

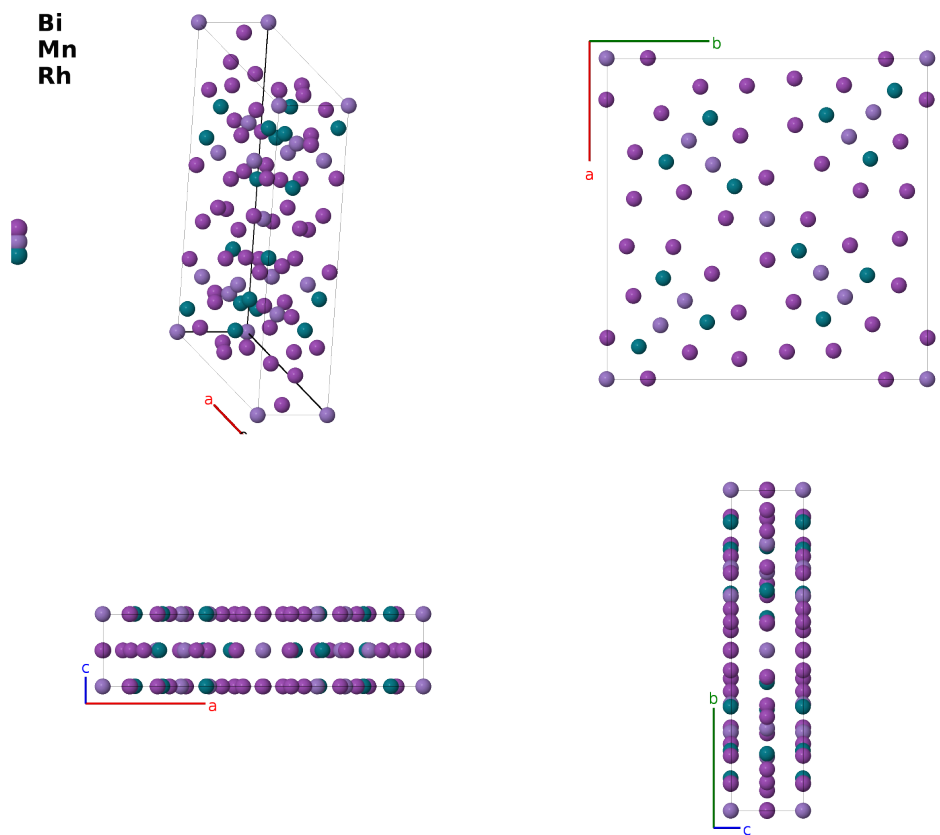
Rh₆Mn₅Bi₁₈ Structure: A18B5C6_tP58_136_f4i_afg_gi-001

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

https://aflow.org/prototype-encyclopedia/A18B5C6_tP58_136_f4i_afg_gi-001

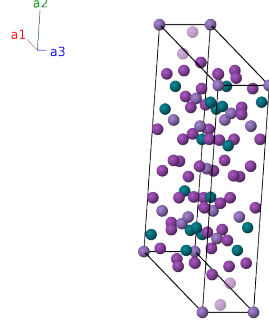


Prototype	Bi ₁₈ Mn ₅ Rh ₆
AFLOW prototype label	A18B5C6_tP58_136_f4i_afg_gi-001
ICSD	130687
CCDC	1850892
Pearson symbol	tP58
Space group number	136
Space group symbol	$P4_2/mnm$
AFLOW prototype command	<code>aflow --proto=A18B5C6_tP58_136_f4i_afg_gi-001 --params=a, c/a, x₂, x₃, x₄, x₅, x₆, y₆, x₇, y₇, x₈, y₈, x₉, y₉, x₁₀, y₁₀</code>

- AFLOW rotates the system by 180° about the x-axis, so that (x y z) ↔ (x -y -z). The practical effect is to interchange the (4f) and (4g) Wyckoff positions.

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(2a)	Mn I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2a)	Mn I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$a x_2 \hat{\mathbf{x}} + a x_2 \hat{\mathbf{y}}$	(4f)	Bi I
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$-a x_2 \hat{\mathbf{x}} - a x_2 \hat{\mathbf{y}}$	(4f)	Bi I
$\mathbf{B}_5$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	Bi I
$\mathbf{B}_6$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	Bi I
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$a x_3 \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}}$	(4f)	Mn II
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-a x_3 \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}}$	(4f)	Mn II
$\mathbf{B}_9$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	Mn II
$\mathbf{B}_{10}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	Mn II
$\mathbf{B}_{11}$	$= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2$	$=$	$a x_4 \hat{\mathbf{x}} - a x_4 \hat{\mathbf{y}}$	(4g)	Mn III
$\mathbf{B}_{12}$	$= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2$	$=$	$-a x_4 \hat{\mathbf{x}} + a x_4 \hat{\mathbf{y}}$	(4g)	Mn III
$\mathbf{B}_{13}$	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	Mn III
$\mathbf{B}_{14}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	Mn III
$\mathbf{B}_{15}$	$= x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2$	$=$	$a x_5 \hat{\mathbf{x}} - a x_5 \hat{\mathbf{y}}$	(4g)	Rh I
$\mathbf{B}_{16}$	$= -x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2$	$=$	$-a x_5 \hat{\mathbf{x}} + a x_5 \hat{\mathbf{y}}$	(4g)	Rh I
$\mathbf{B}_{17}$	$= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	Rh I
$\mathbf{B}_{18}$	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	Rh I
$\mathbf{B}_{19}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2$	$=$	$a x_6 \hat{\mathbf{x}} + a y_6 \hat{\mathbf{y}}$	(8i)	Bi II
$\mathbf{B}_{20}$	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2$	$=$	$-a x_6 \hat{\mathbf{x}} - a y_6 \hat{\mathbf{y}}$	(8i)	Bi II
$\mathbf{B}_{21}$	$= -\left(y_6 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a \left(y_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	Bi II

$\mathbf{B}_{22} =$	$(y_6 + \frac{1}{2}) \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$	$a (y_6 + \frac{1}{2}) \hat{\mathbf{x}} - a (x_6 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	Bi II
$\mathbf{B}_{23} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$	$-a (x_6 - \frac{1}{2}) \hat{\mathbf{x}} + a (y_6 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	Bi II
$\mathbf{B}_{24} =$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$	$a (x_6 + \frac{1}{2}) \hat{\mathbf{x}} - a (y_6 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	Bi II
$\mathbf{B}_{25} =$	$y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 =$	$ay_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}}$	(8i)	Bi II
$\mathbf{B}_{26} =$	$-y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 =$	$-ay_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}}$	(8i)	Bi II
$\mathbf{B}_{27} =$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 =$	$ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}}$	(8i)	Bi III
$\mathbf{B}_{28} =$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 =$	$-ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}}$	(8i)	Bi III
$\mathbf{B}_{29} =$	$-(y_7 - \frac{1}{2}) \mathbf{a}_1 + (x_7 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$	$-a (y_7 - \frac{1}{2}) \hat{\mathbf{x}} + a (x_7 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	Bi III
$\mathbf{B}_{30} =$	$(y_7 + \frac{1}{2}) \mathbf{a}_1 - (x_7 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$	$a (y_7 + \frac{1}{2}) \hat{\mathbf{x}} - a (x_7 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	Bi III
$\mathbf{B}_{31} =$	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$	$-a (x_7 - \frac{1}{2}) \hat{\mathbf{x}} + a (y_7 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	Bi III
$\mathbf{B}_{32} =$	$(x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$	$a (x_7 + \frac{1}{2}) \hat{\mathbf{x}} - a (y_7 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	Bi III
$\mathbf{B}_{33} =$	$y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 =$	$ay_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}}$	(8i)	Bi III
$\mathbf{B}_{34} =$	$-y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 =$	$-ay_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}}$	(8i)	Bi III
$\mathbf{B}_{35} =$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 =$	$ax_8 \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}}$	(8i)	Bi IV
$\mathbf{B}_{36} =$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 =$	$-ax_8 \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}}$	(8i)	Bi IV
$\mathbf{B}_{37} =$	$-(y_8 - \frac{1}{2}) \mathbf{a}_1 + (x_8 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$	$-a (y_8 - \frac{1}{2}) \hat{\mathbf{x}} + a (x_8 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	Bi IV
$\mathbf{B}_{38} =$	$(y_8 + \frac{1}{2}) \mathbf{a}_1 - (x_8 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$	$a (y_8 + \frac{1}{2}) \hat{\mathbf{x}} - a (x_8 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	Bi IV
$\mathbf{B}_{39} =$	$-(x_8 - \frac{1}{2}) \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$	$-a (x_8 - \frac{1}{2}) \hat{\mathbf{x}} + a (y_8 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	Bi IV
$\mathbf{B}_{40} =$	$(x_8 + \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$	$a (x_8 + \frac{1}{2}) \hat{\mathbf{x}} - a (y_8 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	Bi IV
$\mathbf{B}_{41} =$	$y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 =$	$ay_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}}$	(8i)	Bi IV
$\mathbf{B}_{42} =$	$-y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 =$	$-ay_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}}$	(8i)	Bi IV
$\mathbf{B}_{43} =$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 =$	$ax_9 \hat{\mathbf{x}} + ay_9 \hat{\mathbf{y}}$	(8i)	Bi V
$\mathbf{B}_{44} =$	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 =$	$-ax_9 \hat{\mathbf{x}} - ay_9 \hat{\mathbf{y}}$	(8i)	Bi V
$\mathbf{B}_{45} =$	$-(y_9 - \frac{1}{2}) \mathbf{a}_1 + (x_9 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$	$-a (y_9 - \frac{1}{2}) \hat{\mathbf{x}} + a (x_9 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	Bi V
$\mathbf{B}_{46} =$	$(y_9 + \frac{1}{2}) \mathbf{a}_1 - (x_9 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$	$a (y_9 + \frac{1}{2}) \hat{\mathbf{x}} - a (x_9 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	Bi V
$\mathbf{B}_{47} =$	$-(x_9 - \frac{1}{2}) \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$	$-a (x_9 - \frac{1}{2}) \hat{\mathbf{x}} + a (y_9 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	Bi V
$\mathbf{B}_{48} =$	$(x_9 + \frac{1}{2}) \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$	$a (x_9 + \frac{1}{2}) \hat{\mathbf{x}} - a (y_9 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	Bi V
$\mathbf{B}_{49} =$	$y_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 =$	$ay_9 \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}}$	(8i)	Bi V
$\mathbf{B}_{50} =$	$-y_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 =$	$-ay_9 \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}}$	(8i)	Bi V
$\mathbf{B}_{51} =$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 =$	$ax_{10} \hat{\mathbf{x}} + ay_{10} \hat{\mathbf{y}}$	(8i)	Rh II
$\mathbf{B}_{52} =$	$-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 =$	$-ax_{10} \hat{\mathbf{x}} - ay_{10} \hat{\mathbf{y}}$	(8i)	Rh II
$\mathbf{B}_{53} =$	$-(y_{10} - \frac{1}{2}) \mathbf{a}_1 + (x_{10} + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$	$-a (y_{10} - \frac{1}{2}) \hat{\mathbf{x}} + a (x_{10} + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	Rh II
$\mathbf{B}_{54} =$	$(y_{10} + \frac{1}{2}) \mathbf{a}_1 - (x_{10} - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$	$a (y_{10} + \frac{1}{2}) \hat{\mathbf{x}} - a (x_{10} - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	Rh II
$\mathbf{B}_{55} =$	$-(x_{10} - \frac{1}{2}) \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$	$-a (x_{10} - \frac{1}{2}) \hat{\mathbf{x}} + a (y_{10} + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	Rh II

$$\mathbf{B}_{56} = \begin{pmatrix} x_{10} + \frac{1}{2} \\ y_{10} - \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_{10} - \frac{1}{2} \\ x_{10} + \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_{10} + \frac{1}{2} \\ y_{10} - \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \mathbf{a}_3 = a \begin{pmatrix} x_{10} + \frac{1}{2} \\ y_{10} - \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - a \begin{pmatrix} y_{10} - \frac{1}{2} \\ x_{10} + \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \quad (8i) \quad \text{Rh II}$$

$$\mathbf{B}_{57} = y_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 = ay_{10} \hat{\mathbf{x}} + ax_{10} \hat{\mathbf{y}} \quad (8i) \quad \text{Rh II}$$

$$\mathbf{B}_{58} = -y_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 = -ay_{10} \hat{\mathbf{x}} - ax_{10} \hat{\mathbf{y}} \quad (8i) \quad \text{Rh II}$$

References

- [1] P. Kainzbauer, K. W. Richter, H. S. Effenberger, M. C. J. Marker, and H. Ipser, *Single-crystal structure determination of two new ternary bismuthides: $Rh_6Mn_5Bi_{18}$ and $RhMnBi_3$* , Acta Crystallogr. Sect. C **74**, 863–869 (2018), doi:10.1107/S2053229618009087.

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