$MnBi_6Te_{10}$ Structure: A6BC10_hR17_166_3c_a_5c-001

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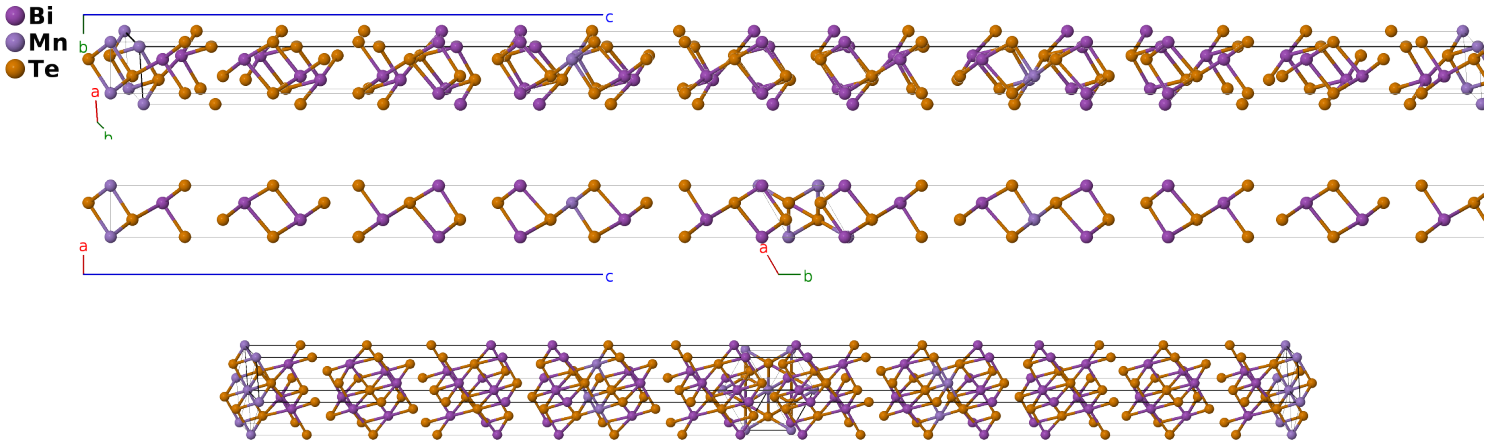
https://aflow.org/p/LD13

https://aflow.org/p/A6BC10_hR17_166_3c_a_5c-001

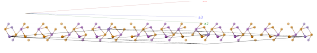


Prototype	Bi_6MnTe_{10}
AFLOW prototype label	A6BC10_hR17_166_3c_a_5c-001
ICSD	37568
Pearson symbol	hR17
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A6BC10_hR17_166_3c_a_5c-001 --params=`$a, c/a, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9$

- The ICSD entry lists $x_9 = 0.4446$, while the text of (Aliev, 2019) gives 0.41446. The difference is large enough that ¡tt¿xprototype¡/tt¿ declares the two lattices unmatchable. The value of 0.41446 gives atomic positions consistent with Fig. 5 of (Alieve, 2019) – all Bi-Mn-Te layers are terminated by Te surfaces – so we use that value.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Mn I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(2c)	Bi I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(2c)	Bi I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	Bi II
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	Bi II
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$cx_4\,\hat{\mathbf{z}}$	(2c)	Bi III
$\mathbf{B_7}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-cx_4\,\hat{\mathbf{z}}$	(2c)	Bi III
$\mathbf{B_8}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$cx_5\,\hat{\mathbf{z}}$	(2c)	Te I
$\mathbf{B_9}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-cx_5\,\hat{\mathbf{z}}$	(2c)	Te I
$\mathbf{B_{10}}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$cx_6\,\hat{\mathbf{z}}$	(2c)	Te II
$\mathbf{B_{11}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$-cx_6\,\hat{\mathbf{z}}$	(2c)	Te II
$\mathbf{B_{12}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$cx_7\,\hat{\mathbf{z}}$	(2c)	Te III
$\mathbf{B_{13}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$-cx_7\,\hat{\mathbf{z}}$	(2c)	Te III
$\mathbf{B_{14}}$	=	$x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	=	$cx_8\,\hat{\mathbf{z}}$	(2c)	Te IV
$\mathbf{B_{15}}$	=	$-x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3$	=	$-cx_8\,\hat{\mathbf{z}}$	(2c)	Te IV
$\mathbf{B_{16}}$	=	$x_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + x_9\,\mathbf{a}_3$	=	$cx_9\,\hat{\mathbf{z}}$	(2c)	Te V
$\mathbf{B_{17}}$	=	$-x_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 - x_9\,\mathbf{a}_3$	=	$-cx_9\,\hat{\mathbf{z}}$	(2c)	Te V

References

[1] Z. S. Alieva, I. R. Amiraslanov, D. I. Nasonova, A. V.Shevelkov, N. A. Abdullayev, Z. A. Jahangirli, E. N. Orujlu, M. M. Otrokov, N. T. Mamedov, M. B. Babanly, and E. V.Chulkov, *Novel ternary layered manganese bismuth tellurides of the $MnTe$-Bi_2Te_3 system: Synthesis and crystal structure*, J. Alloys Compd. **789**, 443–450 (2019), doi:10.1016/j.jallcom.2019.03.030.

Found in

[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.