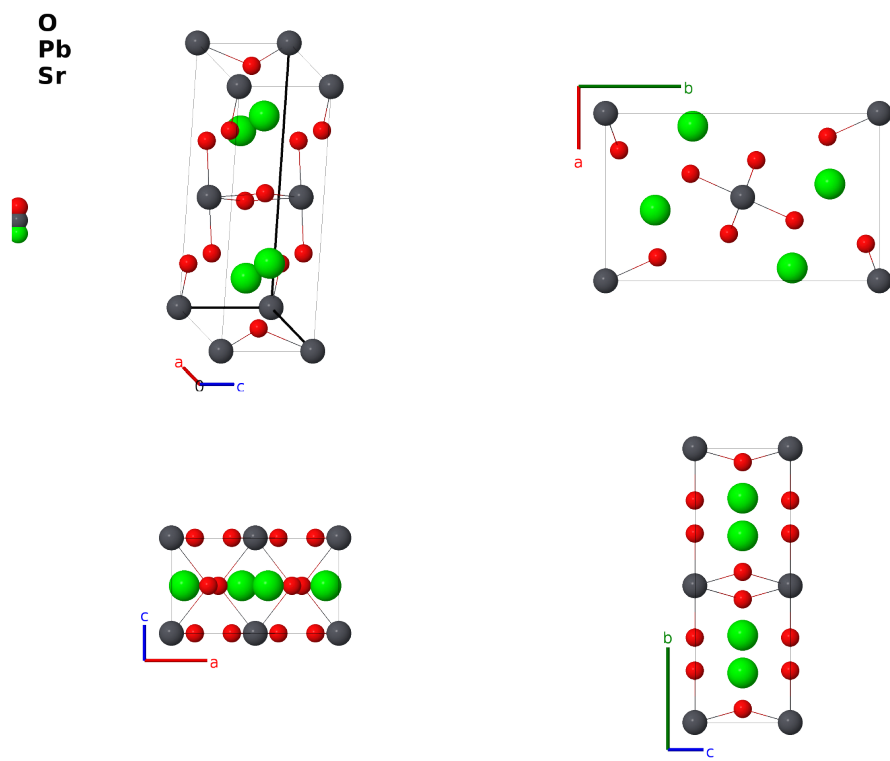
## A4BC2\_oP14\_55\_gh\_a\_h-001

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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/YNA1>

[https://aflow.org/prototype-encyclopedia/A4BC2\\_oP14\\_55\\_gh\\_a\\_h-001](https://aflow.org/prototype-encyclopedia/A4BC2_oP14_55_gh_a_h-001)



|                         |                                                                                                                                                                            |
|-------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prototype               | O <sub>4</sub> PbSb <sub>2</sub>                                                                                                                                           |
| AFLOW prototype label   | A4BC2_oP14_55_gh_a_h-001                                                                                                                                                   |
| ICSD                    | 4418                                                                                                                                                                       |
| CCDC                    | 1593048                                                                                                                                                                    |
| Pearson symbol          | oP14                                                                                                                                                                       |
| Space group number      | 55                                                                                                                                                                         |
| Space group symbol      | <i>Pbam</i>                                                                                                                                                                |
| AFLOW prototype command | <code>aflow --proto=A4BC2_oP14_55_gh_a_h-001</code><br><code>--params=a,b/a,c/a,x<sub>2</sub>,y<sub>2</sub>,x<sub>3</sub>,y<sub>3</sub>,x<sub>4</sub>,y<sub>4</sub></code> |

## Other compounds with this structure

$\text{Ca}_2\text{PbO}_4$ ,  $\text{Ca}_2\text{SnO}_4$ ,  $\text{Cd}_2\text{SnO}_4$ ,  $\text{Li}_2\text{MgH}_4$ ,  $\text{Mg}_2\text{SiO}_4$ ,  $\text{Mn}_2\text{GeO}_4$ ,  $\text{Na}_2\text{CdCl}_4$ ,  $\text{Na}_2\text{MgCl}_4$ ,  $\text{Na}_2\text{MnCl}_4$ ,  $\text{Na}_2\text{UO}_4$ ,  $\text{Sr}_2\text{CeO}_4$ ,  $\text{Sr}_2\text{PrO}_4$

## Simple Orthorhombic primitive vectors



## Basis vectors

|                   | Lattice coordinates                                                                                 |     | Cartesian coordinates                                                                                             | Wyckoff position | Atom type |
|-------------------|-----------------------------------------------------------------------------------------------------|-----|-------------------------------------------------------------------------------------------------------------------|------------------|-----------|
| $\mathbf{B}_1$    | $= 0$                                                                                               | $=$ | $0$                                                                                                               | (2a)             | Pb I      |
| $\mathbf{B}_2$    | $= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$                                             | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}}$                                                 | (2a)             | Pb I      |
| $\mathbf{B}_3$    | $= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$                                                             | $=$ | $ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}}$                                                                   | (4g)             | O I       |
| $\mathbf{B}_4$    | $= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$                                                            | $=$ | $-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}}$                                                                  | (4g)             | O I       |
| $\mathbf{B}_5$    | $= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2$                            | $=$ | $-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}}$                                  | (4g)             | O I       |
| $\mathbf{B}_6$    | $= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2$                             | $=$ | $a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}}$                                   | (4g)             | O I       |
| $\mathbf{B}_7$    | $= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$                                  | $=$ | $ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$                                  | (4h)             | O II      |
| $\mathbf{B}_8$    | $= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$                                 | $=$ | $-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$                                 | (4h)             | O II      |
| $\mathbf{B}_9$    | $= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$ | $=$ | $-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$ | (4h)             | O II      |
| $\mathbf{B}_{10}$ | $= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$  | $=$ | $a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$  | (4h)             | O II      |
| $\mathbf{B}_{11}$ | $= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$                                  | $=$ | $ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$                                  | (4h)             | Sr I      |
| $\mathbf{B}_{12}$ | $= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$                                 | $=$ | $-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$                                 | (4h)             | Sr I      |
| $\mathbf{B}_{13}$ | $= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$ | $=$ | $-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$ | (4h)             | Sr I      |
| $\mathbf{B}_{14}$ | $= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$  | $=$ | $a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$  | (4h)             | Sr I      |

## References

- [1] M. Trömel, *Die Kristallstruktur der Verbindungen vom  $\text{Sr}_2\text{PbO}_4$ -Typ*, Z. Anorganische und Allgemeine Chemie **371**, 237–247 (1969), doi:10.1002/zaac.19693710504.

## Found in

- [1] AFLOW legacy structure.

## First cited in

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