$MnBi_2Te_4$ Structure: A2BC4_hR7_166_c_a_2c-002

This structure originally had the label `A2BC4_hR7_166_c_a_2c`. Calls to that address will be redirected here.

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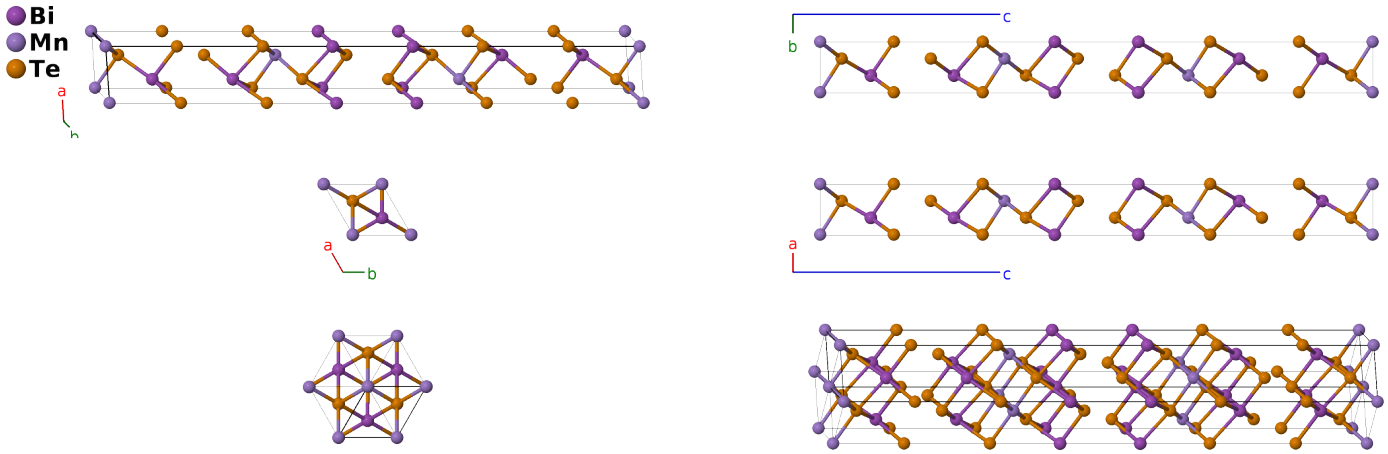
https://aflow.org/p/MU2V

https://aflow.org/p/A2BC4_hR7_166_c_a_2c-002



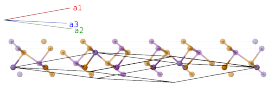
Prototype	Bi_2MnTe_4
AFLOW prototype label	A2BC4_hR7_166_c_a_2c-002
ICSD	37566
Pearson symbol	hR7
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A2BC4_hR7_166_c_a_2c-002 --params=`$a, c/a, x_2, x_3, x_4$

Other compounds with this structure
$GeAs_2Te_4$, $MnSb_2Te_4$, SSe_2Bi_4, Bi_3Se_4, Se_3Bi_4

- We use the data taken at 10K. Except for the magnetic ordering there is no substantial change in the structure up to room temperature.
- The ICSD entry is from the room-temperature measurements of (Aliev, 2019).
- This structure is nearly identical to $GeSb_2Te_4$, but the ordering of the tellurium atoms is different in the two cases.

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)	Te I
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	Te I
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$cx_4\,\hat{\mathbf{z}}$	(2c)	Te II
$\mathbf{B_7}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-cx_4\,\hat{\mathbf{z}}$	(2c)	Te II

References

[1] J.-Q. Yan, Q. Zhang, T. Heitmann, Z. Huang, K. Y. Chen, J.-G. Cheng, W. Wu, D. Vaknin, B. C. Sales, and R. J. McQueeney, *Crystal growth and magnetic structure of $MnBi_2Te_4$*, Phys. Rev. Mat. **3**, 064202 (2019), doi:10.1103/PhysRevMaterials.3.064202.

[2] Z. S. Aliev, 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.