$MnBi_4Te_7$ Structure: A4BC7_hP12_164_2d_a_bc2d-001

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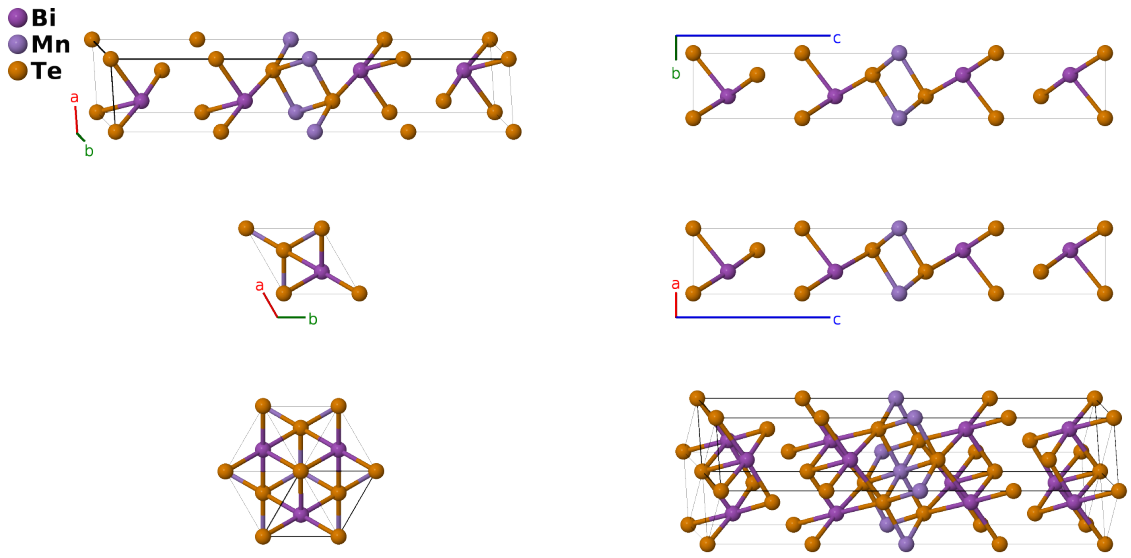
https://aflow.org/p/SPWJ

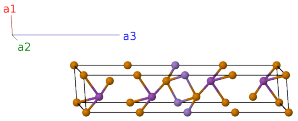
https://aflow.org/p/A4BC7_hP12_164_2d_a_bc2d-001



Prototype	Bi_4MnTe_7
AFLOW prototype label	A4BC7_hP12_164_2d_a_bc2d-001
ICSD	37567
Pearson symbol	hP12
Space group number	164
Space group symbol	$P\bar{3}m1$
AFLOW prototype command	`aflow --proto=A4BC7_hP12_164_2d_a_bc2d-001 --params=`$a, c/a, z_3, z_4, z_5, z_6, z_7$

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$ =	0	=	0	(1a)	Mn I

$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Te I
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(2c)	Te II
$\mathbf{B_4}$	=	$-z_3\,\mathbf{a}_3$	=	$-cz_3\,\hat{\mathbf{z}}$	(2c)	Te II
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2d)	Bi I
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(2d)	Bi I
$\mathbf{B_7}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(2d)	Bi II
$\mathbf{B_8}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(2d)	Bi II
$\mathbf{B_9}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(2d)	Te III
$\mathbf{B_{10}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(2d)	Te III
$\mathbf{B_{11}}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(2d)	Te IV
$\mathbf{B_{12}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(2d)	Te IV

References

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[1] J.-Q. Yan, Y. H. Liu, D. S. Parker, Y. Wu, A. A. Aczel, M. Matsuda, M. A. McGuire, and B. C. Sales, *A-type antiferromagnetic order in $MnBi_4Te_7$ and $MnBi_6Te_{10}$ single crystals*, Phys. Rev. Materials **4**, 054202 (2020), doi:10.1103/PhysRevMaterials.4.054202.