$RhMnBi_3$ Structure: A3BC_oC20_65_gq_ac_i-001

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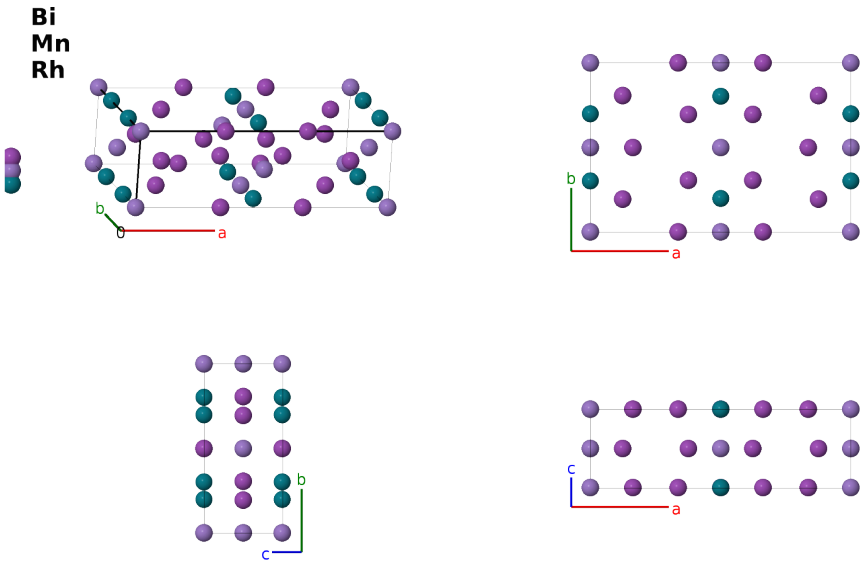
https://aflow.org/prototype-encyclopedia/KTDY

https://aflow.org/prototype-encyclopedia/A3BC_oC20_65_gq_ac_i-001

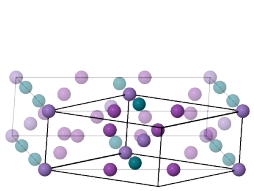


Prototype	Bi_3MnRh
AFLOW prototype label	A3BC_oC20_65_gq_ac_i-001
ICSD	130688
CCDC	1850893
Pearson symbol	oC20
Space group number	65
Space group symbol	$Cmmm$
AFLOW prototype command	`aflow --proto=A3BC_oC20_65_gq_ac_i-001 --params=`$a, b/a, c/a, x_3, y_4, x_5, y_5$

- AFLOW rotates the lattice by 90° about the z-axis compared to the reported structure.

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Mn I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	Mn II
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}}$	(4g)	Bi I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}}$	(4g)	Bi I
$\mathbf{B_5}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2$	=	$by_4\,\hat{\mathbf{y}}$	(4i)	Rh I
$\mathbf{B_6}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2$	=	$-by_4\,\hat{\mathbf{y}}$	(4i)	Rh I
$\mathbf{B_7}$	=	$(x_5 - y_5)\,\mathbf{a}_1 + (x_5 + y_5)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8q)	Bi II
$\mathbf{B_8}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - (x_5 + y_5)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8q)	Bi II
$\mathbf{B_9}$	=	$-(x_5 + y_5)\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8q)	Bi II
$\mathbf{B_{10}}$	=	$(x_5 + y_5)\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8q)	Bi 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.

Found in

[1] P. Kainzbauer, M. C. J. M., and K. W. Richter, *Reassessment of the Binary Mn-Rh Phase Diagram and Experimental Investigations of the Ternary Bi-Mn-Rh System*, J. Phase Equilib. Diffus. **41**, 282–298 (2020), doi:10.1007/s11669-020-00820-6.

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