# High Temperature Metastable $VO_2$ Structure: A2B_tI24_87_2h_h-001

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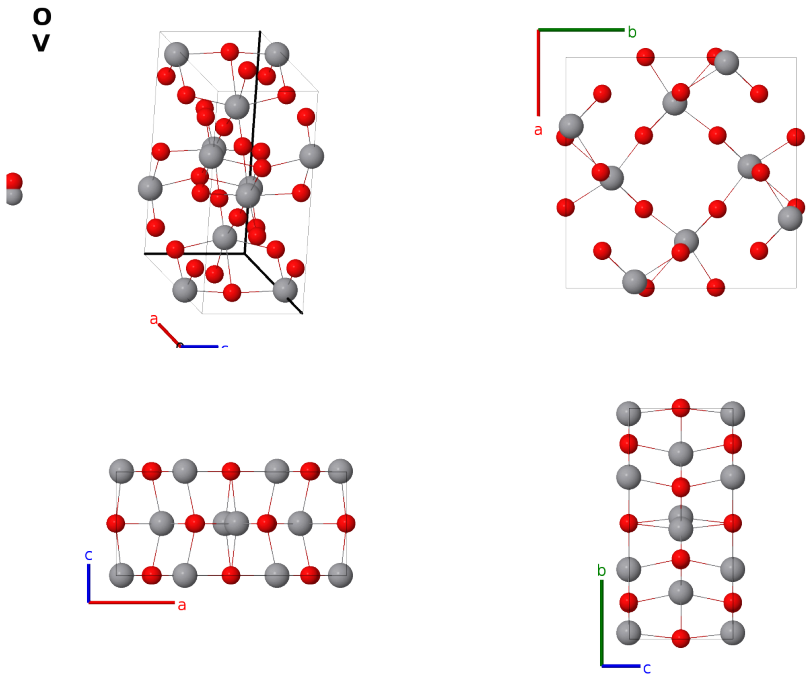
https://aflow.org/prototype-encyclopedia/MHEM

https://aflow.org/prototype-encyclopedia/A2B_tI24_87_2h_h-001




| | |
|---|---|
| **Prototype** | $O_2V$ |
| **AFLOW prototype label** | A2B_tI24_87_2h_h-001 |
| **ICSD** | 51214 |
| **CCDC** | 1616107 |
| **Pearson symbol** | tI24 |
| **Space group number** | 87 |
| **Space group symbol** | $I4/m$ |
| **AFLOW prototype command** | `aflow --proto=A2B_tI24_87_2h_h-001 --params=`$a, c/a, x_1, y_1, x_2, y_2, x_3, y_3$ |

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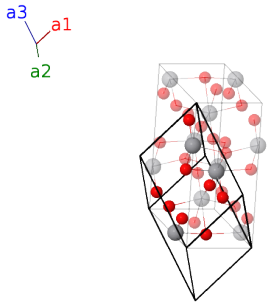
- While the ground state of $VO_2$ is similar to baddeleyite ($C43$) (Villars, 2018), there are several metastable states (Oka, 1998), including this structure, seen at 473K, and another tetragonal structure seen at 298K.
- It has also been seen in the arsenopyrite $E0_7$ structure.

### 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.


### First cited in

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