

Enstatite (MgSiO_3 , $S4_3$) Structure: AB3C_oP80_61_2c_6c_2c-001

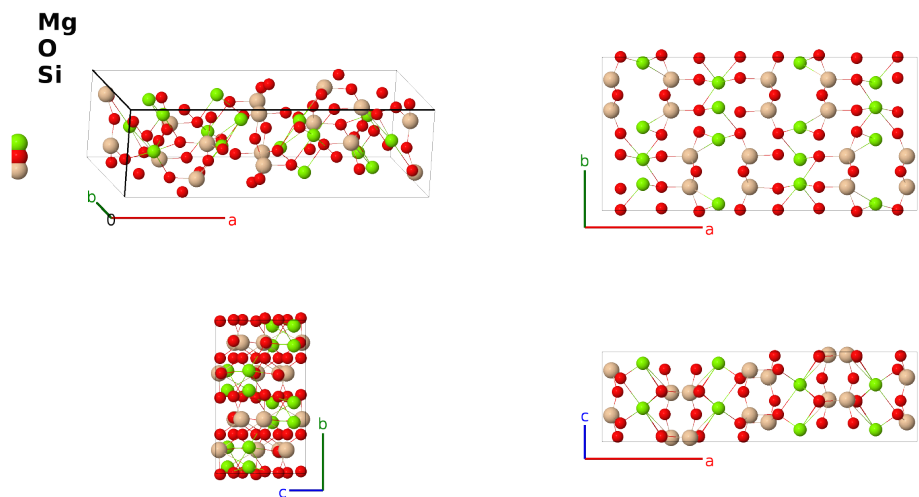
This structure previously used the label(s) AB3C_oP80_61_2c_6c_2c. Calls to these addresses will be redirected here.

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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/N16Y>

https://aflow.org/prototype-encyclopedia/AB3C_oP80_61_2c_6c_2c-001



Prototype	MgO_3Si
AFLOW prototype label	AB3C_oP80_61_2c_6c_2c-001
<i>Strukturbericht</i> designation	$S4_3$
Mineral name	enstatite
ICSD	77344
CCDC	1637782
Pearson symbol	oP80
Space group number	61
Space group symbol	$Pbca$
AFLOW prototype command	<pre>aflow --proto=AB3C_oP80_61_2c_6c_2c-001 --params=a,b/a,c/a,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,y5,z5,x6,y6,z6,x7, y7,z7,x8,y8,z8,x9,y9,z9,x10,y10,z10</pre>

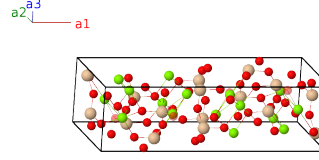
Other compounds with this structure

FeSiO_3 (ferrosilite), CoGeO_3 , CoSiO_3 (Co-pyroxene), MgGeO_3

- Enstatite (properly orthoenstatite) is an end point of orthopyroxene, XYSi_2O_6 , where X and Y are small-radius divalent cations. If either X or Y is replaced by a transition metal the system becomes a monoclinic clinopyroxene, in space group $C2/c$ #15.
- We also have data for a high-pressure, post-perovskite phase of MgSiO_3 .
- The ICSD entry is from (Byström, 1943).

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
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(8c)	Mg I
$\mathbf{B}_2$	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Mg I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Mg I
$\mathbf{B}_4$	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(8c)	Mg I
$\mathbf{B}_5$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(8c)	Mg I
$\mathbf{B}_6$	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 + y_1 \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Mg I
$\mathbf{B}_7$	$= x_1 \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Mg I
$\mathbf{B}_8$	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(8c)	Mg I
$\mathbf{B}_9$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8c)	Mg II
$\mathbf{B}_{10}$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Mg II
$\mathbf{B}_{11}$	$= -x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Mg II
$\mathbf{B}_{12}$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8c)	Mg II
$\mathbf{B}_{13}$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8c)	Mg II
$\mathbf{B}_{14}$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + y_2 \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Mg II
$\mathbf{B}_{15}$	$= x_2 \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Mg II
$\mathbf{B}_{16}$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8c)	Mg II
$\mathbf{B}_{17}$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_{18}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_{19}$	$= -x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O I

$\mathbf{B}_{20} =$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3 =$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_{21} =$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 =$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_{22} =$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3 =$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_{23} =$	$x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3 =$	$ax_3 \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_{24} =$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3 =$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_{25} =$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 =$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{26} =$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3 =$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{27} =$	$-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3 =$	$-ax_4 \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{28} =$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3 =$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{29} =$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 =$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{30} =$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3 =$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{31} =$	$x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3 =$	$ax_4 \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{32} =$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3 =$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{33} =$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 =$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B}_{34} =$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3 =$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B}_{35} =$	$-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3 =$	$-ax_5 \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B}_{36} =$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3 =$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B}_{37} =$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 =$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B}_{38} =$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 + y_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3 =$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B}_{39} =$	$x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3 =$	$ax_5 \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B}_{40} =$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3 =$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B}_{41} =$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 =$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8c)	O IV
$\mathbf{B}_{42} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 =$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O IV
$\mathbf{B}_{43} =$	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3 =$	$-ax_6 \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O IV
$\mathbf{B}_{44} =$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3 =$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8c)	O IV
$\mathbf{B}_{45} =$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 =$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8c)	O IV
$\mathbf{B}_{46} =$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 + y_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3 =$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O IV
$\mathbf{B}_{47} =$	$x_6 \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 =$	$ax_6 \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O IV
$\mathbf{B}_{48} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3 =$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8c)	O IV
$\mathbf{B}_{49} =$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 =$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8c)	O V
$\mathbf{B}_{50} =$	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3 =$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O V
$\mathbf{B}_{51} =$	$-x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3 =$	$-ax_7 \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O V

$\mathbf{B}_{52} =$	$(x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8c)	O V
$\mathbf{B}_{53} =$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8c)	O V
$\mathbf{B}_{54} =$	$(x_7 + \frac{1}{2}) \mathbf{a}_1 + y_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O V
$\mathbf{B}_{55} =$	$x_7 \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O V
$\mathbf{B}_{56} =$	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8c)	O V
$\mathbf{B}_{57} =$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8c)	O VI
$\mathbf{B}_{58} =$	$-(x_8 - \frac{1}{2}) \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O VI
$\mathbf{B}_{59} =$	$-x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O VI
$\mathbf{B}_{60} =$	$(x_8 + \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8c)	O VI
$\mathbf{B}_{61} =$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8c)	O VI
$\mathbf{B}_{62} =$	$(x_8 + \frac{1}{2}) \mathbf{a}_1 + y_8 \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O VI
$\mathbf{B}_{63} =$	$x_8 \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O VI
$\mathbf{B}_{64} =$	$-(x_8 - \frac{1}{2}) \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8c)	O VI
$\mathbf{B}_{65} =$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8c)	Si I
$\mathbf{B}_{66} =$	$-(x_9 - \frac{1}{2}) \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Si I
$\mathbf{B}_{67} =$	$-x_9 \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Si I
$\mathbf{B}_{68} =$	$(x_9 + \frac{1}{2}) \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(8c)	Si I
$\mathbf{B}_{69} =$	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(8c)	Si I
$\mathbf{B}_{70} =$	$(x_9 + \frac{1}{2}) \mathbf{a}_1 + y_9 \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Si I
$\mathbf{B}_{71} =$	$x_9 \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} - b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Si I
$\mathbf{B}_{72} =$	$-(x_9 - \frac{1}{2}) \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$-a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8c)	Si I
$\mathbf{B}_{73} =$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8c)	Si II
$\mathbf{B}_{74} =$	$-(x_{10} - \frac{1}{2}) \mathbf{a}_1 - y_{10} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Si II
$\mathbf{B}_{75} =$	$-x_{10} \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 - (z_{10} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} + b(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Si II
$\mathbf{B}_{76} =$	$(x_{10} + \frac{1}{2}) \mathbf{a}_1 - (y_{10} - \frac{1}{2}) \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{10} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(8c)	Si II
$\mathbf{B}_{77} =$	$-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(8c)	Si II
$\mathbf{B}_{78} =$	$(x_{10} + \frac{1}{2}) \mathbf{a}_1 + y_{10} \mathbf{a}_2 - (z_{10} - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Si II
$\mathbf{B}_{79} =$	$x_{10} \mathbf{a}_1 - (y_{10} - \frac{1}{2}) \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} - b(y_{10} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Si II
$\mathbf{B}_{80} =$	$-(x_{10} - \frac{1}{2}) \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$-a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8c)	Si II

References

- [1] B. E. Warren and D. I. Modell, *The Structure of Enstatite $MgSiO_3$* , Z. Kristallogr. **75**, 1–14 (1930), doi:10.1515/zkri-1930-0102.
- [2] A. Byström, *Roentgenuntersuchung des Systems $MgO-Al_2O_3-SiO_2$* , Berichte Deutsch. Keram. G. **24**, 2–15 (1943).

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