$V_{13}O_{16}$ Structure: A16B13_tI116_141_2hi_a2fh-001

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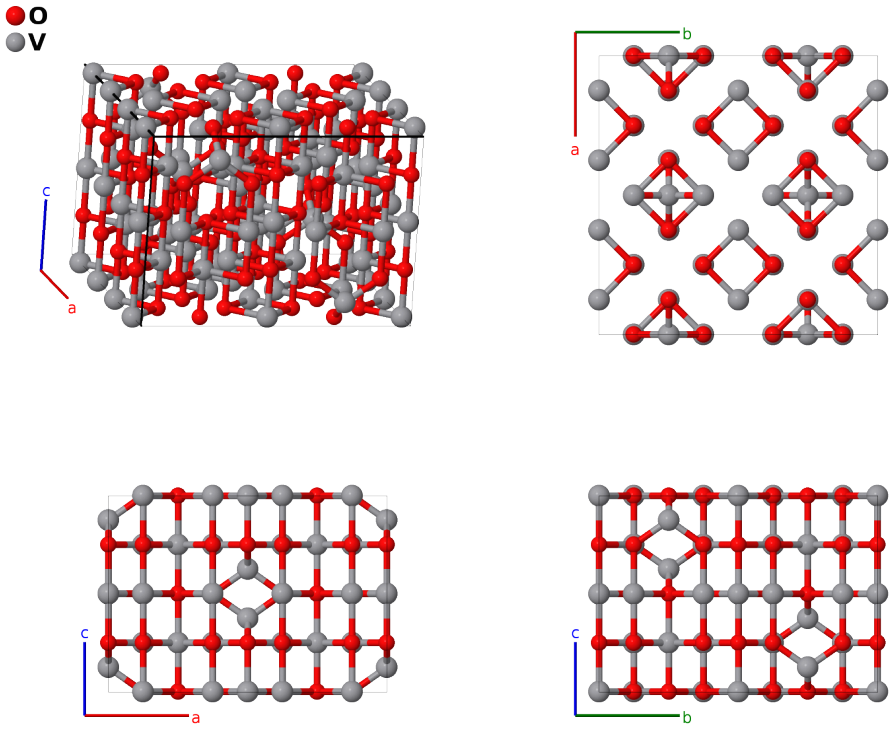
https://aflow.org/p/NCQA

https://aflow.org/p/A16B13_tI116_141_2hi_a2fh-001



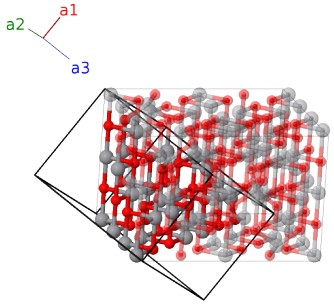
Prototype	$O_{16}V_{13}$
AFLOW prototype label	A16B13_tI116_141_2hi_a2fh-001
ICSD	77708
Pearson symbol	tI116
Space group number	141
Space group symbol	$I4_1/amd$
AFLOW prototype command	`aflow --proto=A16B13_tI116_141_2hi_a2fh-001 --params=`$a, c/a, x_2, x_3, y_4, z_4, y_5, z_5, y_6, z_6, x_7, y_7, z_7$

- There are serveral problems with this structure:
- It is not clear if (Andersson, 1970) put this in the first (4a site at the origin) or second (inversion site at the origin) setting of space group $I4_1/amd$ #141.
- Furthermore, they give values for x and z for the (16h) positions, even though the standard definition is (0 y z) in both settings.

- The ICSD entry assumes the first setting, and that the authors meant "y" rather than "x" for the first coordinate, but kept x as "x" for the other Wyckoff positions.
- We follow this convention, using AFLOW to convert that structure to the standard second setting. The result is shown here.
- However, (Andersson, 1970) call this structure a distorted rock salt ($B1$) structure with vacancies on the vanadium sites and interstitial vanadium atoms on the (4a) sites, and our structure look nothing like this.
- Furthermore, the (presumably relaxed) structure found on the Materials Project page (Jain, 2013) has the same symmetry and occupied Wyckoff positions, but is actually much different than this structure.
- We fill investigate this further. If updates are necessary we will revise this page.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(4a)	V I
$\mathbf{B_2}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(4a)	V I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}}$	(16f)	V II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(16f)	V II
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16f)	V II
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - \frac{1}{4}c\,\hat{\mathbf{z}}$	(16f)	V II
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}}$	(16f)	V II
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(16f)	V II
$\mathbf{B_9}$	=	$-x_2\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16f)	V II
$\mathbf{B_{10}}$	=	$x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - \frac{1}{4}c\,\hat{\mathbf{z}}$	(16f)	V II
$\mathbf{B_{11}}$	=	$x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}$	(16f)	V III
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(16f)	V III
$\mathbf{B_{13}}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16f)	V III
$\mathbf{B_{14}}$	=	$-x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - \frac{1}{4}c\,\hat{\mathbf{z}}$	(16f)	V III
$\mathbf{B_{15}}$	=	$-x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}$	(16f)	V III
$\mathbf{B_{16}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(16f)	V III
$\mathbf{B_{17}}$	=	$-x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16f)	V III
$\mathbf{B_{18}}$	=	$x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - \frac{1}{4}c\,\hat{\mathbf{z}}$	(16f)	V III
$\mathbf{B_{19}}$	=	$(y_4 + z_4)\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16h)	O I

$\mathbf{B_{20}}$	$=$	$\left(-y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_1+z_4\,\mathbf{a}_2-\left(y_4-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(16h)	O I
$\mathbf{B_{21}}$	$=$	$z_4\,\mathbf{a}_1+\left(-y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2-y_4\,\mathbf{a}_3$	$=$	$-a\left(y_4-\frac{1}{4}\right)\,\hat{\mathbf{x}}-\frac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	O I
$\mathbf{B_{22}}$	$=$	$z_4\,\mathbf{a}_1+(y_4+z_4)\,\mathbf{a}_2+\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(y_4+\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_4-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	O I
$\mathbf{B_{23}}$	$=$	$\left(y_4-z_4+\frac{1}{2}\right)\,\mathbf{a}_1-z_4\,\mathbf{a}_2+\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}}$	(16h)	O I
$\mathbf{B_{24}}$	$=$	$-\left(y_4+z_4\right)\,\mathbf{a}_1-z_4\,\mathbf{a}_2-y_4\,\mathbf{a}_3$	$=$	$-ay_4\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}}$	(16h)	O I
$\mathbf{B_{25}}$	$=$	$-z_4\,\mathbf{a}_1+\left(y_4-z_4+\frac{1}{2}\right)\,\mathbf{a}_2+y_4\,\mathbf{a}_3$	$=$	$a\left(y_4+\frac{1}{4}\right)\,\hat{\mathbf{x}}-\frac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	O I
$\mathbf{B_{26}}$	$=$	$-z_4\,\mathbf{a}_1-\left(y_4+z_4\right)\,\mathbf{a}_2-\left(y_4-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(y_4-\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	O I
$\mathbf{B_{27}}$	$=$	$\left(y_5+z_5\right)\,\mathbf{a}_1+z_5\,\mathbf{a}_2+y_5\,\mathbf{a}_3$	$=$	$ay_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(16h)	O II
$\mathbf{B_{28}}$	$=$	$\left(-y_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_1+z_5\,\mathbf{a}_2-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(16h)	O II
$\mathbf{B_{29}}$	$=$	$z_5\,\mathbf{a}_1+\left(-y_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_2-y_5\,\mathbf{a}_3$	$=$	$-a\left(y_5-\frac{1}{4}\right)\,\hat{\mathbf{x}}-\frac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	O II
$\mathbf{B_{30}}$	$=$	$z_5\,\mathbf{a}_1+(y_5+z_5)\,\mathbf{a}_2+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(y_5+\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_5-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	O II
$\mathbf{B_{31}}$	$=$	$\left(y_5-z_5+\frac{1}{2}\right)\,\mathbf{a}_1-z_5\,\mathbf{a}_2+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(16h)	O II
$\mathbf{B_{32}}$	$=$	$-\left(y_5+z_5\right)\,\mathbf{a}_1-z_5\,\mathbf{a}_2-y_5\,\mathbf{a}_3$	$=$	$-ay_5\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(16h)	O II
$\mathbf{B_{33}}$	$=$	$-z_5\,\mathbf{a}_1+\left(y_5-z_5+\frac{1}{2}\right)\,\mathbf{a}_2+y_5\,\mathbf{a}_3$	$=$	$a\left(y_5+\frac{1}{4}\right)\,\hat{\mathbf{x}}-\frac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	O II
$\mathbf{B_{34}}$	$=$	$-z_5\,\mathbf{a}_1-\left(y_5+z_5\right)\,\mathbf{a}_2-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(y_5-\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	O II
$\mathbf{B_{35}}$	$=$	$\left(y_6+z_6\right)\,\mathbf{a}_1+z_6\,\mathbf{a}_2+y_6\,\mathbf{a}_3$	$=$	$ay_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(16h)	V IV
$\mathbf{B_{36}}$	$=$	$\left(-y_6+z_6+\frac{1}{2}\right)\,\mathbf{a}_1+z_6\,\mathbf{a}_2-\left(y_6-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(16h)	V IV
$\mathbf{B_{37}}$	$=$	$z_6\,\mathbf{a}_1+\left(-y_6+z_6+\frac{1}{2}\right)\,\mathbf{a}_2-y_6\,\mathbf{a}_3$	$=$	$-a\left(y_6-\frac{1}{4}\right)\,\hat{\mathbf{x}}-\frac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	V IV
$\mathbf{B_{38}}$	$=$	$z_6\,\mathbf{a}_1+(y_6+z_6)\,\mathbf{a}_2+\left(y_6+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(y_6+\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_6-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	V IV
$\mathbf{B_{39}}$	$=$	$\left(y_6-z_6+\frac{1}{2}\right)\,\mathbf{a}_1-z_6\,\mathbf{a}_2+\left(y_6+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_6\,\hat{\mathbf{z}}$	(16h)	V IV
$\mathbf{B_{40}}$	$=$	$-\left(y_6+z_6\right)\,\mathbf{a}_1-z_6\,\mathbf{a}_2-y_6\,\mathbf{a}_3$	$=$	$-ay_6\,\hat{\mathbf{y}}-cz_6\,\hat{\mathbf{z}}$	(16h)	V IV
$\mathbf{B_{41}}$	$=$	$-z_6\,\mathbf{a}_1+\left(y_6-z_6+\frac{1}{2}\right)\,\mathbf{a}_2+y_6\,\mathbf{a}_3$	$=$	$a\left(y_6+\frac{1}{4}\right)\,\hat{\mathbf{x}}-\frac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_6-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	V IV
$\mathbf{B_{42}}$	$=$	$-z_6\,\mathbf{a}_1-\left(y_6+z_6\right)\,\mathbf{a}_2-\left(y_6-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(y_6-\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_6+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	V IV
$\mathbf{B_{43}}$	$=$	$\left(y_7+z_7\right)\,\mathbf{a}_1+\left(x_7+z_7\right)\,\mathbf{a}_2+\left(x_7+y_7\right)\,\mathbf{a}_3$	$=$	$ax_7\,\hat{\mathbf{x}}+ay_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(32i)	O III
$\mathbf{B_{44}}$	$=$	$\left(-y_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_7-z_7\right)\,\mathbf{a}_2-\left(x_7+y_7-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ax_7\,\hat{\mathbf{x}}-a\left(y_7-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(32i)	O III
$\mathbf{B_{45}}$	$=$	$\left(x_7+z_7\right)\,\mathbf{a}_1+\left(-y_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_7-y_7\right)\,\mathbf{a}_3$	$=$	$-a\left(y_7-\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(x_7-\frac{1}{4}\right)\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32i)	O III
$\mathbf{B_{46}}$	$=$	$-\left(x_7-z_7\right)\,\mathbf{a}_1+\left(y_7+z_7\right)\,\mathbf{a}_2+\left(-x_7+y_7+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(y_7+\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(x_7-\frac{1}{4}\right)\,\hat{\mathbf{y}}+c\left(z_7-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32i)	O III
$\mathbf{B_{47}}$	$=$	$\left(y_7-z_7+\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_7+z_7\right)\,\mathbf{a}_2+\left(-x_7+y_7+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ax_7\,\hat{\mathbf{x}}+a\left(y_7+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}}$	(32i)	O III
$\mathbf{B_{48}}$	$=$	$-\left(y_7+z_7\right)\,\mathbf{a}_1+\left(x_7-z_7\right)\,\mathbf{a}_2+\left(x_7-y_7\right)\,\mathbf{a}_3$	$=$	$ax_7\,\hat{\mathbf{x}}-ay_7\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}}$	(32i)	O III

$$\mathbf{B_{49}} = (x_7 - z_7)\,\mathbf{a}_1 + \left(y_7 - z_7 + \tfrac{1}{2}\right)\mathbf{a}_2 + (x_7 + y_7)\,\mathbf{a}_3 = a\left(y_7 + \tfrac{1}{4}\right)\hat{\mathbf{x}} + a\left(x_7 - \tfrac{1}{4}\right)\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (32i) \quad \text{O III}$$

$$\mathbf{B_{50}} = -(x_7 + z_7)\,\mathbf{a}_1 - (y_7 + z_7)\,\mathbf{a}_2 - \left(x_7 + y_7 - \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(y_7 - \tfrac{1}{4}\right)\hat{\mathbf{x}} - a\left(x_7 - \tfrac{1}{4}\right)\hat{\mathbf{y}} - c\left(z_7 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (32i) \quad \text{O III}$$

$$\mathbf{B_{51}} = -(y_7 + z_7)\,\mathbf{a}_1 - (x_7 + z_7)\,\mathbf{a}_2 - (x_7 + y_7)\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} - ay_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad (32i) \quad \text{O III}$$

$$\mathbf{B_{52}} = \left(y_7 - z_7 + \tfrac{1}{2}\right)\mathbf{a}_1 + (x_7 - z_7)\,\mathbf{a}_2 + \left(x_7 + y_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} + a\left(y_7 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad (32i) \quad \text{O III}$$

$$\mathbf{B_{53}} = -(x_7 + z_7)\,\mathbf{a}_1 + \left(y_7 - z_7 + \tfrac{1}{2}\right)\mathbf{a}_2 - (x_7 - y_7)\,\mathbf{a}_3 = a\left(y_7 + \tfrac{1}{4}\right)\hat{\mathbf{x}} - a\left(x_7 + \tfrac{1}{4}\right)\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (32i) \quad \text{O III}$$

$$\mathbf{B_{54}} = (x_7 - z_7)\,\mathbf{a}_1 - (y_7 + z_7)\,\mathbf{a}_2 + \left(x_7 - y_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(y_7 - \tfrac{1}{4}\right)\hat{\mathbf{x}} + a\left(x_7 + \tfrac{1}{4}\right)\hat{\mathbf{y}} - c\left(z_7 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (32i) \quad \text{O III}$$

$$\mathbf{B_{55}} = \left(-y_7 + z_7 + \tfrac{1}{2}\right)\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2 + \left(x_7 - y_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} - a\left(y_7 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (32i) \quad \text{O III}$$

$$\mathbf{B_{56}} = (y_7 + z_7)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 - (x_7 - y_7)\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} + ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (32i) \quad \text{O III}$$

$$\mathbf{B_{57}} = -(x_7 - z_7)\,\mathbf{a}_1 + \left(-y_7 + z_7 + \tfrac{1}{2}\right)\mathbf{a}_2 - (x_7 + y_7)\,\mathbf{a}_3 = -a\left(y_7 - \tfrac{1}{4}\right)\hat{\mathbf{x}} - a\left(x_7 + \tfrac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (32i) \quad \text{O III}$$

$$\mathbf{B_{58}} = (x_7 + z_7)\,\mathbf{a}_1 + (y_7 + z_7)\,\mathbf{a}_2 + \left(x_7 + y_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(y_7 + \tfrac{1}{4}\right)\hat{\mathbf{x}} + a\left(x_7 + \tfrac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_7 - \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (32i) \quad \text{O III}$$

References

[1] B. Andersson and J. Gj, *Ordered Phases in the Monoxide Region of the Vanadium-Oxygen System*, Acta Chem. Scand. **24**, 2250–2252 (1970), doi:10.3891/acta.chem.scand.24-2250.

Found in

[1] A. Jain, S. Ping, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, and K. A. Persson, *Commentary: The Materials Project: A materials genome approach to accelerating materials innovation*, APL Materials **1**, 011002 (2013), doi:10.1063/1.4812323. $V_{13}O_{16}$, mp-30065.