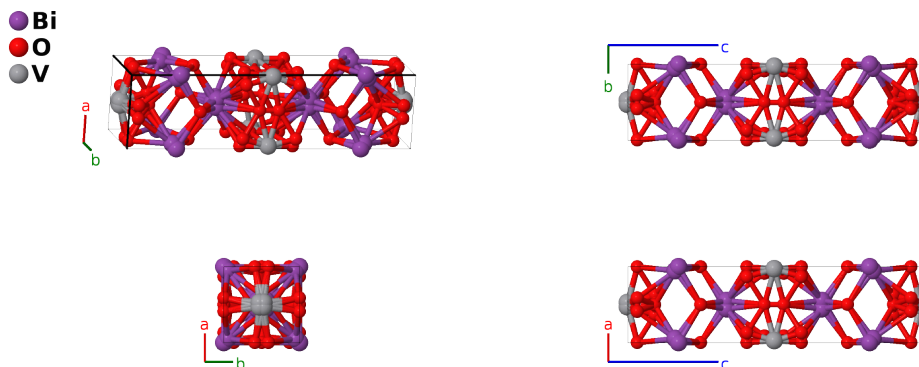


γ -Bi₄V₂O₁₁ Structure: A5B9C2_tI64_139_em_d2n_h-001

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<https://aflow.org/p/0N6E>

https://aflow.org/p/A5B9C2_tI64_139_em_d2n_h-001



Prototype	Bi ₄ O ₁₁ V ₂
AFLOW prototype label	A5B9C2_tI64_139_em_d2n_h-001
ICSD	98587
Pearson symbol	tI64
Space group number	139
Space group symbol	<i>I4/mmm</i>
AFLOW prototype command	<code>aflow --proto=A5B9C2_tI64_139_em_d2n_h-001 --params=a, c/a, z₂, x₃, x₄, z₄, y₅, z₅, y₆, z₆</code>

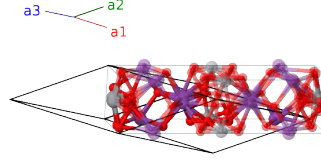
Other compounds with this structure

Bi₂WO₆

- 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, and
 - γ , stable from 555°C up to the melting point at 880°C (this structure).
- The data for this structure was taken at 550°C.
- Most of the Wyckoff positions here are only partially occupied: Bi-I 50%, Bi-II 25%, O-II 23.8%, O-III 19.8%, and V 25%, giving a stoichiometry of Bi₄V₂O_{10.976}. This structure is also sometimes described as Bi₂VO_{5.5}.

Body-centered Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	O I
\mathbf{B}_2	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	O I
\mathbf{B}_3	$= z_2 \mathbf{a}_1 + z_2 \mathbf{a}_2$	$=$	$cz_2 \hat{\mathbf{z}}$	(4e)	Bi I
\mathbf{B}_4	$= -z_2 \mathbf{a}_1 - z_2 \mathbf{a}_2$	$=$	$-cz_2 \hat{\mathbf{z}}$	(4e)	Bi I
\mathbf{B}_5	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + 2x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}}$	(8h)	V I
\mathbf{B}_6	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - 2x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}}$	(8h)	V I
\mathbf{B}_7	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}}$	(8h)	V I
\mathbf{B}_8	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}}$	(8h)	V I
\mathbf{B}_9	$= (x_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + 2x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(16m)	Bi II
\mathbf{B}_{10}	$= -(x_4 - z_4) \mathbf{a}_1 - (x_4 - z_4) \mathbf{a}_2 - 2x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(16m)	Bi II
\mathbf{B}_{11}	$= (x_4 + z_4) \mathbf{a}_1 - (x_4 - z_4) \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(16m)	Bi II
\mathbf{B}_{12}	$= -(x_4 - z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(16m)	Bi II
\mathbf{B}_{13}	$= (x_4 - z_4) \mathbf{a}_1 - (x_4 + z_4) \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(16m)	Bi II
\mathbf{B}_{14}	$= -(x_4 + z_4) \mathbf{a}_1 + (x_4 - z_4) \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(16m)	Bi II
\mathbf{B}_{15}	$= (x_4 - z_4) \mathbf{a}_1 + (x_4 - z_4) \mathbf{a}_2 + 2x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(16m)	Bi II
\mathbf{B}_{16}	$= -(x_4 + z_4) \mathbf{a}_1 - (x_4 + z_4) \mathbf{a}_2 - 2x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(16m)	Bi II
\mathbf{B}_{17}	$= (y_5 + z_5) \mathbf{a}_1 + z_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(16n)	O II
\mathbf{B}_{18}	$= -(y_5 - z_5) \mathbf{a}_1 + z_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(16n)	O II
\mathbf{B}_{19}	$= z_5 \mathbf{a}_1 - (y_5 - z_5) \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} + cz_5 \hat{\mathbf{z}}$	(16n)	O II
\mathbf{B}_{20}	$= z_5 \mathbf{a}_1 + (y_5 + z_5) \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} + cz_5 \hat{\mathbf{z}}$	(16n)	O II
\mathbf{B}_{21}	$= (y_5 - z_5) \mathbf{a}_1 - z_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(16n)	O II
\mathbf{B}_{22}	$= -(y_5 + z_5) \mathbf{a}_1 - z_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(16n)	O II
\mathbf{B}_{23}	$= -z_5 \mathbf{a}_1 + (y_5 - z_5) \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} - cz_5 \hat{\mathbf{z}}$	(16n)	O II
\mathbf{B}_{24}	$= -z_5 \mathbf{a}_1 - (y_5 + z_5) \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} - cz_5 \hat{\mathbf{z}}$	(16n)	O II
\mathbf{B}_{25}	$= (y_6 + z_6) \mathbf{a}_1 + z_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(16n)	O III
\mathbf{B}_{26}	$= -(y_6 - z_6) \mathbf{a}_1 + z_6 \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(16n)	O III
\mathbf{B}_{27}	$= z_6 \mathbf{a}_1 - (y_6 - z_6) \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} + cz_6 \hat{\mathbf{z}}$	(16n)	O III
\mathbf{B}_{28}	$= z_6 \mathbf{a}_1 + (y_6 + z_6) \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} + cz_6 \hat{\mathbf{z}}$	(16n)	O III
\mathbf{B}_{29}	$= (y_6 - z_6) \mathbf{a}_1 - z_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(16n)	O III

$$\mathbf{B}_{30} = -(y_6 + z_6) \mathbf{a}_1 - z_6 \mathbf{a}_2 - y_6 \mathbf{a}_3 = -ay_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} \quad (16n) \quad \text{O III}$$

$$\mathbf{B}_{31} = -z_6 \mathbf{a}_1 + (y_6 - z_6) \mathbf{a}_2 + y_6 \mathbf{a}_3 = ay_6 \hat{\mathbf{x}} - cz_6 \hat{\mathbf{z}} \quad (16n) \quad \text{O III}$$

$$\mathbf{B}_{32} = -z_6 \mathbf{a}_1 - (y_6 + z_6) \mathbf{a}_2 - y_6 \mathbf{a}_3 = -ay_6 \hat{\mathbf{x}} - cz_6 \hat{\mathbf{z}} \quad (16n) \quad \text{O III}$$

References

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