

Mg₆MnO₈ Structure:

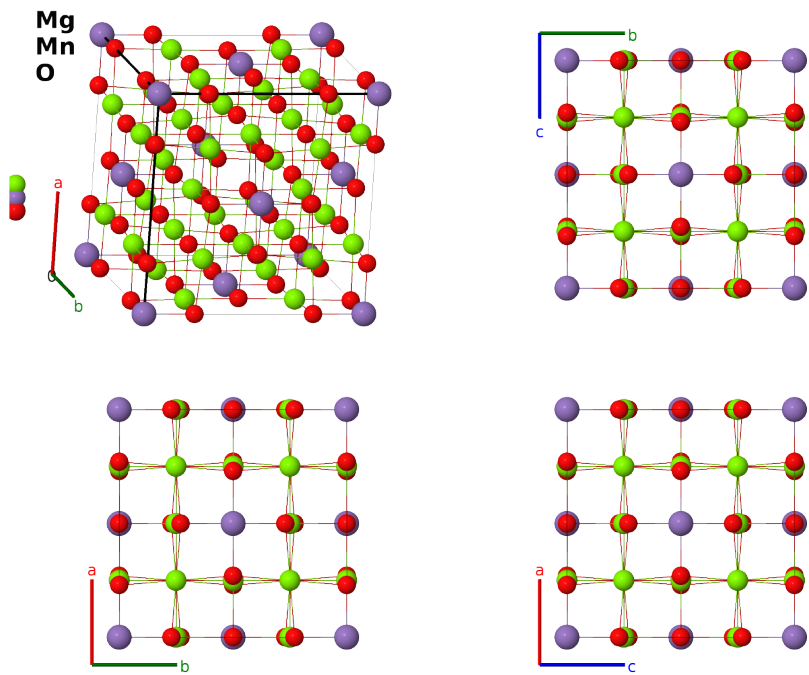
A6BC8_cF60_225_d_a_ce-001

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<https://aflow.org/prototype-encyclopedia/4YGB>

https://aflow.org/prototype-encyclopedia/A6BC8_cF60_225_d_a_ce-001



Prototype	Mg ₆ MnO ₈
AFLOW prototype label	A6BC8_cF60_225_d_a_ce-001
ICSD	24710
CCDC	1600723
Pearson symbol	cF60
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A6BC8_cF60_225_d_a_ce-001</code> <code>--params=a, x_4</code>

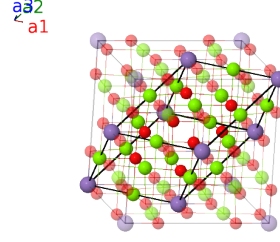
Other compounds with this structure

Na₆CdCl₈, Na₆FeCl₈, Na₆MgCl₈, Na₆MnCl₈

- This can be seen as a distortion of the rock salt ($B1$) structure with four atoms removed. Adding atoms to the (4b) site and setting $x_4 = 1/4$ places all of the atoms on the sites of the rock salt crystal.

Face-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(4a) Mn I
$\mathbf{B}_2$	$=$	$\frac{1}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(8c) O I
$\mathbf{B}_3$	$=$	$\frac{3}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}a\hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{y}} + \frac{3}{4}a\hat{\mathbf{z}}$	(8c) O I
$\mathbf{B}_4$	$=$	$\frac{1}{2}\mathbf{a}_1$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d) Mg I
$\mathbf{B}_5$	$=$	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d) Mg I
$\mathbf{B}_6$	$=$	$\frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d) Mg I
$\mathbf{B}_7$	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d) Mg I
$\mathbf{B}_8$	$=$	$\frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}}$	(24d) Mg I
$\mathbf{B}_9$	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24d) Mg I
$\mathbf{B}_{10}$	$=$	$-x_4\mathbf{a}_1 + x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$ax_4\hat{\mathbf{x}}$	(24e) O II
$\mathbf{B}_{11}$	$=$	$x_4\mathbf{a}_1 - x_4\mathbf{a}_2 - x_4\mathbf{a}_3$	$=$	$-ax_4\hat{\mathbf{x}}$	(24e) O II
$\mathbf{B}_{12}$	$=$	$x_4\mathbf{a}_1 - x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$ax_4\hat{\mathbf{y}}$	(24e) O II
$\mathbf{B}_{13}$	$=$	$-x_4\mathbf{a}_1 + x_4\mathbf{a}_2 - x_4\mathbf{a}_3$	$=$	$-ax_4\hat{\mathbf{y}}$	(24e) O II
$\mathbf{B}_{14}$	$=$	$x_4\mathbf{a}_1 + x_4\mathbf{a}_2 - x_4\mathbf{a}_3$	$=$	$ax_4\hat{\mathbf{z}}$	(24e) O II
$\mathbf{B}_{15}$	$=$	$-x_4\mathbf{a}_1 - x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$-ax_4\hat{\mathbf{z}}$	(24e) O II

References

- [1] J. S. Kasper and J. S. Prener, *The Crystal Structure of Mg_6MnO_8* , Acta Cryst. **7**, 246–248 (1954), doi:10.1107/S0365110X54000722.

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