

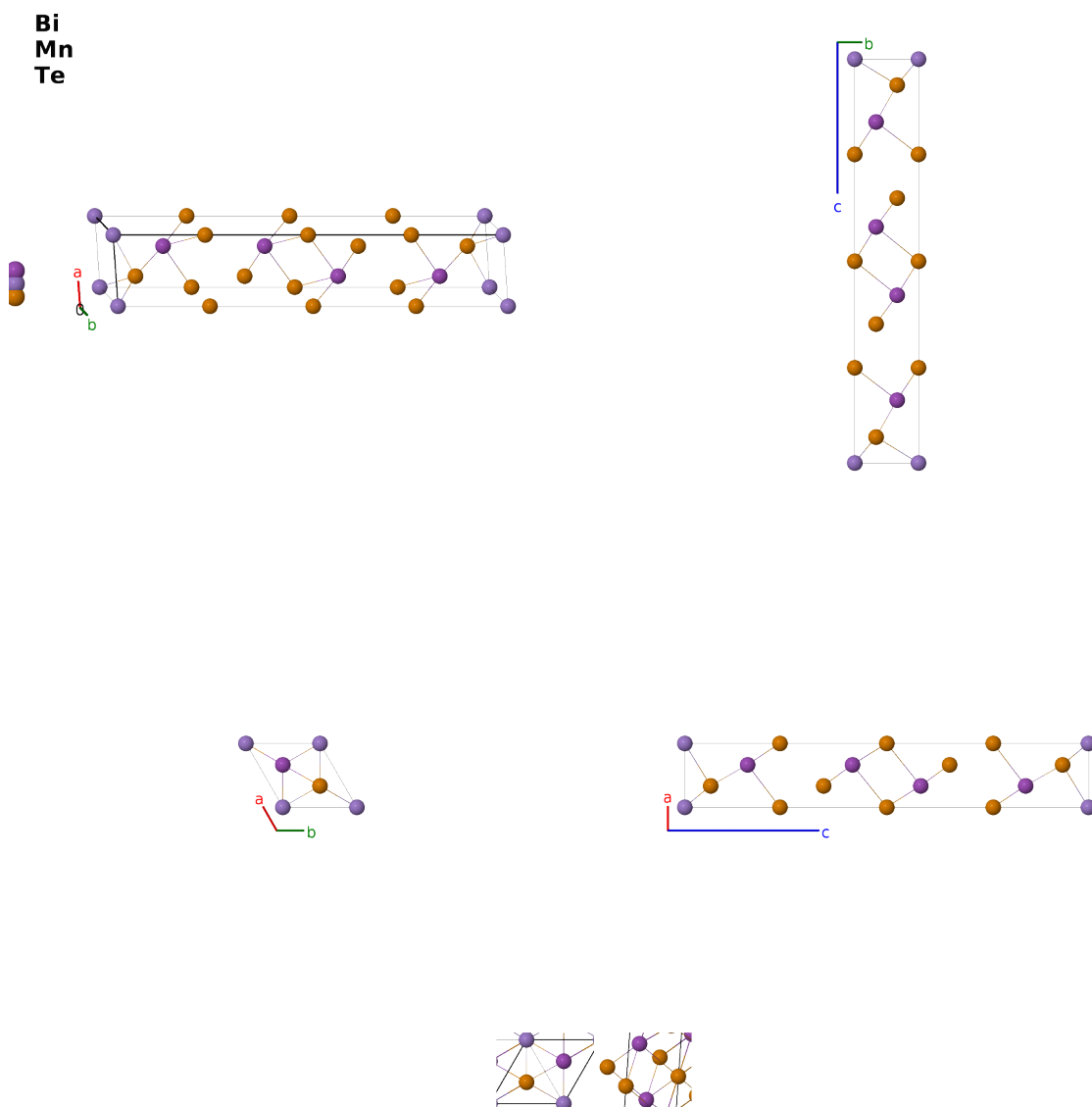
MnBi₄Te₇ Structure: A4BC7_hP12_164_2d_a_bc2d-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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

https://aflow.org/prototype-encyclopedia/A4BC7_hP12_164_2d_a_bc2d-001



Prototype

Bi₄MnTe₇

AFLOW prototype label

A4BC7_hP12_164_2d_a_bc2d-001

ICSD

37567

CCDC

2227557

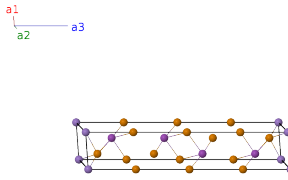
Pearson symbol	hP12
Space group number	164
Space group symbol	$P\bar{3}m1$
AFLOW prototype command	<code>aflow --proto=A4BC7_hP12_164_2d_a_bc2d-001</code> <code>--params=a, c/a, z₃, z₄, z₅, z₆, z₇</code>

Other compounds with this structure

GeAs₄Te₇, GeBi₄Te₇, GeSb₄Te₇, PbBi₄Te₇, SnBi₄Te₇

- The ICSD says places these compounds under the Bohdanowiczite (AgBiSe₂) structure, which is true in the sense that the same Wyckoff positions are occupied. We arbitrarily chose MnBi₄Te₇ as the prototype for this stoichiometry.

Trigonal (Hexagonal) primitive vectors

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
 \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$


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

- [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-Bi₂Te₃ 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.

First cited in

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.