

α -Bi₄V₂O₁₁ Structure:

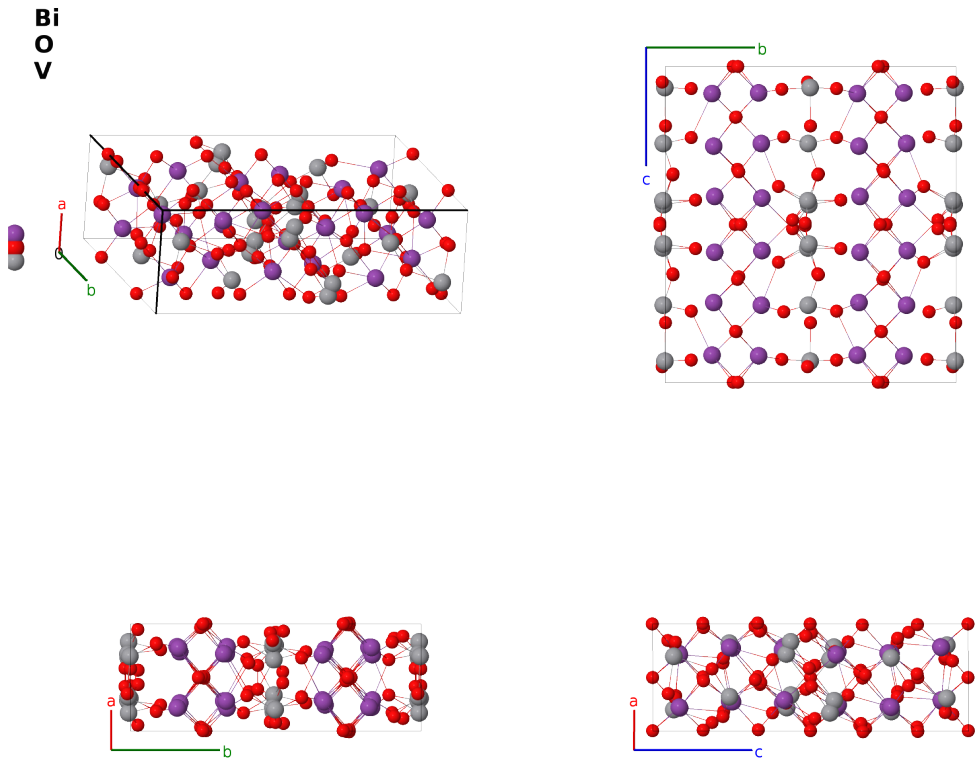
A3B9C2_mC112_5_6c_2a2b16c_4c-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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.

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

https://aflow.org/prototype-encyclopedia/A3B9C2_mC112_5_6c_2a2b16c_4c-001



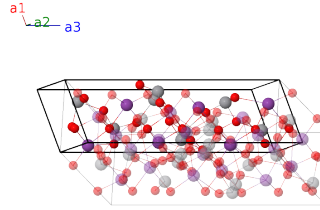
Prototype	Bi ₄ O ₁₁ V ₂
AFLOW prototype label	A3B9C2_mC112_5_6c_2a2b16c_4c-001
ICSD	98589
CCDC	1657853
Pearson symbol	mC112
Space group number	5
Space group symbol	C2

AFLOW prototype command `aflow --proto=A3B9C2_mC112_5_6c_2a2b16c_4c-001`
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- There are three known varieties of Bi₄V₂O₁₁ (Villars, 2018):
 - α , the ground state structure, stable up to 450°C (this structure),
 - β , stable between 450°C and 555°C, and
 - γ , 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 α -Bi₄V₂O₁₁ 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

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



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
$\mathbf{B}_{15} =$	$(x_{10} - y_{10}) \mathbf{a}_1 + (x_{10} + y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(4c)	Bi VI
$\mathbf{B}_{16} =$	$-(x_{10} + y_{10}) \mathbf{a}_1 - (x_{10} - y_{10}) \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} - cz_{10} \sin \beta \hat{\mathbf{z}}$	(4c)	Bi VI
$\mathbf{B}_{17} =$	$(x_{11} - y_{11}) \mathbf{a}_1 + (x_{11} + y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(4c)	O V
$\mathbf{B}_{18} =$	$-(x_{11} + y_{11}) \mathbf{a}_1 - (x_{11} - y_{11}) \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} - cz_{11} \sin \beta \hat{\mathbf{z}}$	(4c)	O V
$\mathbf{B}_{19} =$	$(x_{12} - y_{12}) \mathbf{a}_1 + (x_{12} + y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(4c)	O VI
$\mathbf{B}_{20} =$	$-(x_{12} + y_{12}) \mathbf{a}_1 - (x_{12} - y_{12}) \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} - cz_{12} \sin \beta \hat{\mathbf{z}}$	(4c)	O VI
$\mathbf{B}_{21} =$	$(x_{13} - y_{13}) \mathbf{a}_1 + (x_{13} + y_{13}) \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \sin \beta \hat{\mathbf{z}}$	(4c)	O VII
$\mathbf{B}_{22} =$	$-(x_{13} + y_{13}) \mathbf{a}_1 - (x_{13} - y_{13}) \mathbf{a}_2 - z_{13} \mathbf{a}_3$	$=$	$-(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} - cz_{13} \sin \beta \hat{\mathbf{z}}$	(4c)	O VII
$\mathbf{B}_{23} =$	$(x_{14} - y_{14}) \mathbf{a}_1 + (x_{14} + y_{14}) \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \sin \beta \hat{\mathbf{z}}$	(4c)	O VIII
$\mathbf{B}_{24} =$	$-(x_{14} + y_{14}) \mathbf{a}_1 - (x_{14} - y_{14}) \mathbf{a}_2 - z_{14} \mathbf{a}_3$	$=$	$-(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} - cz_{14} \sin \beta \hat{\mathbf{z}}$	(4c)	O VIII
$\mathbf{B}_{25} =$	$(x_{15} - y_{15}) \mathbf{a}_1 + (x_{15} + y_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3$	$=$	$(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} + cz_{15} \sin \beta \hat{\mathbf{z}}$	(4c)	O IX
$\mathbf{B}_{26} =$	$-(x_{15} + y_{15}) \mathbf{a}_1 - (x_{15} - y_{15}) \mathbf{a}_2 - z_{15} \mathbf{a}_3$	$=$	$-(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} - cz_{15} \sin \beta \hat{\mathbf{z}}$	(4c)	O IX
$\mathbf{B}_{27} =$	$(x_{16} - y_{16}) \mathbf{a}_1 + (x_{16} + y_{16}) \mathbf{a}_2 + z_{16} \mathbf{a}_3$	$=$	$(ax_{16} + cz_{16} \cos \beta) \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} + cz_{16} \sin \beta \hat{\mathbf{z}}$	(4c)	O X
$\mathbf{B}_{28} =$	$-(x_{16} + y_{16}) \mathbf{a}_1 - (x_{16} - y_{16}) \mathbf{a}_2 - z_{16} \mathbf{a}_3$	$=$	$-(ax_{16} + cz_{16} \cos \beta) \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} - cz_{16} \sin \beta \hat{\mathbf{z}}$	(4c)	O X
$\mathbf{B}_{29} =$	$(x_{17} - y_{17}) \mathbf{a}_1 + (x_{17} + y_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3$	$=$	$(ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} + cz_{17} \sin \beta \hat{\mathbf{z}}$	(4c)	O XI
$\mathbf{B}_{30} =$	$-(x_{17} + y_{17}) \mathbf{a}_1 - (x_{17} - y_{17}) \mathbf{a}_2 - z_{17} \mathbf{a}_3$	$=$	$-(ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} - cz_{17} \sin \beta \hat{\mathbf{z}}$	(4c)	O XI
$\mathbf{B}_{31} =$	$(x_{18} - y_{18}) \mathbf{a}_1 + (x_{18} + y_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3$	$=$	$(ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} + cz_{18} \sin \beta \hat{\mathbf{z}}$	(4c)	O XII
$\mathbf{B}_{32} =$	$-(x_{18} + y_{18}) \mathbf{a}_1 - (x_{18} - y_{18}) \mathbf{a}_2 - z_{18} \mathbf{a}_3$	$=$	$-(ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} - cz_{18} \sin \beta \hat{\mathbf{z}}$	(4c)	O XII
$\mathbf{B}_{33} =$	$(x_{19} - y_{19}) \mathbf{a}_1 + (x_{19} + y_{19}) \mathbf{a}_2 + z_{19} \mathbf{a}_3$	$=$	$(ax_{19} + cz_{19} \cos \beta) \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} + cz_{19} \sin \beta \hat{\mathbf{z}}$	(4c)	O XIII
$\mathbf{B}_{34} =$	$-(x_{19} + y_{19}) \mathbf{a}_1 - (x_{19} - y_{19}) \mathbf{a}_2 - z_{19} \mathbf{a}_3$	$=$	$-(ax_{19} + cz_{19} \cos \beta) \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} - cz_{19} \sin \beta \hat{\mathbf{z}}$	(4c)	O XIII

$\mathbf{B}_{35} =$	$(x_{20} - y_{20}) \mathbf{a}_1 +$ $(x_{20} + y_{20}) \mathbf{a}_2 + z_{20} \mathbf{a}_3$	$=$	$(ax_{20} + cz_{20} \cos \beta) \hat{\mathbf{x}} + by_{20} \hat{\mathbf{y}} + cz_{20} \sin \beta \hat{\mathbf{z}}$	(4c)	O XIV
$\mathbf{B}_{36} =$	$-(x_{20} + y_{20}) \mathbf{a}_1 -$ $(x_{20} - y_{20}) \mathbf{a}_2 - z_{20} \mathbf{a}_3$	$=$	$-(ax_{20} + cz_{20} \cos \beta) \hat{\mathbf{x}} + by_{20} \hat{\mathbf{y}} -$ $cz_{20} \sin \beta \hat{\mathbf{z}}$	(4c)	O XIV
$\mathbf{B}_{37} =$	$(x_{21} - y_{21}) \mathbf{a}_1 +$ $(x_{21} + y_{21}) \mathbf{a}_2 + z_{21} \mathbf{a}_3$	$=$	$(ax_{21} + cz_{21} \cos \beta) \hat{\mathbf{x}} + by_{21} \hat{\mathbf{y}} + cz_{21} \sin \beta \hat{\mathbf{z}}$	(4c)	O XV
$\mathbf{B}_{38} =$	$-(x_{21} + y_{21}) \mathbf{a}_1 -$ $(x_{21} - y_{21}) \mathbf{a}_2 - z_{21} \mathbf{a}_3$	$=$	$-(ax_{21} + cz_{21} \cos \beta) \hat{\mathbf{x}} + by_{21} \hat{\mathbf{y}} -$ $cz_{21} \sin \beta \hat{\mathbf{z}}$	(4c)	O XV
$\mathbf{B}_{39} =$	$(x_{22} - y_{22}) \mathbf{a}_1 +$ $(x_{22} + y_{22}) \mathbf{a}_2 + z_{22} \mathbf{a}_3$	$=$	$(ax_{22} + cz_{22} \cos \beta) \hat{\mathbf{x}} + by_{22} \hat{\mathbf{y}} + cz_{22} \sin \beta \hat{\mathbf{z}}$	(4c)	O XVI
$\mathbf{B}_{40} =$	$-(x_{22} + y_{22}) \mathbf{a}_1 -$ $(x_{22} - y_{22}) \mathbf{a}_2 - z_{22} \mathbf{a}_3$	$=$	$-(ax_{22} + cz_{22} \cos \beta) \hat{\mathbf{x}} + by_{22} \hat{\mathbf{y}} -$ $cz_{22} \sin \beta \hat{\mathbf{z}}$	(4c)	O XVI
$\mathbf{B}_{41} =$	$(x_{23} - y_{23}) \mathbf{a}_1 +$ $(x_{23} + y_{23}) \mathbf{a}_2 + z_{23} \mathbf{a}_3$	$=$	$(ax_{23} + cz_{23} \cos \beta) \hat{\mathbf{x}} + by_{23} \hat{\mathbf{y}} + cz_{23} \sin \beta \hat{\mathbf{z}}$	(4c)	O XVII
$\mathbf{B}_{42} =$	$-(x_{23} + y_{23}) \mathbf{a}_1 -$ $(x_{23} - y_{23}) \mathbf{a}_2 - z_{23} \mathbf{a}_3$	$=$	$-(ax_{23} + cz_{23} \cos \beta) \hat{\mathbf{x}} + by_{23} \hat{\mathbf{y}} -$ $cz_{23} \sin \beta \hat{\mathbf{z}}$	(4c)	O XVII
$\mathbf{B}_{43} =$	$(x_{24} - y_{24}) \mathbf{a}_1 +$ $(x_{24} + y_{24}) \mathbf{a}_2 + z_{24} \mathbf{a}_3$	$=$	$(ax_{24} + cz_{24} \cos \beta) \hat{\mathbf{x}} + by_{24} \hat{\mathbf{y}} + cz_{24} \sin \beta \hat{\mathbf{z}}$	(4c)	O XVIII
$\mathbf{B}_{44} =$	$-(x_{24} + y_{24}) \mathbf{a}_1 -$ $(x_{24} - y_{24}) \mathbf{a}_2 - z_{24} \mathbf{a}_3$	$=$	$-(ax_{24} + cz_{24} \cos \beta) \hat{\mathbf{x}} + by_{24} \hat{\mathbf{y}} -$ $cz_{24} \sin \beta \hat{\mathbf{z}}$	(4c)	O XVIII
$\mathbf{B}_{45} =$	$(x_{25} - y_{25}) \mathbf{a}_1 +$ $(x_{25} + y_{25}) \mathbf{a}_2 + z_{25} \mathbf{a}_3$	$=$	$(ax_{25} + cz_{25} \cos \beta) \hat{\mathbf{x}} + by_{25} \hat{\mathbf{y}} + cz_{25} \sin \beta \hat{\mathbf{z}}$	(4c)	O XIX
$\mathbf{B}_{46} =$	$-(x_{25} + y_{25}) \mathbf{a}_1 -$ $(x_{25} - y_{25}) \mathbf{a}_2 - z_{25} \mathbf{a}_3$	$=$	$-(ax_{25} + cz_{25} \cos \beta) \hat{\mathbf{x}} + by_{25} \hat{\mathbf{y}} -$ $cz_{25} \sin \beta \hat{\mathbf{z}}$	(4c)	O XIX
$\mathbf{B}_{47} =$	$(x_{26} - y_{26}) \mathbf{a}_1 +$ $(x_{26} + y_{26}) \mathbf{a}_2 + z_{26} \mathbf{a}_3$	$=$	$(ax_{26} + cz_{26} \cos \beta) \hat{\mathbf{x}} + by_{26} \hat{\mathbf{y}} + cz_{26} \sin \beta \hat{\mathbf{z}}$	(4c)	O XX
$\mathbf{B}_{48} =$	$-(x_{26} + y_{26}) \mathbf{a}_1 -$ $(x_{26} - y_{26}) \mathbf{a}_2 - z_{26} \mathbf{a}_3$	$=$	$-(ax_{26} + cz_{26} \cos \beta) \hat{\mathbf{x}} + by_{26} \hat{\mathbf{y}} -$ $cz_{26} \sin \beta \hat{\mathbf{z}}$	(4c)	O XX
$\mathbf{B}_{49} =$	$(x_{27} - y_{27}) \mathbf{a}_1 +$ $(x_{27} + y_{27}) \mathbf{a}_2 + z_{27} \mathbf{a}_3$	$=$	$(ax_{27} + cz_{27} \cos \beta) \hat{\mathbf{x}} + by_{27} \hat{\mathbf{y}} + cz_{27} \sin \beta \hat{\mathbf{z}}$	(4c)	V I
$\mathbf{B}_{50} =$	$-(x_{27} + y_{27}) \mathbf{a}_1 -$ $(x_{27} - y_{27}) \mathbf{a}_2 - z_{27} \mathbf{a}_3$	$=$	$-(ax_{27} + cz_{27} \cos \beta) \hat{\mathbf{x}} + by_{27} \hat{\mathbf{y}} -$ $cz_{27} \sin \beta \hat{\mathbf{z}}$	(4c)	V I
$\mathbf{B}_{51} =$	$(x_{28} - y_{28}) \mathbf{a}_1 +$ $(x_{28} + y_{28}) \mathbf{a}_2 + z_{28} \mathbf{a}_3$	$=$	$(ax_{28} + cz_{28} \cos \beta) \hat{\mathbf{x}} + by_{28} \hat{\mathbf{y}} + cz_{28} \sin \beta \hat{\mathbf{z}}$	(4c)	V II
$\mathbf{B}_{52} =$	$-(x_{28} + y_{28}) \mathbf{a}_1 -$ $(x_{28} - y_{28}) \mathbf{a}_2 - z_{28} \mathbf{a}_3$	$=$	$-(ax_{28} + cz_{28} \cos \beta) \hat{\mathbf{x}} + by_{28} \hat{\mathbf{y}} -$ $cz_{28} \sin \beta \hat{\mathbf{z}}$	(4c)	V II
$\mathbf{B}_{53} =$	$(x_{29} - y_{29}) \mathbf{a}_1 +$ $(x_{29} + y_{29}) \mathbf{a}_2 + z_{29} \mathbf{a}_3$	$=$	$(ax_{29} + cz_{29} \cos \beta) \hat{\mathbf{x}} + by_{29} \hat{\mathbf{y}} + cz_{29} \sin \beta \hat{\mathbf{z}}$	(4c)	V III
$\mathbf{B}_{54} =$	$-(x_{29} + y_{29}) \mathbf{a}_1 -$ $(x_{29} - y_{29}) \mathbf{a}_2 - z_{29} \mathbf{a}_3$	$=$	$-(ax_{29} + cz_{29} \cos \beta) \hat{\mathbf{x}} + by_{29} \hat{\mathbf{y}} -$ $cz_{29} \sin \beta \hat{\mathbf{z}}$	(4c)	V III
$\mathbf{B}_{55} =$	$(x_{30} - y_{30}) \mathbf{a}_1 +$ $(x_{30} + y_{30}) \mathbf{a}_2 + z_{30} \mathbf{a}_3$	$=$	$(ax_{30} + cz_{30} \cos \beta) \hat{\mathbf{x}} + by_{30} \hat{\mathbf{y}} + cz_{30} \sin \beta \hat{\mathbf{z}}$	(4c)	V IV
$\mathbf{B}_{56} =$	$-(x_{30} + y_{30}) \mathbf{a}_1 -$ $(x_{30} - y_{30}) \mathbf{a}_2 - z_{30} \mathbf{a}_3$	$=$	$-(ax_{30} + cz_{30} \cos \beta) \hat{\mathbf{x}} + by_{30} \hat{\mathbf{y}} -$ $cz_{30} \sin \beta \hat{\mathbf{z}}$	(4c)	V IV

References

- [1] G. Mairesse, P. Roussel, R. N. Vannier, M. Anne, and G. Nowogrocki, *Crystal structure determination of α -, β - and γ - $\text{Bi}_4\text{V}_2\text{O}_{11}$ polymorphs. Part II: crystal structure of α - $\text{Bi}_4\text{V}_2\text{O}_{11}$* , Solid State Sci. **5**, 861–869 (2003), doi:10.1016/S1293-

2558(03)00016-5.

- [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.

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