

Forsterite (Mg_2SiO_4 , $S1_2$) Structure: A2B4C_oP28_62_ac_2cd_c-001

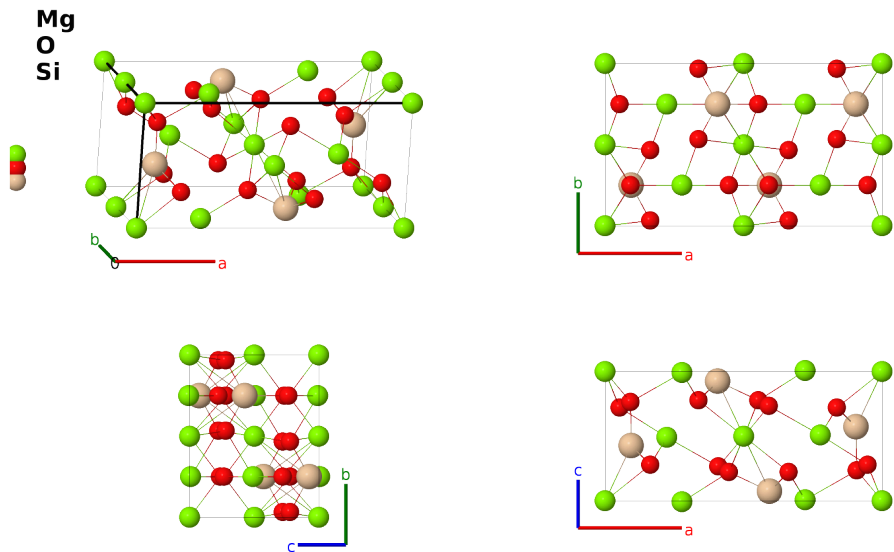
This structure previously used the label(s) **A2B4C_oP28_62_ac_2cd_c**. Calls to these addresses will be redirected here.

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/V88M>

https://aflow.org/prototype-encyclopedia/A2B4C_oP28_62_ac_2cd_c-001



Prototype	$\text{Mg}_2\text{O}_4\text{Si}$
AFLOW prototype label	A2B4C_oP28_62_ac_2cd_c-001
<i>Strukturbericht</i> designation	$S1_2$
Mineral name	forsterite
ICSD	64744
CCDC	1626923
Pearson symbol	oP28
Space group number	62
Space group symbol	$Pnma$
AFLOW prototype command	<pre>aflow --proto=A2B4C_oP28_62_ac_2cd_c-001 --params=a,b/a,c/a,x2,z2,x3,z3,x4,z4,x5,z5,x6,y6,z6</pre>

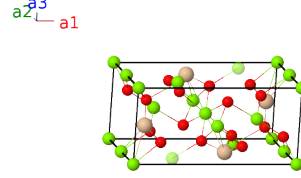
Other compounds with this structure

Al_2BeO_4 , Fe_2SiO_4 (fayalite), Fe_2SiS_4 , Mg_2GeO_4 , Mg_2GeS_4 , Mg_2GeS_4 , Mn_2GeS_4 , Tm_2ZnS_4

- This structure is the magnesium end-point of olivine, $(\text{Mg,Fe})_2\text{SiO}_4$.
- We use the structural data taken by (Hazen, 1976) at 23°C.
- For olivine structures where the (2a) and (2c) sites have different species, see the monticellite structure page.
- (Hazen, 1976) reports the structure in the $Pbnm$ setting of space group #62. We have transformed this into the standard $Pnma$ setting.

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
$\mathbf{B}_1$	$= 0$	$=$	0	(4a)	Mg I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4a)	Mg I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}b \hat{\mathbf{y}}$	(4a)	Mg I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4a)	Mg 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)	Mg II
$\mathbf{B}_6$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Mg II
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4c)	Mg II
$\mathbf{B}_8$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Mg II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_{10}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O 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)	O I
$\mathbf{B}_{12}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_{14}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_{16}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B}_{18}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B}_{19}$	$= -x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B}_{20}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B}_{21}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8d)	O III

$$\begin{aligned}
\mathbf{B}_{22} &= \begin{matrix} -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 - y_6 \mathbf{a}_2 + \\ \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 \end{matrix} &= & -a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{O III} \\
\mathbf{B}_{23} &= -x_6 \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 - z_6 \mathbf{a}_3 &= & -ax_6 \hat{\mathbf{x}} + b \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (8d) & \text{O III} \\
\mathbf{B}_{24} &= \begin{matrix} \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 - \\ \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3 \end{matrix} &= & a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_6 - \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_6 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{O III} \\
\mathbf{B}_{25} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= & -ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (8d) & \text{O III} \\
\mathbf{B}_{26} &= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 + y_6 \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3 &= & a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c \left(z_6 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{O III} \\
\mathbf{B}_{27} &= x_6 \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 + z_6 \mathbf{a}_3 &= & ax_6 \hat{\mathbf{x}} - b \left(y_6 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (8d) & \text{O III} \\
\mathbf{B}_{28} &= \begin{matrix} -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 + \\ \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 \end{matrix} &= & -a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{O III}
\end{aligned}$$

References

- [1] R. M. Hazen, *Effects of temperature and pressure on the crystal structure of forsterite*, Am. Mineral. **61**, 1280–1293 (1976).

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043