$MnPS_3$ Structure: ABC3_mC20_12_g_i_ij-001

This structure originally had the label `ABC3_mC20_12_g_i_ij`. Calls to that address will be redirected here.

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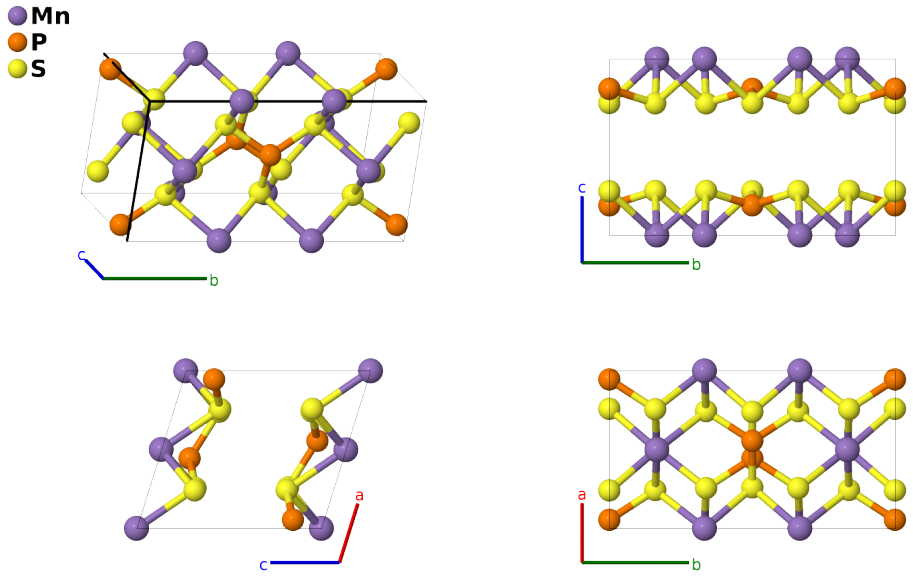
https://aflow.org/p/UPGR

https://aflow.org/p/ABC3_mC20_12_g_i_ij-001



Prototype	$MnPS_3$
AFLOW prototype label	ABC3_mC20_12_g_i_ij-001
ICSD	61391
Pearson symbol	mC20
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=ABC3_mC20_12_g_i_ij-001 --params=`$a, b/a, c/a, \beta, y_1, x_2, z_2, x_3, z_3, x_4, y_4, z_4$

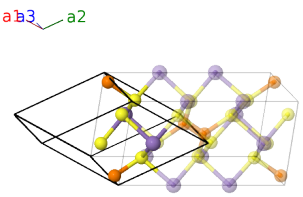
Other compounds with this structure

$CdPS_3$, $CdPSe_3$, $CoPS_3$, $CoPSe_3$, $CrGeTe_3$, $CrPS_3$, $FePS_3$, $FePSe_3$, $MnPS_3$, $MnPSe_3$, $NiPS_3$, $NiPSe_3$, $ZnPS_3$

- $FePS_3$ is often used as the prototype for this structure, but (Ouvrard, 1985) lists $MnPS_3$ first, so we use that compound.

Base-centered Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2$	=	$by_1\,\hat{\mathbf{y}}$	(4g)	Mn I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2$	=	$-by_1\,\hat{\mathbf{y}}$	(4g)	Mn I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	P I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	P I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	S I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	S I
$\mathbf{B_7}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(8j)	S II
$\mathbf{B_8}$	=	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(8j)	S II
$\mathbf{B_9}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(8j)	S II
$\mathbf{B_{10}}$	=	$(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(8j)	S II

References

[1] G. Ouvrard, R. Brec, and J. Rouxel, *Structural determination of some MPS_3 layered phases (M = Mn, Fe, Co, Ni and Cd)*, Mater. Res. Bull. **20**, 1181–1189 (1985), doi:10.1016/0025-5408(85)90092-3.

Found in

[1] V. Zhukov, S. Alvarez, and D. Novikov, *Electronic band structure of the magnetic layered semiconductors MPS_3 (M = Mn, Fe and Ni)*, J. Phys. Chem. Solids **57**, 647–652 (1996), doi:10.1016/0022-3697(95)00203-0.