MnP ($B31$) Structure: AB_oP8_62_c_c-002

This structure originally had the label `AB_oP8_62_c_c.MnP`. Calls to that address will be redirected here.

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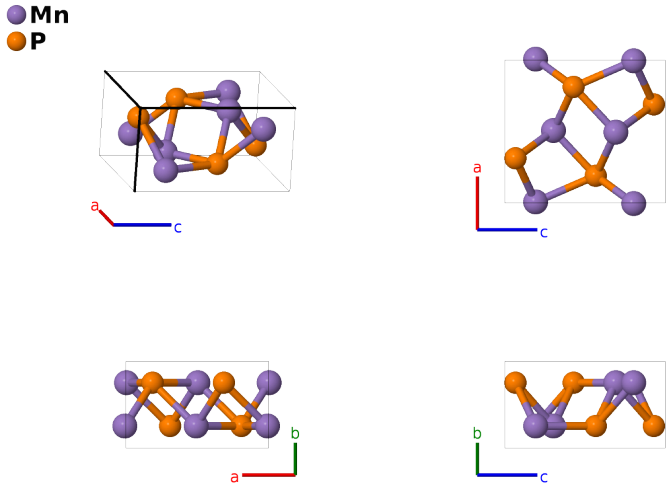
https://aflow.org/p/36ZK

https://aflow.org/p/AB_oP8_62_c_c-002



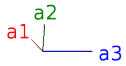
Prototype	MnP
AFLOW prototype label	AB_oP8_62_c_c-002
***Strukturbericht* designation**	$B31$
ICSD	76091
Pearson symbol	oP8
Space group number	62
Space group symbol	*Pnma*
AFLOW prototype command	`aflow --proto=AB_oP8_62_c_c-002 --params=`$a, b/a, c/a, x_1, z_1, x_2, z_2$

Other compounds with this structure
AsCo, AsCr, AsFe, AsMn, AsRh, AsRu, AsV, AuGa, CoP, CrP, FeP, FeS, GeIr, GeNi, GePd, GePt, GeRh, IrSi, $Nb_{1-x}S$ (HT), NiSi, PRu, PW, PdSi, PdSn, PtSi, RhSb, RhSi, SV, SeTi

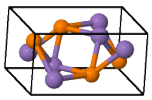
- (Hermann, 1937) assigns the prototype FeAs and the Strukturbericht designation $B14$ to this structure. This was superseded by the similar MnP structure in (Gottfried, 1937, pp. 17-18), where it is designated $B31$. (Parthé, 1993) prefers $B14$.
- We inadvertainly used the wrong atomic coordinates in the previous version of this structure. These have now been corrected to match the 10K data of (Fjellvag, 1984).

- FeAs ($B14$), GeS ($B16$), FeB ($B27$), SnS ($B29$), MnP ($B31$), and η-NiSi (B_d) all share the same AFLOW label, AB_oP8_62_c_c. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Orthorhombic primitive vectors



$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4c)	Mn I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Mn I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4c)	Mn I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Mn I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	P I

References

[1] H. Fjellvåg and A. Kjekshus, *Magnetic and Structural Properties of Transition Metal Substituted MnP. I. $Mn_{1-t}Co_tP$ (0.00 <= t <= 0.30).*, Acta Chem. Scand. A **38**, 563–573 (1984), doi:10.3891/acta.chem.scand.38a-0563.