γ-$Bi_4V_2O_{11}$ Structure: A5B9C2_tI64_139_em_d2n_h-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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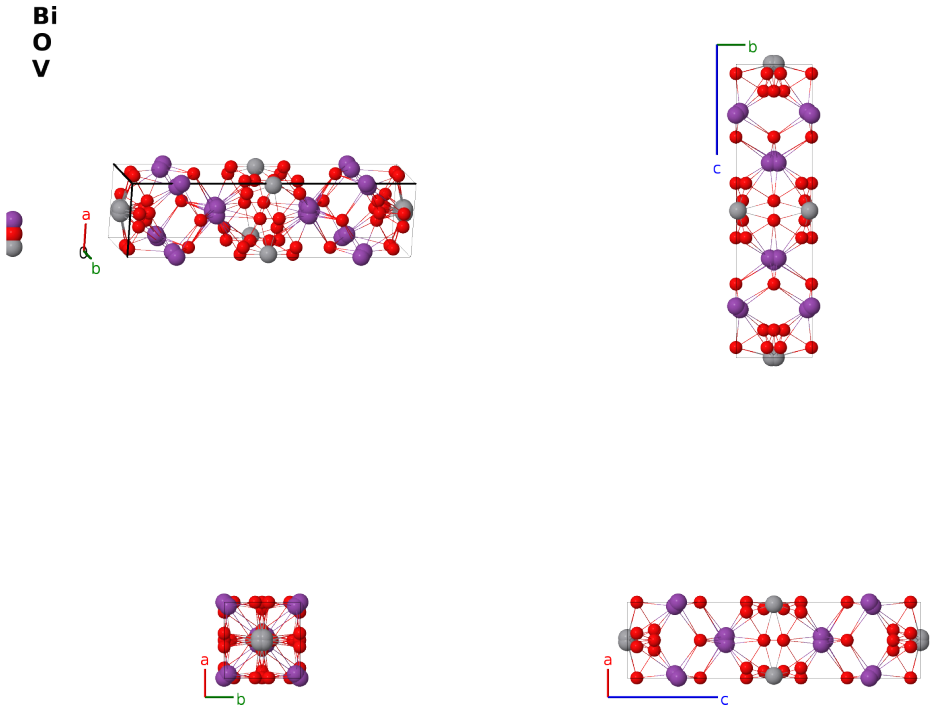
https://aflow.org/prototype-encyclopedia/0N6E

https://aflow.org/prototype-encyclopedia/A5B9C2_tI64_139_em_d2n_h-001



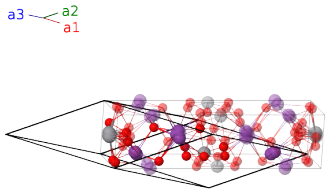
Prototype	$Bi_4O_{11}V_2$
AFLOW prototype label	A5B9C2_tI64_139_em_d2n_h-001
ICSD	98587
CCDC	1657851
Pearson symbol	tI64
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=A5B9C2_tI64_139_em_d2n_h-001 --params=`$a, c/a, z_2, x_3, x_4, z_4, y_5, z_5, y_6, z_6$

Other compounds with this structure
Bi_2WO_6

- There are three known varieties of $Bi_4V_2O_{11}$ (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 $Bi_4V_2O_{10.976}$. This structure is also sometimes described as $Bi_2VO_{5.5}$.

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
$\mathbf{B_1}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{30}}$	=	$-(y_6+z_6)\,\mathbf{a}_1-z_6\,\mathbf{a}_2-y_6\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{y}}-cz_6\,\hat{\mathbf{z}}$	(16n)	O III
$\mathbf{B_{31}}$	=	$-z_6\,\mathbf{a}_1+(y_6-z_6)\,\mathbf{a}_2+y_6\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}}-cz_6\,\hat{\mathbf{z}}$	(16n)	O III
$\mathbf{B_{32}}$	=	$-z_6\,\mathbf{a}_1-(y_6+z_6)\,\mathbf{a}_2-y_6\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}}-cz_6\,\hat{\mathbf{z}}$	(16n)	O III

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First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.