

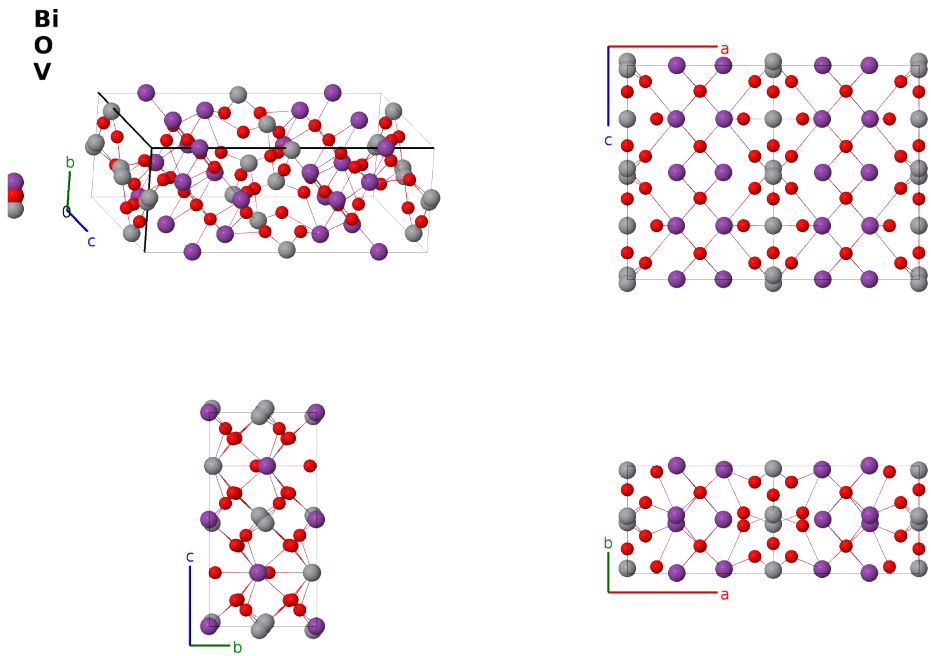
β -Bi₄V₂O₁₁ Structure: A4B12C3_oC76_63_eg_fg2h_cf-001

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<https://aflow.org/prototype-encyclopedia/AB76>

https://aflow.org/prototype-encyclopedia/A4B12C3_oC76_63_eg_fg2h_cf-001



Prototype	Bi ₄ O ₁₁ V ₂
AFLOW prototype label	A4B12C3_oC76_63_eg_fg2h_cf-001
ICSD	98588
CCDC	1657852
Pearson symbol	oC76
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	<code>aflow --proto=A4B12C3_oC76_63_eg_fg2h_cf-001</code> <code>--params=a, b/a, c/a, y₁, x₂, y₃, z₃, y₄, z₄, x₅, y₅, x₆, y₆, x₇, y₇, z₇, x₈, y₈, z₈</code>

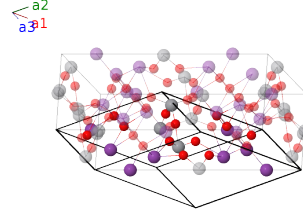
- There are three known varieties of Bi₄V₂O₁₁ (Villars, 2018):
 - α , the ground state structure, stable up to 450°C,
 - β , stable between 450°C and 555°C (this structure), and

– γ , stable from 555°C up to the melting point at 880°C.

- The data for this structure was taken at 550°C.
- Several of the Wyckoff positions listed here are only partially occupied: V-I: 25%, V-II: 50%, and O-IV 75%.
- (Mairesee, 2003) describe this structure in the *Amam* setting of space group #63. We used FINDSYM to transform this to the standard *Cmcm* setting.

Base-centered Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	V I
$\mathbf{B}_2$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	V I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{x}}$	(8e)	Bi I
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8e)	Bi I
$\mathbf{B}_5$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}}$	(8e)	Bi I
$\mathbf{B}_6$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8e)	Bi I
$\mathbf{B}_7$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B}_8$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B}_9$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B}_{10}$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B}_{11}$	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8f)	V II
$\mathbf{B}_{12}$	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	V II
$\mathbf{B}_{13}$	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	V II
$\mathbf{B}_{14}$	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8f)	V II
$\mathbf{B}_{15}$	$= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	Bi II
$\mathbf{B}_{16}$	$= -(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	Bi II
$\mathbf{B}_{17}$	$= -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	Bi II
$\mathbf{B}_{18}$	$= (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	Bi II
$\mathbf{B}_{19}$	$= (x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B}_{20}$	$= -(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B}_{21}$	$= -(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	O II

$$\begin{aligned}
\mathbf{B}_{22} &= (x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 = ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8g) & \quad \text{O II} \\
\mathbf{B}_{23} &= (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3 = ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (16h) & \quad \text{O III} \\
\mathbf{B}_{24} &= -(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 = -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} & (16h) & \quad \text{O III} \\
\mathbf{B}_{25} &= -(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 = -ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} & (16h) & \quad \text{O III} \\
\mathbf{B}_{26} &= (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3 = ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (16h) & \quad \text{O III} \\
\mathbf{B}_{27} &= -(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3 = -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (16h) & \quad \text{O III} \\
\mathbf{B}_{28} &= (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 = ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} & (16h) & \quad \text{O III} \\
\mathbf{B}_{29} &= (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 = ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} & (16h) & \quad \text{O III} \\
\mathbf{B}_{30} &= -(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3 = -ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (16h) & \quad \text{O III} \\
\mathbf{B}_{31} &= (x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3 = ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (16h) & \quad \text{O IV} \\
\mathbf{B}_{32} &= -(x_8 - y_8) \mathbf{a}_1 - (x_8 + y_8) \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3 = -ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c \left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}} & (16h) & \quad \text{O IV} \\
\mathbf{B}_{33} &= -(x_8 + y_8) \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3 = -ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c \left(z_8 - \frac{1}{2}\right) \hat{\mathbf{z}} & (16h) & \quad \text{O IV} \\
\mathbf{B}_{34} &= (x_8 + y_8) \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3 = ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (16h) & \quad \text{O IV} \\
\mathbf{B}_{35} &= -(x_8 - y_8) \mathbf{a}_1 - (x_8 + y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3 = -ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (16h) & \quad \text{O IV} \\
\mathbf{B}_{36} &= (x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3 = ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c \left(z_8 - \frac{1}{2}\right) \hat{\mathbf{z}} & (16h) & \quad \text{O IV} \\
\mathbf{B}_{37} &= (x_8 + y_8) \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3 = ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c \left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}} & (16h) & \quad \text{O IV} \\
\mathbf{B}_{38} &= -(x_8 + y_8) \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3 = -ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (16h) & \quad \text{O IV}
\end{aligned}$$

References

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