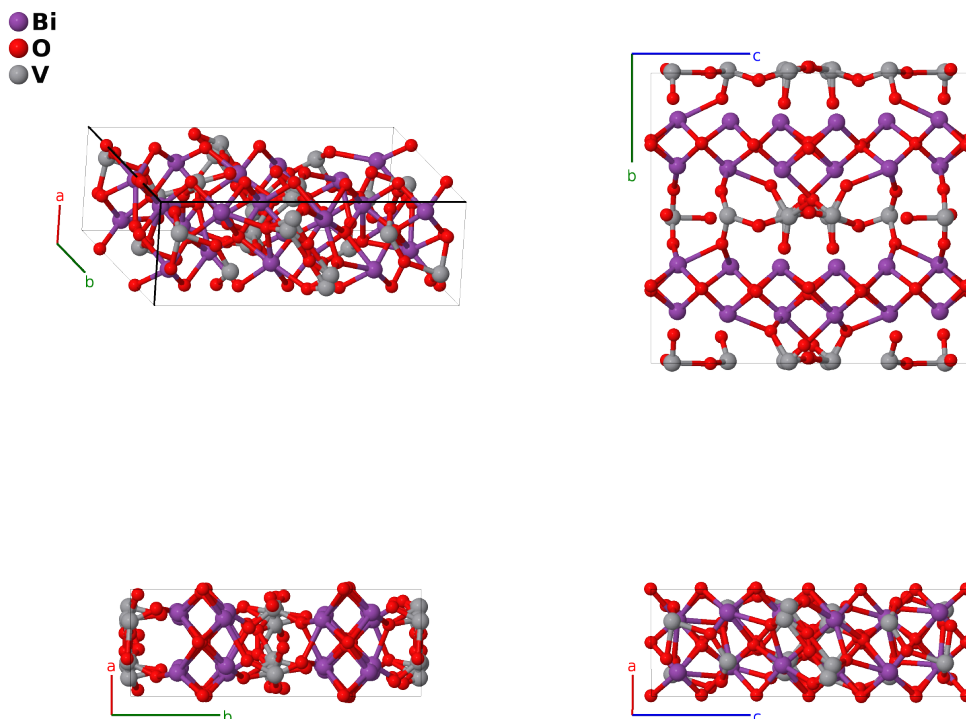


# $\alpha$ -Bi<sub>4</sub>V<sub>2</sub>O<sub>11</sub> Structure: A3B9C2\_mC112\_5\_6c\_2a2b16c\_4c-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

<https://aflow.org/p/JBQX>

[https://aflow.org/p/A3B9C2\\_mC112\\_5\\_6c\\_2a2b16c\\_4c-001](https://aflow.org/p/A3B9C2_mC112_5_6c_2a2b16c_4c-001)



Prototype	Bi <sub>4</sub> O <sub>11</sub> V <sub>2</sub>
AFLOW prototype label	A3B9C2_mC112_5_6c_2a2b16c_4c-001
ICSD	98589
Pearson symbol	mC112
Space group number	5
Space group symbol	C2
AFLOW prototype command	<pre>aflow --proto=A3B9C2_mC112_5_6c_2a2b16c_4c-001       --params=a, b/a, c/a, beta, y1, y2, y3, y4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9,       x10, y10, z10, x11, y11, z11, x12, y12, z12, x13, y13, z13, x14, y14, z14, x15, y15, z15, x16, y16, z16, x17,       y17, z17, x18, y18, z18, x19, y19, z19, x20, y20, z20, x21, y21, z21, x22, y22, z22, x23, y23, z23, x24, y24,       z24, x25, y25, z25, x26, y26, z26, x27, y27, z27, x28, y28, z28, x29, y29, z29, x30, y30, z30</pre>

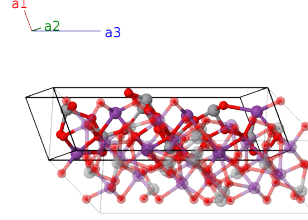
- There are three known varieties of Bi<sub>4</sub>V<sub>2</sub>O<sub>11</sub> (Villars, 2018):

- $\alpha$ , the ground state structure, stable up to 450°C (this structure),
  - $\beta$ , stable between 450°C and 555°C, and
  - $\gamma$ , stable from 555°C up to the melting point at 880°C.
- The sites we have labeled O-XXIV, O-XXV, O-XXVI, V-III, and V-IV are each only occupied 50% of the time in any one primitive cell.
  - (Mairesse, 2003) describe the structure of  $\alpha$ -Bi<sub>4</sub>V<sub>2</sub>O<sub>11</sub> in the *A2* setting of space group #5 with unique axis *c*. We describe it in our standard setting, *C2* with unique axis *b*.

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### Base-centered Monoclinic primitive vectors

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




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### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2$	$=$	$by_1 \hat{\mathbf{y}}$	(2a)	O I
$\mathbf{B}_2$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	$=$	$by_2 \hat{\mathbf{y}}$	(2a)	O II
$\mathbf{B}_3$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(2b)	O III
$\mathbf{B}_4$	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(2b)	O IV
$\mathbf{B}_5$	$= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4c)	Bi I
$\mathbf{B}_6$	$= -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4c)	Bi I
$\mathbf{B}_7$	$= (x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4c)	Bi II
$\mathbf{B}_8$	$= -(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4c)	Bi II
$\mathbf{B}_9$	$= (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4c)	Bi III
$\mathbf{B}_{10}$	$= -(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(4c)	Bi III
$\mathbf{B}_{11}$	$= (x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(4c)	Bi IV
$\mathbf{B}_{12}$	$= -(x_8 + y_8) \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(4c)	Bi IV
$\mathbf{B}_{13}$	$= (x_9 - y_9) \mathbf{a}_1 + (x_9 + y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(4c)	Bi V
$\mathbf{B}_{14}$	$= -(x_9 + y_9) \mathbf{a}_1 - (x_9 - y_9) \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}}$	(4c)	Bi V



$$\begin{aligned}
\mathbf{B}_{39} &= \begin{pmatrix} (x_{22} - y_{22}) \mathbf{a}_1 + \\ (x_{22} + y_{22}) \mathbf{a}_2 + z_{22} \mathbf{a}_3 \end{pmatrix} &= (ax_{22} + cz_{22} \cos \beta) \hat{\mathbf{x}} + by_{22} \hat{\mathbf{y}} + cz_{22} \sin \beta \hat{\mathbf{z}} &(4c) & \text{O XVI} \\
\mathbf{B}_{40} &= \begin{pmatrix} -(x_{22} + y_{22}) \mathbf{a}_1 - \\ (x_{22} - y_{22}) \mathbf{a}_2 - z_{22} \mathbf{a}_3 \end{pmatrix} &= \begin{pmatrix} -(ax_{22} + cz_{22} \cos \beta) \hat{\mathbf{x}} + by_{22} \hat{\mathbf{y}} - \\ cz_{22} \sin \beta \hat{\mathbf{z}} \end{pmatrix} &(4c) & \text{O XVI} \\
\mathbf{B}_{41} &= \begin{pmatrix} (x_{23} - y_{23}) \mathbf{a}_1 + \\ (x_{23} + y_{23}) \mathbf{a}_2 + z_{23} \mathbf{a}_3 \end{pmatrix} &= (ax_{23} + cz_{23} \cos \beta) \hat{\mathbf{x}} + by_{23} \hat{\mathbf{y}} + cz_{23} \sin \beta \hat{\mathbf{z}} &(4c) & \text{O XVII} \\
\mathbf{B}_{42} &= \begin{pmatrix} -(x_{23} + y_{23}) \mathbf{a}_1 - \\ (x_{23} - y_{23}) \mathbf{a}_2 - z_{23} \mathbf{a}_3 \end{pmatrix} &= \begin{pmatrix} -(ax_{23} + cz_{23} \cos \beta) \hat{\mathbf{x}} + by_{23} \hat{\mathbf{y}} - \\ cz_{23} \sin \beta \hat{\mathbf{z}} \end{pmatrix} &(4c) & \text{O XVII} \\
\mathbf{B}_{43} &= \begin{pmatrix} (x_{24} - y_{24}) \mathbf{a}_1 + \\ (x_{24} + y_{24}) \mathbf{a}_2 + z_{24} \mathbf{a}_3 \end{pmatrix} &= (ax_{24} + cz_{24} \cos \beta) \hat{\mathbf{x}} + by_{24} \hat{\mathbf{y}} + cz_{24} \sin \beta \hat{\mathbf{z}} &(4c) & \text{O XVIII} \\
\mathbf{B}_{44} &= \begin{pmatrix} -(x_{24} + y_{24}) \mathbf{a}_1 - \\ (x_{24} - y_{24}) \mathbf{a}_2 - z_{24} \mathbf{a}_3 \end{pmatrix} &= \begin{pmatrix} -(ax_{24} + cz_{24} \cos \beta) \hat{\mathbf{x}} + by_{24} \hat{\mathbf{y}} - \\ cz_{24} \sin \beta \hat{\mathbf{z}} \end{pmatrix} &(4c) & \text{O XVIII} \\
\mathbf{B}_{45} &= \begin{pmatrix} (x_{25} - y_{25}) \mathbf{a}_1 + \\ (x_{25} + y_{25}) \mathbf{a}_2 + z_{25} \mathbf{a}_3 \end{pmatrix} &= (ax_{25} + cz_{25} \cos \beta) \hat{\mathbf{x}} + by_{25} \hat{\mathbf{y}} + cz_{25} \sin \beta \hat{\mathbf{z}} &(4c) & \text{O XIX} \\
\mathbf{B}_{46} &= \begin{pmatrix} -(x_{25} + y_{25}) \mathbf{a}_1 - \\ (x_{25} - y_{25}) \mathbf{a}_2 - z_{25} \mathbf{a}_3 \end{pmatrix} &= \begin{pmatrix} -(ax_{25} + cz_{25} \cos \beta) \hat{\mathbf{x}} + by_{25} \hat{\mathbf{y}} - \\ cz_{25} \sin \beta \hat{\mathbf{z}} \end{pmatrix} &(4c) & \text{O XIX} \\
\mathbf{B}_{47} &= \begin{pmatrix} (x_{26} - y_{26}) \mathbf{a}_1 + \\ (x_{26} + y_{26}) \mathbf{a}_2 + z_{26} \mathbf{a}_3 \end{pmatrix} &= (ax_{26} + cz_{26} \cos \beta) \hat{\mathbf{x}} + by_{26} \hat{\mathbf{y}} + cz_{26} \sin \beta \hat{\mathbf{z}} &(4c) & \text{O XX} \\
\mathbf{B}_{48} &= \begin{pmatrix} -(x_{26} + y_{26}) \mathbf{a}_1 - \\ (x_{26} - y_{26}) \mathbf{a}_2 - z_{26} \mathbf{a}_3 \end{pmatrix} &= \begin{pmatrix} -(ax_{26} + cz_{26} \cos \beta) \hat{\mathbf{x}} + by_{26} \hat{\mathbf{y}} - \\ cz_{26} \sin \beta \hat{\mathbf{z}} \end{pmatrix} &(4c) & \text{O XX} \\
\mathbf{B}_{49} &= \begin{pmatrix} (x_{27} - y_{27}) \mathbf{a}_1 + \\ (x_{27} + y_{27}) \mathbf{a}_2 + z_{27} \mathbf{a}_3 \end{pmatrix} &= (ax_{27} + cz_{27} \cos \beta) \hat{\mathbf{x}} + by_{27} \hat{\mathbf{y}} + cz_{27} \sin \beta \hat{\mathbf{z}} &(4c) & \text{V I} \\
\mathbf{B}_{50} &= \begin{pmatrix} -(x_{27} + y_{27}) \mathbf{a}_1 - \\ (x_{27} - y_{27}) \mathbf{a}_2 - z_{27} \mathbf{a}_3 \end{pmatrix} &= \begin{pmatrix} -(ax_{27} + cz_{27} \cos \beta) \hat{\mathbf{x}} + by_{27} \hat{\mathbf{y}} - \\ cz_{27} \sin \beta \hat{\mathbf{z}} \end{pmatrix} &(4c) & \text{V I} \\
\mathbf{B}_{51} &= \begin{pmatrix} (x_{28} - y_{28}) \mathbf{a}_1 + \\ (x_{28} + y_{28}) \mathbf{a}_2 + z_{28} \mathbf{a}_3 \end{pmatrix} &= (ax_{28} + cz_{28} \cos \beta) \hat{\mathbf{x}} + by_{28} \hat{\mathbf{y}} + cz_{28} \sin \beta \hat{\mathbf{z}} &(4c) & \text{V II} \\
\mathbf{B}_{52} &= \begin{pmatrix} -(x_{28} + y_{28}) \mathbf{a}_1 - \\ (x_{28} - y_{28}) \mathbf{a}_2 - z_{28} \mathbf{a}_3 \end{pmatrix} &= \begin{pmatrix} -(ax_{28} + cz_{28} \cos \beta) \hat{\mathbf{x}} + by_{28} \hat{\mathbf{y}} - \\ cz_{28} \sin \beta \hat{\mathbf{z}} \end{pmatrix} &(4c) & \text{V II} \\
\mathbf{B}_{53} &= \begin{pmatrix} (x_{29} - y_{29}) \mathbf{a}_1 + \\ (x_{29} + y_{29}) \mathbf{a}_2 + z_{29} \mathbf{a}_3 \end{pmatrix} &= (ax_{29} + cz_{29} \cos \beta) \hat{\mathbf{x}} + by_{29} \hat{\mathbf{y}} + cz_{29} \sin \beta \hat{\mathbf{z}} &(4c) & \text{V III} \\
\mathbf{B}_{54} &= \begin{pmatrix} -(x_{29} + y_{29}) \mathbf{a}_1 - \\ (x_{29} - y_{29}) \mathbf{a}_2 - z_{29} \mathbf{a}_3 \end{pmatrix} &= \begin{pmatrix} -(ax_{29} + cz_{29} \cos \beta) \hat{\mathbf{x}} + by_{29} \hat{\mathbf{y}} - \\ cz_{29} \sin \beta \hat{\mathbf{z}} \end{pmatrix} &(4c) & \text{V III} \\
\mathbf{B}_{55} &= \begin{pmatrix} (x_{30} - y_{30}) \mathbf{a}_1 + \\ (x_{30} + y_{30}) \mathbf{a}_2 + z_{30} \mathbf{a}_3 \end{pmatrix} &= (ax_{30} + cz_{30} \cos \beta) \hat{\mathbf{x}} + by_{30} \hat{\mathbf{y}} + cz_{30} \sin \beta \hat{\mathbf{z}} &(4c) & \text{V IV} \\
\mathbf{B}_{56} &= \begin{pmatrix} -(x_{30} + y_{30}) \mathbf{a}_1 - \\ (x_{30} - y_{30}) \mathbf{a}_2 - z_{30} \mathbf{a}_3 \end{pmatrix} &= \begin{pmatrix} -(ax_{30} + cz_{30} \cos \beta) \hat{\mathbf{x}} + by_{30} \hat{\mathbf{y}} - \\ cz_{30} \sin \beta \hat{\mathbf{z}} \end{pmatrix} &(4c) & \text{V IV}
\end{aligned}$$

## References

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- [2] P. Villars, H. Okamoto, and K. Cenzual, eds., *ASM Alloy Phase Diagram Database* (ASM International, 2018), chap. Bismuth-Oxygen-Vanadium Ternary, Vertical Section (1987 Blinovskov Y.N.). Copyright ©2006-2018 ASM International.