

PbV₂O₆ Structure:

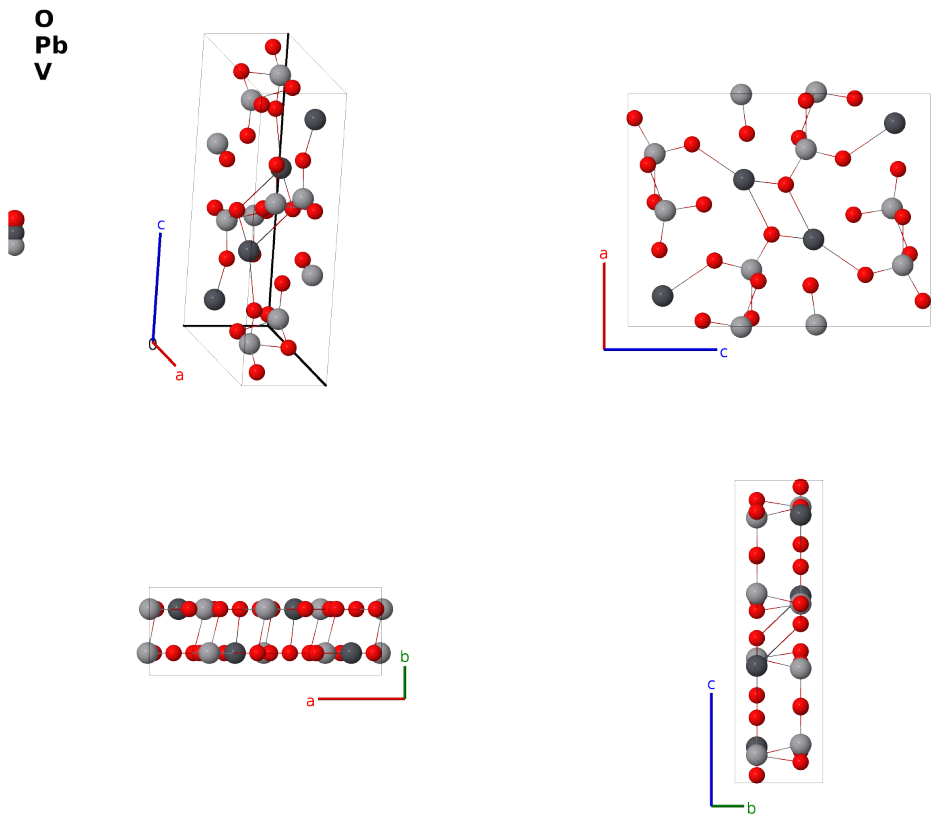
A6BC2_oP36_62_6c_c_2c-001

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<https://aflow.org/prototype-encyclopedia/XXTA>

https://aflow.org/prototype-encyclopedia/A6BC2_oP36_62_6c_c_2c-001



Prototype	O ₆ PbV ₂
AFLOW prototype label	A6BC2_oP36_62_6c_c_2c-001
ICSD	6109
CCDC	1593617
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</code> <code>--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

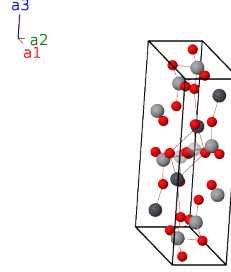
- This is the ground state structure of PbV₂O₆, stable up to 490°C. (Villars, 2018) There is also a metastable monoclinic structure.

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
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_6$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_8$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{10}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{12}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{14}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{16}$	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{18}$	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{26} =$	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 +$ $(z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_7 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c (z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	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)	Pb I
$\mathbf{B}_{28} =$	$(x_7 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_7 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c (z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	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)	V I
$\mathbf{B}_{30} =$	$-(x_8 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 +$ $(z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_8 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c (z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	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)	V I
$\mathbf{B}_{32} =$	$(x_8 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_8 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c (z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	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)	V II
$\mathbf{B}_{34} =$	$-(x_9 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 +$ $(z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_9 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c (z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	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)	V II
$\mathbf{B}_{36} =$	$(x_9 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_9 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c (z_9 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	V II

References

- [1] B. D. Joran and C. Calvo, *Crystal Structure of Lead meta Vanadate, PbV₂O₆*, Can. J. Chem. **52**, 2071–2074 (1974), doi:10.1139/v74-393.

Found in

- [1] P. Villars, H. Okamoto, and K. Cenxual, 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.

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