Room Temperature V_3O_5 Structure: A5B3_mP32_13_ef4g_ab2g-001

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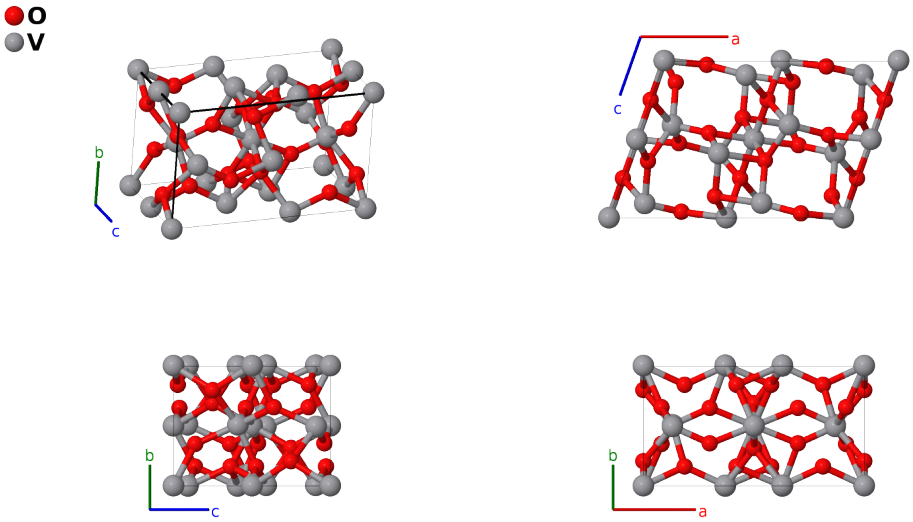
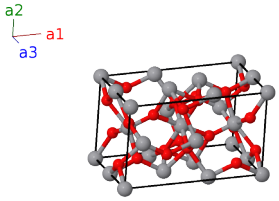


Prototype	O_5V_3
AFLOW prototype label	A5B3_mP32_13_ef4g_ab2g-001
ICSD	16445
Pearson symbol	mP32
Space group number	13
Space group symbol	$P2/c$
AFLOW prototype command	`aflow --proto=A5B3_mP32_13_ef4g_ab2g-001 --params=`$a, b/a, c/a, \beta, y_3, y_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}$

- This is the ground state structure of V_3O_5. In the range 423-433K it transforms into oxyvanite, which is metastable at room temperature (Armbruster, 2009). V_3O_5 can also be found in the metastable form of anosovite, which has the Fe_2TiO_5 ($E4_1$) structure (Weber, 2012).
- (Åsbrink, 1980) places the first two types of vanadium atoms on the (2c) and (2d) Wyckoff positions of space group $P2/c$ #13. We shifted the origin so that these atoms are on the (2a) and (2b) sites.

Simple Monoclinic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= a\,\hat{\mathbf{x}} \\
\mathbf{a_2} &= b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	V I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2a)	V I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(2b)	V II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}\left(a + c\cos\beta\right)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2b)	V II
$\mathbf{B_5}$	=	$y_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(2e)	O I
$\mathbf{B_6}$	=	$-y_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(2e)	O I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\left(\frac{a}{2} + \frac{c\cos\beta}{4}\right)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(2f)	O II
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\left(\frac{a}{2} + \frac{3c\cos\beta}{4}\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(2f)	O II
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\left(ax_5 + cz_5\cos\beta\right)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4g)	O III
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_5 + c\left(z_5 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O III
$\mathbf{B_{11}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-\left(ax_5 + cz_5\cos\beta\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4g)	O III
$\mathbf{B_{12}}$	=	$x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_5 + c\left(z_5 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O III
$\mathbf{B_{13}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\left(ax_6 + cz_6\cos\beta\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4g)	O IV
$\mathbf{B_{14}}$	=	$-x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_6 + c\left(z_6 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O IV
$\mathbf{B_{15}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-\left(ax_6 + cz_6\cos\beta\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(4g)	O IV
$\mathbf{B_{16}}$	=	$x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_6 + c\left(z_6 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O IV
$\mathbf{B_{17}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\left(ax_7 + cz_7\cos\beta\right)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(4g)	O V
$\mathbf{B_{18}}$	=	$-x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_7 + c\left(z_7 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O V
$\mathbf{B_{19}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-\left(ax_7 + cz_7\cos\beta\right)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(4g)	O V
$\mathbf{B_{20}}$	=	$x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_7 + c\left(z_7 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O V
$\mathbf{B_{21}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\left(ax_8 + cz_8\cos\beta\right)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(4g)	O VI
$\mathbf{B_{22}}$	=	$-x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_8 + c\left(z_8 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O VI
$\mathbf{B_{23}}$	=	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-\left(ax_8 + cz_8\cos\beta\right)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(4g)	O VI
$\mathbf{B_{24}}$	=	$x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_8 + c\left(z_8 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O VI
$\mathbf{B_{25}}$	=	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$\left(ax_9 + cz_9\cos\beta\right)\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(4g)	V III

$$\mathbf{B_{26}} = -x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 - \left(z_9 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = -\left(ax_9 + c\left(z_9 - \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} - c\left(z_9 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (4g) \quad \text{V III}$$

$$\mathbf{B_{27}} = -x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3 = -\left(ax_9 + cz_9\cos\beta\right)\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} - cz_9\sin\beta\,\hat{\mathbf{z}} \quad (4g) \quad \text{V III}$$

$$\mathbf{B_{28}} = x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + \left(z_9 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = \left(ax_9 + c\left(z_9 + \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + c\left(z_9 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (4g) \quad \text{V III}$$

$$\mathbf{B_{29}} = x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = \left(ax_{10} + cz_{10}\cos\beta\right)\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\sin\beta\,\hat{\mathbf{z}} \quad (4g) \quad \text{V IV}$$

$$\mathbf{B_{30}} = -x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 - \left(z_{10} - \tfrac{1}{2}\right)\,\mathbf{a}_3 = -\left(ax_{10} + c\left(z_{10} - \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} - c\left(z_{10} - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (4g) \quad \text{V IV}$$

$$\mathbf{B_{31}} = -x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 = -\left(ax_{10} + cz_{10}\cos\beta\right)\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} - cz_{10}\sin\beta\,\hat{\mathbf{z}} \quad (4g) \quad \text{V IV}$$

$$\mathbf{B_{32}} = x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 + \left(z_{10} + \tfrac{1}{2}\right)\,\mathbf{a}_3 = \left(ax_{10} + c\left(z_{10} + \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (4g) \quad \text{V IV}$$

References

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[2] D. Weber, C. Wessel, C. Reimann, C. Schwickert, A. Müller, T. Ressler, R. Pöttgen, T. Bredow, R. Dronskowski, , and M. Lerch, *Anosovite-Type V_3O_5: A New Binary Oxide of Vanadium* **51**, 8524–8529 (2012), doi:10.1021/ic301096d.

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