High Temperature Metastable VO_2 Structure: A2B_tI24_87_2h_h-001

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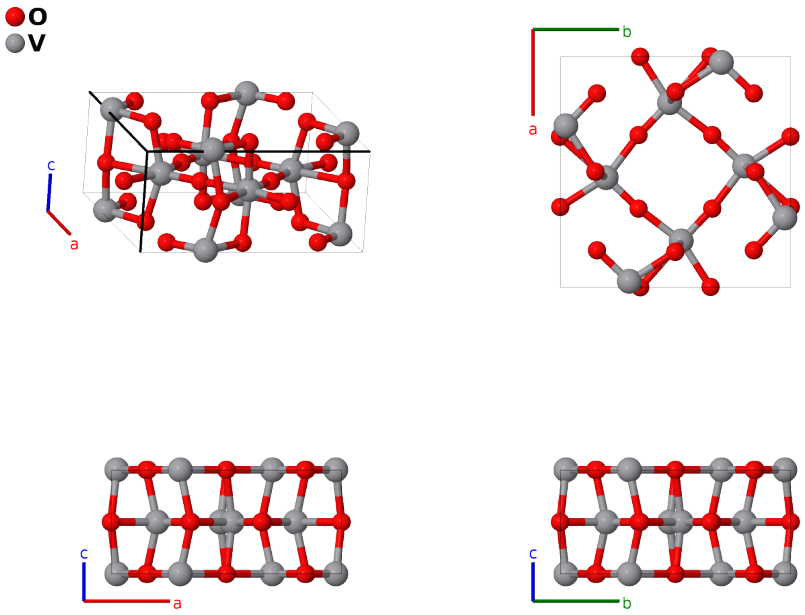
https://aflow.org/p/MHEM

https://aflow.org/p/A2B_tI24_87_2h_h-001

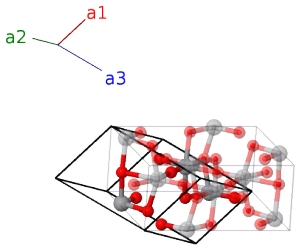


Prototype	O_2V
AFLOW prototype label	A2B_tI24_87_2h_h-001
ICSD	51214
Pearson symbol	tI24
Space group number	87
Space group symbol	$I4/m$
AFLOW prototype command	`aflow --proto=A2B_tI24_87_2h_h-001 --params=`$a, c/a, x_1, y_1, x_2, y_2, x_3, y_3$

- While the ground state of VO_2 is similar to baddeleyite ($C43$) (Villars, 2018), there are several metastable states (Oka, 1998), including this structure, seen at 473K, and another tetragonal structure seen at 298K.
- It has also been seen in the arsenopyrite $E0_7$ structure.

Body-centered Tetragonal primitive vectors

$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$y_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + (x_1+y_1)\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ay_1\,\hat{\mathbf{y}}$	(8h)	O I
$\mathbf{B_2}$	=	$-y_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - (x_1+y_1)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - ay_1\,\hat{\mathbf{y}}$	(8h)	O I
$\mathbf{B_3}$	=	$x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + (x_1-y_1)\,\mathbf{a}_3$	=	$-ay_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}}$	(8h)	O I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 - (x_1-y_1)\,\mathbf{a}_3$	=	$ay_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}}$	(8h)	O I
$\mathbf{B_5}$	=	$y_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + (x_2+y_2)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_6}$	=	$-y_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - (x_2+y_2)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_7}$	=	$x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + (x_2-y_2)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_8}$	=	$-x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 - (x_2-y_2)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_9}$	=	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + (x_3+y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}}$	(8h)	V I
$\mathbf{B_{10}}$	=	$-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - (x_3+y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}}$	(8h)	V I
$\mathbf{B_{11}}$	=	$x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + (x_3-y_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(8h)	V I
$\mathbf{B_{12}}$	=	$-x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - (x_3-y_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(8h)	V I

References

[1] Y. Oka, S. Sato, T. Yao, and N. Yamamoto, *Crystal Structures and Transition Mechanism of VO_2 (A)*, J. Solid State Chem. **141**, 594–598 (1998), doi:10.1006/jssc.1998.8025.

[2] 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.