

α' -V₈O Structure:

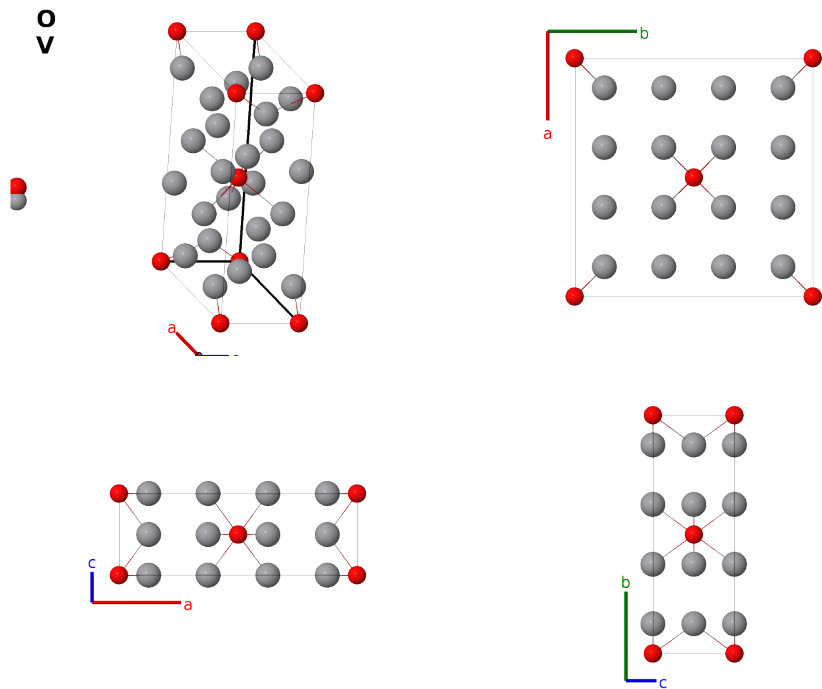
AB8_tP18_136_a_2fi-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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/WVZU>

https://aflow.org/prototype-encyclopedia/AB8_tP18_136_a_2fi-001



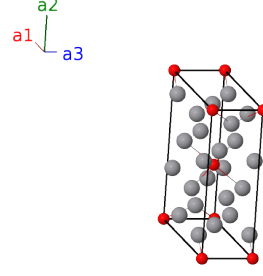
Prototype	OV ₈
AFLOW prototype label	AB8_tP18_136_a_2fi-001
ICSD	166600
CCDC	1682582
Pearson symbol	tP18
Space group number	136
Space group symbol	$P4_2/mnm$
AFLOW prototype command	<code>aflow --proto=AB8_tP18_136_a_2fi-001</code> <code>--params=a, c/a, x₂, x₃, x₄, y₄</code>

- (Villars, 2018) calls this β -V₈O, and refers to it as the room-temperature tetragonal structure. They also refer to a room-temperature triclinic structure.

- This is a supercell of the body-centered cubic (A2) lattice, with periodic interstitial oxygen atoms at the octahedral sites. In the real structure it is likely that there is considerable relaxation around the oxygen atoms.

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(2a) O I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2a) O I
$\mathbf{B}_3$	$=$	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}}$	(4f) V I
$\mathbf{B}_4$	$=$	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}}$	(4f) V I
$\mathbf{B}_5$	$=$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f) V I
$\mathbf{B}_6$	$=$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f) V I
$\mathbf{B}_7$	$=$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}}$	(4f) V II
$\mathbf{B}_8$	$=$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}}$	(4f) V II
$\mathbf{B}_9$	$=$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f) V II
$\mathbf{B}_{10}$	$=$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f) V II
$\mathbf{B}_{11}$	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}}$	(8i) V III
$\mathbf{B}_{12}$	$=$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}}$	(8i) V III
$\mathbf{B}_{13}$	$=$	$-(y_4 - \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i) V III
$\mathbf{B}_{14}$	$=$	$(y_4 + \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(y_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i) V III
$\mathbf{B}_{15}$	$=$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i) V III
$\mathbf{B}_{16}$	$=$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i) V III
$\mathbf{B}_{17}$	$=$	$y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2$	$=$	$ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}}$	(8i) V III
$\mathbf{B}_{18}$	$=$	$-y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2$	$=$	$-ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}}$	(8i) V III

References

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Found in

- [1] P. Villars, H. Okamoto, and K. Cenzual, eds., *ASM Alloy Phase Diagram Database* (ASM International, 2018), chap. Oxygen-Vanadium Binary Phase Diagram (1990 Wriedt H.A.). Copyright ©2006-2018 ASM International.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.