$PbMnTeO_6$ Structure: AB6CD_hP9_149_a_l_d_e-001

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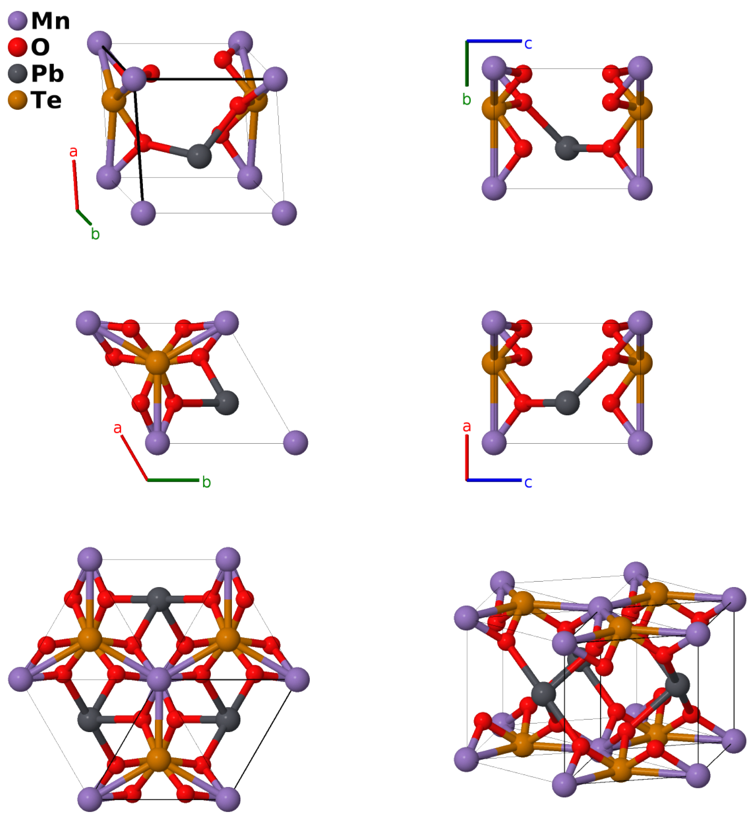
https://aflow.org/p/63FP

https://aflow.org/p/AB6CD_hP9_149_a_l_d_e-001



Prototype MnO_6PbTe

AFLOW prototype label AB6CD_hP9_149_a_l_d_e-001

ICSD 5923

Pearson symbol hP9

Space group number 149

Space group symbol $P312$

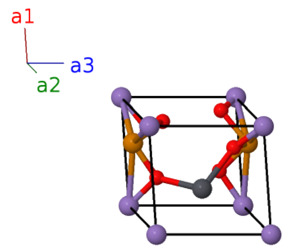
AFLOW prototype command `aflow --proto=AB6CD_hP9_149_a_l_d_e-001`
`--params=`$a, c/a, x_4, y_4, z_4$

Other compounds with this structure
$BaGeTeO_6$, $NaNiIO_6$, $PbGeTeO_6$, $SrGeTeO_6$, $SrMnTeO_6$

- In the sample studied by (Kuchugura, 2019) the site we have labeled "Mn (1f)" is actually 90.6% manganese and 9.4% tellurium, while the "Te (1d)" site is 90.6% tellurium and 9.4% manganese.
- The mineral kuranakhite (Xinchun, 1998) also has this composition. While it was tentatively indexed as a body-centered orthorhombic structure, its lattice constants are very close to the trigonal structure described here, indicating that this may be the structure of kuranakhite.

Trigonal (Hexagonal) primitive vectors

$$\begin{aligned} \mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_3} &= c\,\hat{\mathbf{z}} \end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Mn I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(1d)	Pb I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(1e)	Te I
$\mathbf{B_4}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(6l)	O I
$\mathbf{B_5}$	=	$-y_4\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - 2y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(6l)	O I
$\mathbf{B_6}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(6l)	O I
$\mathbf{B_7}$	=	$-y_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(6l)	O I
$\mathbf{B_8}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_4 + 2y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(6l)	O I
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(6l)	O I

References

[1] M. D. Kuchugura, A. I. Kurbakov, E. A. Zvereva, T. M. Vasilchikova, G. V. Raganyan, A. N. Vasiliev, V. A. Barchukf, and V. B. Nalbandyan, *$PbMnTeO_6$: a chiral quasi 2D magnet with all cations in octahedral coordination and the space group problem of trigonal layered $A^{2+}M^{4+}TeO^6$*, Dalton Trans. **48**, 17070–17077 (2019), doi:10.1039/c9dt03154e.

[2] Z. Xinchun, L. Liang, W. Shizhong, W. Yan, Y. Jiankun, G. Nenglin, L. Guanghui, and H. Jianmin, *Kuranakhite discovered in China for the first time*, Chinese J. Geochem. **17**, 77–80 (1998), doi:10.1007/BF02834625.