Room Temperature Metastable VO_2 Structure: A2B_tP48_130_2g_g-001

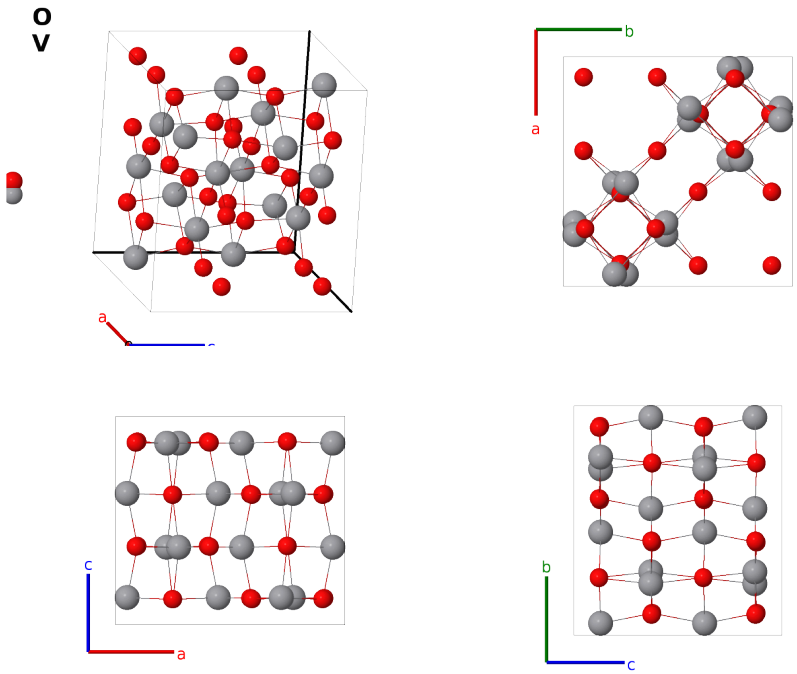
Cite this page as:

- 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.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, 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/P5YW

https://aflow.org/prototype-encyclopedia/A2B_tP48_130_2g_g-001

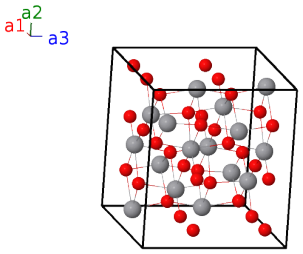


Prototype	O_2V
AFLOW prototype label	A2B_tP48_130_2g_g-001
ICSD	51213
CCDC	1616106
Pearson symbol	tP48
Space group number	130
Space group symbol	$P4/ncc$
AFLOW prototype command	`aflow --proto=A2B_tP48_130_2g_g-001 --params=`$a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3$

- 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 298K, and another tetragonal structure seen at 473K.
- It has also been seen in the arsenopyrite $E0_7$ structure.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ay_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B_2}$	=	$-\left(x_1-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_1-\frac{1}{2}\right)\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_1-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B_3}$	=	$-\left(y_1-\frac{1}{2}\right)\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$-a\left(y_1-\frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B_4}$	=	$y_1\,\mathbf{a}_1 - \left(x_1-\frac{1}{2}\right)\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ay_1\,\hat{\mathbf{x}} - a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_1 + \left(y_1+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_1-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + a\left(y_1+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_1-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B_6}$	=	$\left(x_1+\frac{1}{2}\right)\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - \left(z_1-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{x}} - ay_1\,\hat{\mathbf{y}} - c\left(z_1-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B_7}$	=	$\left(y_1+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_1+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_1-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_1+\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_1-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B_8}$	=	$-y_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - \left(z_1-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} - c\left(z_1-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B_9}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - ay_1\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B_{10}}$	=	$\left(x_1+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_1+\frac{1}{2}\right)\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_1+\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B_{11}}$	=	$\left(y_1+\frac{1}{2}\right)\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$a\left(y_1+\frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B_{12}}$	=	$-y_1\,\mathbf{a}_1 + \left(x_1+\frac{1}{2}\right)\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-ay_1\,\hat{\mathbf{x}} + a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B_{13}}$	=	$x_1\,\mathbf{a}_1 - \left(y_1-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} - a\left(y_1-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B_{14}}$	=	$-\left(x_1-\frac{1}{2}\right)\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{x}} + ay_1\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B_{15}}$	=	$-\left(y_1-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_1-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_1-\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B_{16}}$	=	$y_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B_{17}}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(16g)	O II
$\mathbf{B_{18}}$	=	$-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2-\frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_2-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(16g)	O II
$\mathbf{B_{19}}$	=	$-\left(y_2-\frac{1}{2}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-a\left(y_2-\frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(16g)	O II
$\mathbf{B_{20}}$	=	$y_2\,\mathbf{a}_1 - \left(x_2-\frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} - a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(16g)	O II
$\mathbf{B_{21}}$	=	$-x_2\,\mathbf{a}_1 + \left(y_2+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + a\left(y_2+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	O II
$\mathbf{B_{22}}$	=	$\left(x_2+\frac{1}{2}\right)\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - \left(z_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}} - c\left(z_2-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	O II

$\mathbf{B_{23}}$	$=$	$\left(y_2+\frac{1}{2}\right)\mathbf{a}_1+\left(x_2+\frac{1}{2}\right)\mathbf{a}_2-\left(z_2-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(y_2+\frac{1}{2}\right)\hat{\mathbf{x}}+a\left(x_2+\frac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_2-\frac{1}{2}\right)\hat{\mathbf{z}}$	(16g)	O II
$\mathbf{B_{24}}$	$=$	$-y_2\,\mathbf{a}_1-x_2\,\mathbf{a}_2-\left(z_2-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-ay_2\,\hat{\mathbf{x}}-ax_2\,\hat{\mathbf{y}}-c\left(z_2-\frac{1}{2}\right)\hat{\mathbf{z}}$	(16g)	O II
$\mathbf{B_{25}}$	$=$	$-x_2\,\mathbf{a}_1-y_2\,\mathbf{a}_2-z_2\,\mathbf{a}_3$	$=$	$-ax_2\,\hat{\mathbf{x}}-ay_2\,\hat{\mathbf{y}}-cz_2\,\hat{\mathbf{z}}$	(16g)	O II
$\mathbf{B_{26}}$	$=$	$\left(x_2+\frac{1}{2}\right)\mathbf{a}_1+\left(y_2+\frac{1}{2}\right)\mathbf{a}_2-z_2\,\mathbf{a}_3$	$=$	$a\left(x_2+\frac{1}{2}\right)\hat{\mathbf{x}}+a\left(y_2+\frac{1}{2}\right)\hat{\mathbf{y}}-cz_2\,\hat{\mathbf{z}}$	(16g)	O II
$\mathbf{B_{27}}$	$=$	$\left(y_2+\frac{1}{2}\right)\mathbf{a}_1-x_2\,\mathbf{a}_2-z_2\,\mathbf{a}_3$	$=$	$a\left(y_2+\frac{1}{2}\right)\hat{\mathbf{x}}-ax_2\,\hat{\mathbf{y}}-cz_2\,\hat{\mathbf{z}}$	(16g)	O II
$\mathbf{B_{28}}$	$=$	$-y_2\,\mathbf{a}_1+\left(x_2+\frac{1}{2}\right)\mathbf{a}_2-z_2\,\mathbf{a}_3$	$=$	$-ay_2\,\hat{\mathbf{x}}+a\left(x_2+\frac{1}{2}\right)\hat{\mathbf{y}}-cz_2\,\hat{\mathbf{z}}$	(16g)	O II
$\mathbf{B_{29}}$	$=$	$x_2\,\mathbf{a}_1-\left(y_2-\frac{1}{2}\right)\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$ax_2\,\hat{\mathbf{x}}-a\left(y_2-\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\hat{\mathbf{z}}$	(16g)	O II
$\mathbf{B_{30}}$	$=$	$-\left(x_2-\frac{1}{2}\right)\mathbf{a}_1+y_2\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(x_2-\frac{1}{2}\right)\hat{\mathbf{x}}+ay_2\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\hat{\mathbf{z}}$	(16g)	O II
$\mathbf{B_{31}}$	$=$	$-\left(y_2-\frac{1}{2}\right)\mathbf{a}_1-\left(x_2-\frac{1}{2}\right)\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(y_2-\frac{1}{2}\right)\hat{\mathbf{x}}-a\left(x_2-\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\hat{\mathbf{z}}$	(16g)	O II
$\mathbf{B_{32}}$	$=$	$y_2\,\mathbf{a}_1+x_2\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$ay_2\,\hat{\mathbf{x}}+ax_2\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\hat{\mathbf{z}}$	(16g)	O II
$\mathbf{B_{33}}$	$=$	$x_3\,\mathbf{a}_1+y_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	$=$	$ax_3\,\hat{\mathbf{x}}+ay_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(16g)	V I
$\mathbf{B_{34}}$	$=$	$-\left(x_3-\frac{1}{2}\right)\mathbf{a}_1-\left(y_3-\frac{1}{2}\right)\mathbf{a}_2+z_3\,\mathbf{a}_3$	$=$	$-a\left(x_3-\frac{1}{2}\right)\hat{\mathbf{x}}-a\left(y_3-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(16g)	V I
$\mathbf{B_{35}}$	$=$	$-\left(y_3-\frac{1}{2}\right)\mathbf{a}_1+x_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	$=$	$-a\left(y_3-\frac{1}{2}\right)\hat{\mathbf{x}}+ax_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(16g)	V I
$\mathbf{B_{36}}$	$=$	$y_3\,\mathbf{a}_1-\left(x_3-\frac{1}{2}\right)\mathbf{a}_2+z_3\,\mathbf{a}_3$	$=$	$ay_3\,\hat{\mathbf{x}}-a\left(x_3-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(16g)	V I
$\mathbf{B_{37}}$	$=$	$-x_3\,\mathbf{a}_1+\left(y_3+\frac{1}{2}\right)\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-ax_3\,\hat{\mathbf{x}}+a\left(y_3+\frac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_3-\frac{1}{2}\right)\hat{\mathbf{z}}$	(16g)	V I
$\mathbf{B_{38}}$	$=$	$\left(x_3+\frac{1}{2}\right)\mathbf{a}_1-y_3\,\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_3+\frac{1}{2}\right)\hat{\mathbf{x}}-ay_3\,\hat{\mathbf{y}}-c\left(z_3-\frac{1}{2}\right)\hat{\mathbf{z}}$	(16g)	V I
$\mathbf{B_{39}}$	$=$	$\left(y_3+\frac{1}{2}\right)\mathbf{a}_1+\left(x_3+\frac{1}{2}\right)\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(y_3+\frac{1}{2}\right)\hat{\mathbf{x}}+a\left(x_3+\frac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_3-\frac{1}{2}\right)\hat{\mathbf{z}}$	(16g)	V I
$\mathbf{B_{40}}$	$=$	$-y_3\,\mathbf{a}_1-x_3\,\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-ay_3\,\hat{\mathbf{x}}-ax_3\,\hat{\mathbf{y}}-c\left(z_3-\frac{1}{2}\right)\hat{\mathbf{z}}$	(16g)	V I
$\mathbf{B_{41}}$	$=$	$-x_3\,\mathbf{a}_1-y_3\,\mathbf{a}_2-z_3\,\mathbf{a}_3$	$=$	$-ax_3\,\hat{\mathbf{x}}-ay_3\,\hat{\mathbf{y}}-cz_3\,\hat{\mathbf{z}}$	(16g)	V I
$\mathbf{B_{42}}$	$=$	$\left(x_3+\frac{1}{2}\right)\mathbf{a}_1+\left(y_3+\frac{1}{2}\right)\mathbf{a}_2-z_3\,\mathbf{a}_3$	$=$	$a\left(x_3+\frac{1}{2}\right)\hat{\mathbf{x}}+a\left(y_3+\frac{1}{2}\right)\hat{\mathbf{y}}-cz_3\,\hat{\mathbf{z}}$	(16g)	V I
$\mathbf{B_{43}}$	$=$	$\left(y_3+\frac{1}{2}\right)\mathbf{a}_1-x_3\,\mathbf{a}_2-z_3\,\mathbf{a}_3$	$=$	$a\left(y_3+\frac{1}{2}\right)\hat{\mathbf{x}}-ax_3\,\hat{\mathbf{y}}-cz_3\,\hat{\mathbf{z}}$	(16g)	V I
$\mathbf{B_{44}}$	$=$	$-y_3\,\mathbf{a}_1+\left(x_3+\frac{1}{2}\right)\mathbf{a}_2-z_3\,\mathbf{a}_3$	$=$	$-ay_3\,\hat{\mathbf{x}}+a\left(x_3+\frac{1}{2}\right)\hat{\mathbf{y}}-cz_3\,\hat{\mathbf{z}}$	(16g)	V I
$\mathbf{B_{45}}$	$=$	$x_3\,\mathbf{a}_1-\left(y_3-\frac{1}{2}\right)\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$ax_3\,\hat{\mathbf{x}}-a\left(y_3-\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\hat{\mathbf{z}}$	(16g)	V I
$\mathbf{B_{46}}$	$=$	$-\left(x_3-\frac{1}{2}\right)\mathbf{a}_1+y_3\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(x_3-\frac{1}{2}\right)\hat{\mathbf{x}}+ay_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\hat{\mathbf{z}}$	(16g)	V I
$\mathbf{B_{47}}$	$=$	$-\left(y_3-\frac{1}{2}\right)\mathbf{a}_1-\left(x_3-\frac{1}{2}\right)\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(y_3-\frac{1}{2}\right)\hat{\mathbf{x}}-a\left(x_3-\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\hat{\mathbf{z}}$	(16g)	V I
$\mathbf{B_{48}}$	$=$	$y_3\,\mathbf{a}_1+x_3\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$ay_3\,\hat{\mathbf{x}}+ax_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\hat{\mathbf{z}}$	(16g)	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

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.