

MnCuP Structure:

ABC_oP12_62_c_c_c-003

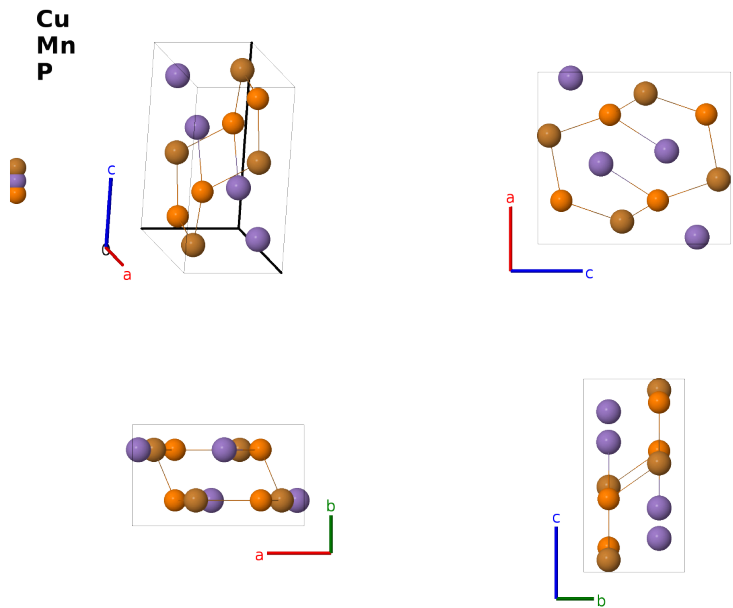
This structure previously used the label(s) **ABC_oP12_62_c_c_c**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/BN2H>

https://aflow.org/prototype-encyclopedia/ABC_oP12_62_c_c_c-003



Prototype	CuMnP
AFLOW prototype label	ABC_oP12_62_c_c_c-003
ICSD	72411
CCDC	1633272
Pearson symbol	oP12
Space group number	62
Space group symbol	<i>Pnma</i>
AFLOW prototype command	<code>aflow --proto=ABC_oP12_62_c_c_c-003</code> <code>--params=a, b/a, c/a, x₁, z₁, x₂, z₂, x₃, z₃</code>

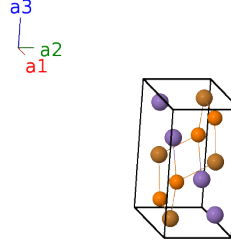
Other compounds with this structure

CoNiSi, CrCoSi, CrNiSi, DyMnGe, ErMnGe, FeCoSi, FeNiSi, HoMnGe, MgSrSi, MnCoSi, MnNiSi, NbCoAs, NbFeAs, NbNiAs, ScCoSi, ScNiSi, ScRuSi, SmMnGe, TaCoAs, TaFeAs, TaNiAs, TiCoAs, TiCoSi, TiNiAs, TiNiSi, TmMnGe, UCoGe, URhGe, VCoSi, VNiSi, ZrFeP, CuMnP_xAs_{1-x}

- This is our prototype for the ternary form of the Co_2Si ($C7$) structure. See that page for similar binary compounds.
- MnCuP and laudite (CuAsS) have the same AFLOW label, $\text{ABC}_{\text{oP12.62.c.c.c.}}$. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- The ICSD lists this structure under the prototype $\text{TiNiSi}\#\text{MgSrSi}$.

Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	Cu 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)	Cu 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)	Cu 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)	Cu 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)	Mn 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)	Mn 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)	Mn 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)	Mn I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B}_{10}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B}_{12}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	P I

References

- [1] J. Mündelein and H.-U. Schuster, *Darstellung und Kristallstruktur der Verbindungen MnCuX ($X = \text{P}, \text{As}, \text{P}_x\text{As}_{1-x}$)*, Z. Naturforsch. B **47**, 925–928 (1992), doi:10.1515/znb-1992-0705.

Found in

- [1] F. Máca, J. Mašek, O. Stelmakhovich, X. Martí, H.Reichlová, K.Uhlířová, P. Beran, P. Wadley, V. Novák, and T. Jungwirth, *Room-temperature antiferromagnetism in CuMnAs* , J. Magn. Magn. Mater. **324**, 1606–1612 (2012), doi:10.1016/j.jmmm.2011.12.017.

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