# $MnPS_3$ Structure: ABC3_mC20_12_g_i_ij-001

This structure previously used the label(s) `ABC3_mC20_12_g_i_ij`. Calls to these addresses will be redirected here.

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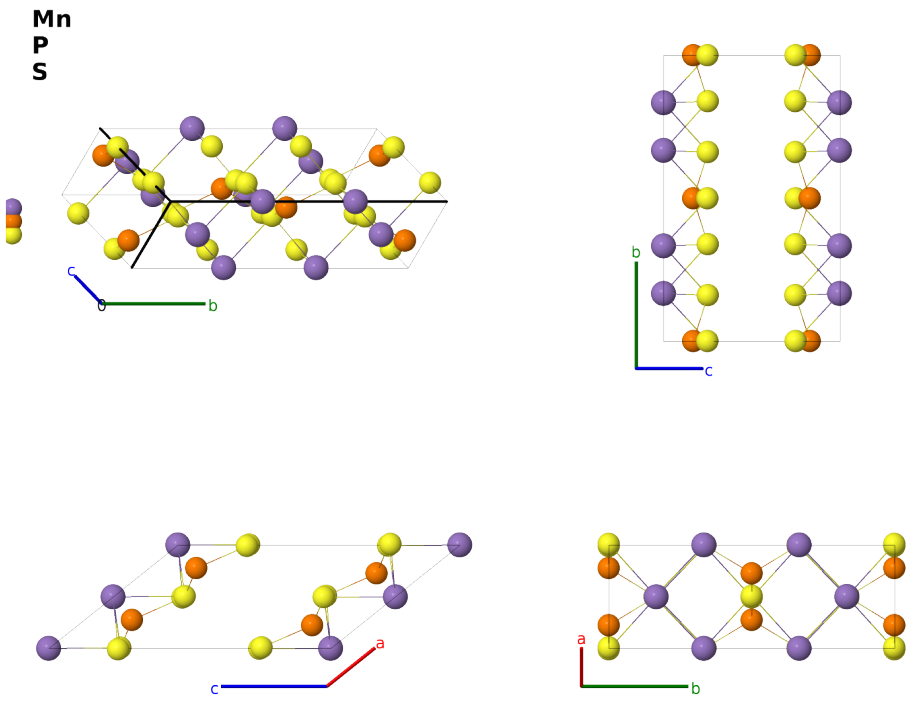
https://aflow.org/prototype-encyclopedia/UPGR

https://aflow.org/prototype-encyclopedia/ABC3_mC20_12_g_i_ij-001



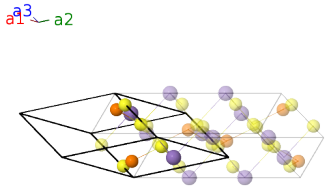

| | |
|---|---|
| **Prototype** | $MnPS_3$ |
| **AFLOW prototype label** | ABC3_mC20_12_g_i_ij-001 |
| **ICSD** | 61391 |
| **CCDC** | 1624918 |
| **Pearson symbol** | mC20 |
| **Space group number** | 12 |
| **Space group symbol** | $C2/m$ |
| **AFLOW prototype command** | `aflow --proto=ABC3_mC20_12_g_i_ij-001 --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**

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




**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.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