

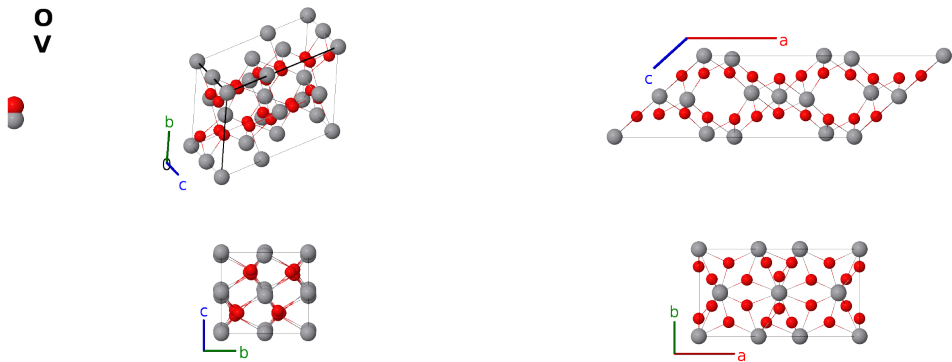
Room Temperature V_3O_5 Structure: A5B3_mP32_13_ef4g_ab2g-001

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<https://aflow.org/prototype-encyclopedia/3J3M>

https://aflow.org/prototype-encyclopedia/A5B3_mP32_13_ef4g_ab2g-001

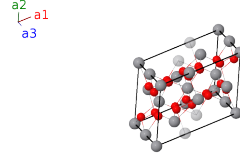


Prototype	O_5V_3
AFLOW prototype label	A5B3_mP32_13_ef4g_ab2g-001
ICSD	16445
CCDC	1597025
Pearson symbol	mP32
Space group number	13
Space group symbol	$P2/c$
AFLOW prototype command	<pre>aflow --proto=A5B3_mP32_13_ef4g_ab2g-001 --params=a,b/a,c/a,β,y₃,y₄,x₅,y₅,z₅,x₆,y₆,z₆,x₇,y₇,z₇,x₈,y₈,z₈,x₉,y₉,z₉,x₁₀, y₁₀,z₁₀</pre>

- 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
$\mathbf{B}_4$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} (a + c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \sin \beta \hat{\mathbf{z}}$	(2b)	V II
$\mathbf{B}_5$	$y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} c \cos \beta \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} + \frac{1}{4} c \sin \beta \hat{\mathbf{z}}$	(2e)	O I
$\mathbf{B}_6$	$-y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} c \cos \beta \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} + \frac{3}{4} c \sin \beta \hat{\mathbf{z}}$	(2e)	O I
$\mathbf{B}_7$	$\frac{1}{2} \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\left(\frac{a}{2} + \frac{c \cos \beta}{4}\right) \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} + \frac{1}{4} c \sin \beta \hat{\mathbf{z}}$	(2f)	O II
$\mathbf{B}_8$	$\frac{1}{2} \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\left(\frac{a}{2} + \frac{3c \cos \beta}{4}\right) \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} + \frac{3}{4} c \sin \beta \hat{\mathbf{z}}$	(2f)	O II
$\mathbf{B}_9$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(a x_5 + c z_5 \cos \beta) \hat{\mathbf{x}} + b y_5 \hat{\mathbf{y}} + c z_5 \sin \beta \hat{\mathbf{z}}$	(4g)	O III
$\mathbf{B}_{10}$	$-x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-(a x_5 + c \left(z_5 - \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} + b y_5 \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}}$	(4g)	O III
$\mathbf{B}_{11}$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(a x_5 + c z_5 \cos \beta) \hat{\mathbf{x}} - b y_5 \hat{\mathbf{y}} - c z_5 \sin \beta \hat{\mathbf{z}}$	(4g)	O III
$\mathbf{B}_{12}$	$x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$(a x_5 + c \left(z_5 + \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} - b y_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}}$	(4g)	O III
$\mathbf{B}_{13}$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(a x_6 + c z_6 \cos \beta) \hat{\mathbf{x}} + b y_6 \hat{\mathbf{y}} + c z_6 \sin \beta \hat{\mathbf{z}}$	(4g)	O IV
$\mathbf{B}_{14}$	$-x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-(a x_6 + c \left(z_6 - \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} + b y_6 \hat{\mathbf{y}} - c \left(z_6 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}}$	(4g)	O IV
$\mathbf{B}_{15}$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(a x_6 + c z_6 \cos \beta) \hat{\mathbf{x}} - b y_6 \hat{\mathbf{y}} - c z_6 \sin \beta \hat{\mathbf{z}}$	(4g)	O IV
$\mathbf{B}_{16}$	$x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$(a x_6 + c \left(z_6 + \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} - b y_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}}$	(4g)	O IV
$\mathbf{B}_{17}$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(a x_7 + c z_7 \cos \beta) \hat{\mathbf{x}} + b y_7 \hat{\mathbf{y}} + c z_7 \sin \beta \hat{\mathbf{z}}$	(4g)	O V
$\mathbf{B}_{18}$	$-x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-(a x_7 + c \left(z_7 - \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} + b y_7 \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}}$	(4g)	O V
$\mathbf{B}_{19}$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(a x_7 + c z_7 \cos \beta) \hat{\mathbf{x}} - b y_7 \hat{\mathbf{y}} - c z_7 \sin \beta \hat{\mathbf{z}}$	(4g)	O V
$\mathbf{B}_{20}$	$x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$(a x_7 + c \left(z_7 + \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} - b y_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}}$	(4g)	O V
$\mathbf{B}_{21}$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(a x_8 + c z_8 \cos \beta) \hat{\mathbf{x}} + b y_8 \hat{\mathbf{y}} + c z_8 \sin \beta \hat{\mathbf{z}}$	(4g)	O VI
$\mathbf{B}_{22}$	$-x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-(a x_8 + c \left(z_8 - \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} + b y_8 \hat{\mathbf{y}} - c \left(z_8 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}}$	(4g)	O VI
$\mathbf{B}_{23}$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(a x_8 + c z_8 \cos \beta) \hat{\mathbf{x}} - b y_8 \hat{\mathbf{y}} - c z_8 \sin \beta \hat{\mathbf{z}}$	(4g)	O VI
$\mathbf{B}_{24}$	$x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$(a x_8 + c \left(z_8 + \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} - b y_8 \hat{\mathbf{y}} + c \left(z_8 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}}$	(4g)	O VI
$\mathbf{B}_{25}$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(a x_9 + c z_9 \cos \beta) \hat{\mathbf{x}} + b y_9 \hat{\mathbf{y}} + c z_9 \sin \beta \hat{\mathbf{z}}$	(4g)	V III
$\mathbf{B}_{26}$	$-x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-(a x_9 + c \left(z_9 - \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} + b y_9 \hat{\mathbf{y}} - c \left(z_9 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}}$	(4g)	V III

$$\begin{aligned}
\mathbf{B}_{27} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 &= - (ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}} &(4g) &\text{V III} \\
\mathbf{B}_{28} &= x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 &= (ax_9 + c \left(z_9 + \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + &(4g) &\text{V III} \\
&&& c \left(z_9 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{29} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= (ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}} &(4g) &\text{V IV} \\
\mathbf{B}_{30} &= -x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_3 &= - (ax_{10} + c \left(z_{10} - \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} - &(4g) &\text{V IV} \\
&&& c \left(z_{10} - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{31} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= - (ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} - &(4g) &\text{V IV} \\
&&& cz_{10} \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{32} &= x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 &= (ax_{10} + c \left(z_{10} + \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + &(4g) &\text{V IV} \\
&&& c \left(z_{10} + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}}
\end{aligned}$$

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