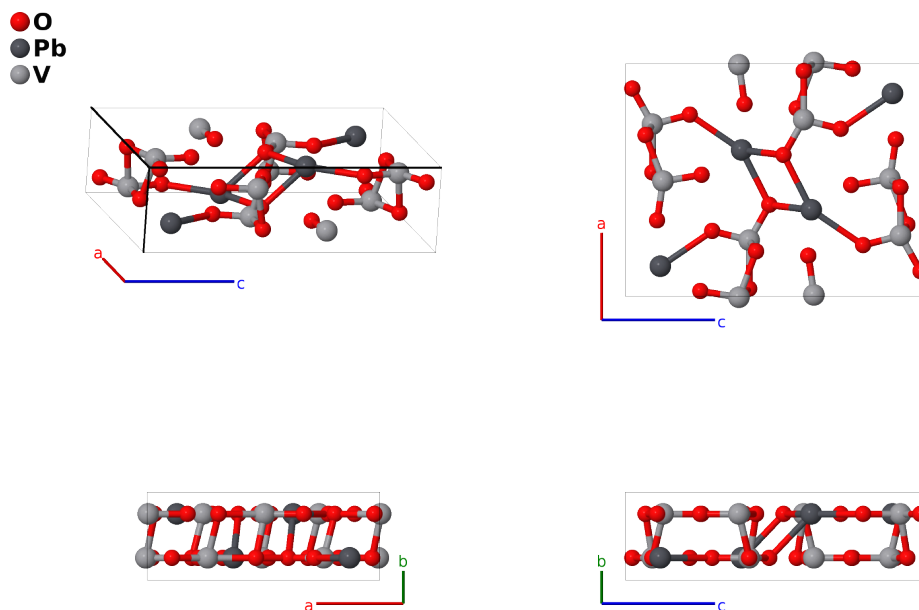


PbV₂O₆ Structure: A6BC2_oP36_62_6c_c_2c-001

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/XXTA>

https://aflow.org/p/A6BC2_oP36_62_6c_c_2c-001



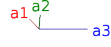
Prototype	O ₆ PbV ₂
AFLOW prototype label	A6BC2_oP36_62_6c_c_2c-001
ICSD	6109
Pearson symbol	oP36
Space group number	62
Space group symbol	<i>Pnma</i>
AFLOW prototype command	<code>aflow --proto=A6BC2_oP36_62_6c_c_2c-001 --params=a, b/a, c/a, x₁, z₁, x₂, z₂, x₃, z₃, x₄, z₄, x₅, z₅, x₆, z₆, x₇, z₇, x₈, z₈, x₉, z₉</code>

Other compounds with this structure

BaV₂O₆, CdV₂O₆, CaV₂O₆, SrV₂O₆, MnSeTeO₆

- This is the ground state structure of PbV₂O₆, stable up to 490°C. (Villars, 2018) There is also a metastable monoclinic structure.

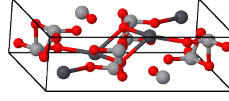
Simple Orthorhombic primitive vectors



$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_2	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_3	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_4	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_6	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_7	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_8	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	O III
\mathbf{B}_{10}	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O III
\mathbf{B}_{11}	$= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4c)	O III
\mathbf{B}_{12}	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O III
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	O IV
\mathbf{B}_{14}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O IV
\mathbf{B}_{15}	$= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4c)	O IV
\mathbf{B}_{16}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O IV
\mathbf{B}_{17}	$= x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	O V
\mathbf{B}_{18}	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O V
\mathbf{B}_{19}	$= -x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4c)	O V
\mathbf{B}_{20}	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O V
\mathbf{B}_{21}	$= x_6 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4c)	O VI
\mathbf{B}_{22}	$= -(x_6 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O VI
\mathbf{B}_{23}	$= -x_6 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4c)	O VI
\mathbf{B}_{24}	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O VI
\mathbf{B}_{25}	$= x_7 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4c)	Pb I

$$\begin{aligned}
\mathbf{B}_{26} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\text{Pb I} \\
\mathbf{B}_{27} &= -x_7 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -ax_7 \hat{\mathbf{x}} + \frac{3}{4}b\hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} &(4c) &\text{Pb I} \\
\mathbf{B}_{28} &= \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\text{Pb I} \\
\mathbf{B}_{29} &= x_8 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_8 \mathbf{a}_3 &= ax_8 \hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} &(4c) &\text{V I} \\
\mathbf{B}_{30} &= -\left(x_8 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\text{V I} \\
\mathbf{B}_{31} &= -x_8 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_8 \mathbf{a}_3 &= -ax_8 \hat{\mathbf{x}} + \frac{3}{4}b\hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} &(4c) &\text{V I} \\
\mathbf{B}_{32} &= \left(x_8 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\text{V I} \\
\mathbf{B}_{33} &= x_9 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_9 \mathbf{a}_3 &= ax_9 \hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} &(4c) &\text{V II} \\
\mathbf{B}_{34} &= -\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\text{V II} \\
\mathbf{B}_{35} &= -x_9 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_9 \mathbf{a}_3 &= -ax_9 \hat{\mathbf{x}} + \frac{3}{4}b\hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} &(4c) &\text{V II} \\
\mathbf{B}_{36} &= \left(x_9 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} - c\left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\text{V II}
\end{aligned}$$

References

- [1] B. D. Joran and C. Calvo, *Crystal Structure of Lead meta Vanadate*, PbV_2O_6 , Can. J. Chem. **52**, 2071–2074 (1974), doi:10.1139/v74-393.

Found in

- [1] P. Villars, H. Okamoto, and K. Cenzual, eds., *ASM Alloy Phase Diagram Database* (ASM International, 2018), chap. Oxygen-Lead-Vanadium Ternary, Vertical Section (1986 Slobodin B.V.). Copyright ©2006-2018 ASM International.