Metastable PbV_2O_6 Structure: A6BC2_mC36_12_6i_i_2i-001

https://aflow.org/p/X6VQ

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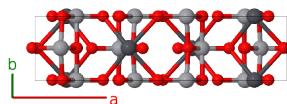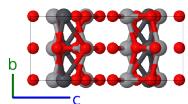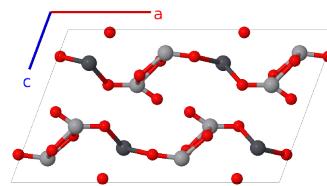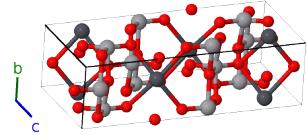
Prototype	O_6PbV_2
AFLOW prototype label	A6BC2_mC36_12_6i_i_2i-001
ICSD	36464
Pearson symbol	mC36
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	aflow --proto=A6BC2_mC36_12_6i_i_2i-001 --params=$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9$

**Other compounds with this structure**

Bi_2WO_6

- This is a metastable phase of PbV_2O_6 (Villars, 2018). The ground state has an orthorhombic structure.

- The ICSD entry sets $x_1 = 0.093$ for the position of the O I atom, while (Calenstani, 1985) has the value 0.93. We use the later value here.

Base-centered Monoclinic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$
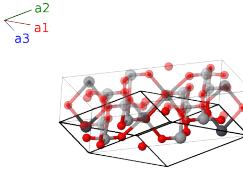
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$x_1\,\mathbf{a_1} + x_1\,\mathbf{a_2} + z_1\,\mathbf{a_3}$	$=$	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(4i)	O I
$\mathbf{B_2}$	$=$	$-x_1\,\mathbf{a_1} - x_1\,\mathbf{a_2} - z_1\,\mathbf{a_3}$	$=$	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(4i)	O I
$\mathbf{B_3}$	$=$	$x_2\,\mathbf{a_1} + x_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	$=$	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	O II
$\mathbf{B_4}$	$=$	$-x_2\,\mathbf{a_1} - x_2\,\mathbf{a_2} - z_2\,\mathbf{a_3}$	$=$	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	O II
$\mathbf{B_5}$	$=$	$x_3\,\mathbf{a_1} + x_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	O III
$\mathbf{B_6}$	$=$	$-x_3\,\mathbf{a_1} - x_3\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	O III
$\mathbf{B_7}$	$=$	$x_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	O IV
$\mathbf{B_8}$	$=$	$-x_4\,\mathbf{a_1} - x_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	O IV
$\mathbf{B_9}$	$=$	$x_5\,\mathbf{a_1} + x_5\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	$=$	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	O V
$\mathbf{B_{10}}$	$=$	$-x_5\,\mathbf{a_1} - x_5\,\mathbf{a_2} - z_5\,\mathbf{a_3}$	$=$	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	O V
$\mathbf{B_{11}}$	$=$	$x_6\,\mathbf{a_1} + x_6\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	$=$	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4i)	O VI
$\mathbf{B_{12}}$	$=$	$-x_6\,\mathbf{a_1} - x_6\,\mathbf{a_2} - z_6\,\mathbf{a_3}$	$=$	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(4i)	O VI
$\mathbf{B_{13}}$	$=$	$x_7\,\mathbf{a_1} + x_7\,\mathbf{a_2} + z_7\,\mathbf{a_3}$	$=$	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pb I
$\mathbf{B_{14}}$	$=$	$-x_7\,\mathbf{a_1} - x_7\,\mathbf{a_2} - z_7\,\mathbf{a_3}$	$=$	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pb I
$\mathbf{B_{15}}$	$=$	$x_8\,\mathbf{a_1} + x_8\,\mathbf{a_2} + z_8\,\mathbf{a_3}$	$=$	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(4i)	V I
$\mathbf{B_{16}}$	$=$	$-x_8\,\mathbf{a_1} - x_8\,\mathbf{a_2} - z_8\,\mathbf{a_3}$	$=$	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(4i)	V I
$\mathbf{B_{17}}$	$=$	$x_9\,\mathbf{a_1} + x_9\,\mathbf{a_2} + z_9\,\mathbf{a_3}$	$=$	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(4i)	V II
$\mathbf{B_{18}}$	$=$	$-x_9\,\mathbf{a_1} - x_9\,\mathbf{a_2} - z_9\,\mathbf{a_3}$	$=$	$-(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} - cz_9\sin\beta\,\hat{\mathbf{z}}$	(4i)	V II

References

[1] G. Calestani, G. D. Andreetti, A. Montenero, and M. Bettinelli, *Structure of metastable lead metavanadates: the monoclinic PbV_2O_6 (II) modification*, Acta Crystallogr. Sect. C **41**, 177–179 (1985), doi:10.1107/S0108270185003225.

[2] 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.

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[1] P. Villars and K. Cenzual, *PbV2O6 (V2PbO6 m mon) Crystal Structure: Datasheet from "PAULING FILE Multinaries Edition – 2012" in SpringerMaterials* (2016). Copyright 2016 Springer-Verlag Berlin Heidelberg & Material Phases Data System (MPDS), Switzerland & National Institute for Materials Science (NIMS), Japan.