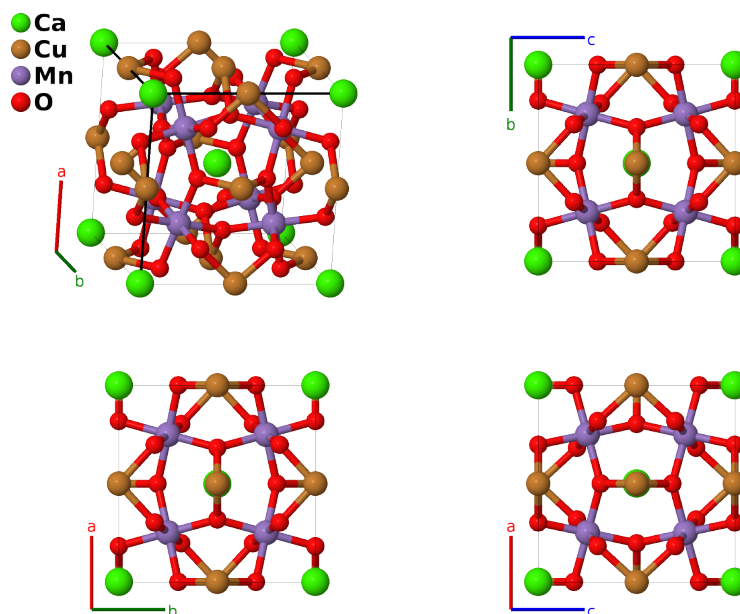


# CaCu<sub>3</sub>Mn<sub>4</sub>O<sub>12</sub> Structure: AB3C4D12\_cI40\_204\_a\_b\_c\_g-001

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<https://afLOW.org/p/RGPS>

[https://afLOW.org/p/AB3C4D12\\_cI40\\_204\\_a\\_b\\_c\\_g-001](https://afLOW.org/p/AB3C4D12_cI40_204_a_b_c_g-001)



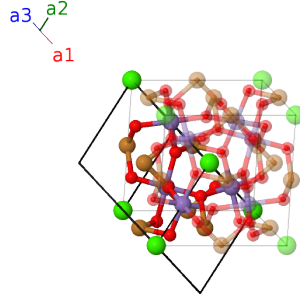
Prototype	CaCu <sub>3</sub> Mn <sub>4</sub> O <sub>12</sub>
AFLOW prototype label	AB3C4D12_cI40_204_a_b_c_g-001
ICSD	15757
Pearson symbol	cI40
Space group number	204
Space group symbol	$Im\bar{3}$
AFLOW prototype command	<pre>afLOW --proto=AB3C4D12_cI40_204_a_b_c_g-001 --params=a, y4, z4</pre>

## Other compounds with this structure

CaCu<sub>3</sub>Co<sub>4</sub>O<sub>12</sub>, CaCu<sub>3</sub>Cr<sub>4</sub>O<sub>12</sub>, CaCu<sub>3</sub>Fe<sub>4</sub>O<sub>12</sub>, CaCu<sub>3</sub>Ge<sub>4</sub>O<sub>12</sub>, CaCu<sub>3</sub>Ir<sub>4</sub>O<sub>12</sub>, CaCu<sub>3</sub>Pt<sub>4</sub>O<sub>12</sub>, CaCu<sub>3</sub>Rh<sub>4</sub>O<sub>12</sub>, CaCu<sub>3</sub>Ru<sub>4</sub>O<sub>12</sub>, CaCu<sub>3</sub>Sn<sub>4</sub>O<sub>12</sub>, CaCu<sub>3</sub>Ti<sub>4</sub>O<sub>12</sub>, CaCu<sub>3</sub>V<sub>4</sub>O<sub>12</sub>, CaCu<sub>3</sub>Zn<sub>4</sub>O<sub>12</sub>, LaCu<sub>3</sub>Ir<sub>4</sub>O<sub>12</sub>, LaCu<sub>3</sub>Mn<sub>4</sub>O<sub>12</sub>, LaCu<sub>3</sub>Ru<sub>4</sub>O<sub>12</sub>, NaCu<sub>3</sub>Ir<sub>4</sub>O<sub>12</sub>, NaCu<sub>3</sub>Ru<sub>4</sub>O<sub>12</sub>, SrCu<sub>3</sub>Fe<sub>4</sub>O<sub>12</sub>

- This is the quaternary form of the double perovskite NaMn<sub>7</sub>O<sub>12</sub>.

## Body-centered Cubic primitive vectors



$$\begin{aligned}
 \mathbf{a}_1 &= -\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}} \\
 \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}} \\
 \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - \frac{1}{2}a \hat{\mathbf{z}}
 \end{aligned}$$

## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$0$	$=$	$0$	(2a)	Ca I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}}$	(6b)	Cu I
$\mathbf{B}_3$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}}$	(6b)	Cu I
$\mathbf{B}_4$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{z}}$	(6b)	Cu I
$\mathbf{B}_5$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(8c)	Mn I
$\mathbf{B}_6$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - \frac{1}{4}a \hat{\mathbf{z}}$	(8c)	Mn I
$\mathbf{B}_7$	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(8c)	Mn I
$\mathbf{B}_8$	$\frac{1}{2} \mathbf{a}_1$	$=$	$-\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(8c)	Mn I
$\mathbf{B}_9$	$(y_4 + z_4) \mathbf{a}_1 + z_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}}$	(24g)	O I
$\mathbf{B}_{10}$	$-(y_4 - z_4) \mathbf{a}_1 + z_4 \mathbf{a}_2 - y_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}}$	(24g)	O I
$\mathbf{B}_{11}$	$(y_4 - z_4) \mathbf{a}_1 - z_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}}$	(24g)	O I
$\mathbf{B}_{12}$	$-(y_4 + z_4) \mathbf{a}_1 - z_4 \mathbf{a}_2 - y_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}}$	(24g)	O I
$\mathbf{B}_{13}$	$y_4 \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$az_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{z}}$	(24g)	O I
$\mathbf{B}_{14}$	$-y_4 \mathbf{a}_1 - (y_4 - z_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$az_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{z}}$	(24g)	O I
$\mathbf{B}_{15}$	$y_4 \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-az_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{z}}$	(24g)	O I
$\mathbf{B}_{16}$	$-y_4 \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-az_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{z}}$	(24g)	O I
$\mathbf{B}_{17}$	$z_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + (y_4 + z_4) \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}}$	(24g)	O I
$\mathbf{B}_{18}$	$z_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - (y_4 - z_4) \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}}$	(24g)	O I
$\mathbf{B}_{19}$	$-z_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + (y_4 - z_4) \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}}$	(24g)	O I
$\mathbf{B}_{20}$	$-z_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - (y_4 + z_4) \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}}$	(24g)	O I

## References

- [1] J. Chenavas, J. C. Joubert, and M. M. B. Bochu, *The synthesis and crystal structure of  $\text{CaCu}_3\text{Mn}_4\text{O}_{12}$ : A new ferromagnetic-perovskite-like compound*, J. Solid State Chem. **14**, 25–32 (1975), doi:10.1016/0022-4596(75)90358-8.