

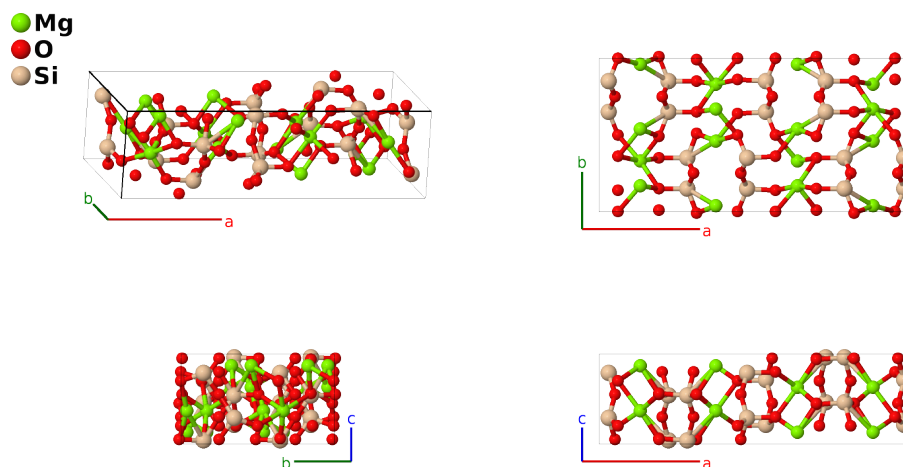
# Enstatite ( $\text{MgSiO}_3$ , $S4_3$ ) Structure: AB3C\_oP80\_61\_2c\_6c\_2c-001

This structure originally had the label AB3C\_oP80\_61\_2c\_6c\_2c. Calls to that address will be redirected here.

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<https://afLOW.org/p/N16Y>

[https://afLOW.org/p/AB3C\\_oP80\\_61\\_2c\\_6c\\_2c-001](https://afLOW.org/p/AB3C_oP80_61_2c_6c_2c-001)



Prototype	$\text{MgO}_3\text{Si}$
AFLOW prototype label	AB3C_oP80_61_2c_6c_2c-001
<i>Strukturbericht</i> designation	$S4_3$
Mineral name	enstatite
ICSD	77344
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

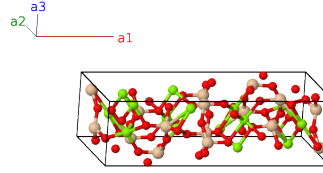
$\text{FeSiO}_3$  (ferrosilite),  $\text{CoGeO}_3$ ,  $\text{CoSiO}_3$  (Co-pyroxene),  $\text{MgGeO}_3$

- Enstatite (properly orthoenstatite) is an end point of orthopyroxene,  $\text{XYSi}_2\text{O}_6$ , 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  $\text{MgSiO}_3$ .

- 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
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Mg I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + b \left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Mg I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(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
$\mathbf{B}_6$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + y_1 \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Mg I
$\mathbf{B}_7$	$= x_1 \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} - b \left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Mg I
$\mathbf{B}_8$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{10}$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Mg II
$\mathbf{B}_{11}$	$= -x_2 \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + b \left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Mg II
$\mathbf{B}_{12}$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{14}$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + y_2 \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Mg II
$\mathbf{B}_{15}$	$= x_2 \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - b \left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Mg II
$\mathbf{B}_{16}$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{18}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_{19}$	$= -x_3 \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + b \left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_{20}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{22}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + y_3 \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_{23}$	$= x_3 \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - b \left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O I



$$\begin{aligned}
\mathbf{B}_{56} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right) \mathbf{a}_2 + z_7 \mathbf{a}_3 &= -a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_7 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} &(8c) & \text{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) & \text{O VI} \\
\mathbf{B}_{58} &= -\left(x_8 - \frac{1}{2}\right) \mathbf{a}_1 - y_8 \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3 &= -a \left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c \left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8c) & \text{O VI} \\
\mathbf{B}_{59} &= -x_8 \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3 &= -ax_8 \hat{\mathbf{x}} + b \left(y_8 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_8 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8c) & \text{O VI} \\
\mathbf{B}_{60} &= \left(x_8 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right) \mathbf{a}_2 - z_8 \mathbf{a}_3 &= a \left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_8 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} &(8c) & \text{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) & \text{O VI} \\
\mathbf{B}_{62} &= \left(x_8 + \frac{1}{2}\right) \mathbf{a}_1 + y_8 \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3 &= a \left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c \left(z_8 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8c) & \text{O VI} \\
\mathbf{B}_{63} &= x_8 \mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3 &= ax_8 \hat{\mathbf{x}} - b \left(y_8 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8c) & \text{O VI} \\
\mathbf{B}_{64} &= -\left(x_8 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 + z_8 \mathbf{a}_3 &= -a \left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_8 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} &(8c) & \text{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) & \text{Si I} \\
\mathbf{B}_{66} &= -\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 - y_9 \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 &= -a \left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c \left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8c) & \text{Si I} \\
\mathbf{B}_{67} &= -x_9 \mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3 &= -ax_9 \hat{\mathbf{x}} + b \left(y_9 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8c) & \text{Si I} \\
\mathbf{B}_{68} &= \left(x_9 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 - z_9 \mathbf{a}_3 &= a \left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_9 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} &(8c) & \text{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) & \text{Si I} \\
\mathbf{B}_{70} &= \left(x_9 + \frac{1}{2}\right) \mathbf{a}_1 + y_9 \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3 &= a \left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - c \left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8c) & \text{Si I} \\
\mathbf{B}_{71} &= x_9 \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 &= ax_9 \hat{\mathbf{x}} - b \left(y_9 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8c) & \text{Si I} \\
\mathbf{B}_{72} &= -\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_2 + z_9 \mathbf{a}_3 &= -a \left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_9 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} &(8c) & \text{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) & \text{Si II} \\
\mathbf{B}_{74} &= -\left(x_{10} - \frac{1}{2}\right) \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 &= -a \left(x_{10} - \frac{1}{2}\right) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c \left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}} &(8c) & \text{Si II} \\
\mathbf{B}_{75} &= -x_{10} \mathbf{a}_1 + \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_3 &= -ax_{10} \hat{\mathbf{x}} + b \left(y_{10} + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_{10} - \frac{1}{2}\right) \hat{\mathbf{z}} &(8c) & \text{Si II} \\
\mathbf{B}_{76} &= \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{10} - \frac{1}{2}\right) \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= a \left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_{10} - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} &(8c) & \text{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) & \text{Si II} \\
\mathbf{B}_{78} &= \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_1 + y_{10} \mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_3 &= a \left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} - c \left(z_{10} - \frac{1}{2}\right) \hat{\mathbf{z}} &(8c) & \text{Si II} \\
\mathbf{B}_{79} &= x_{10} \mathbf{a}_1 - \left(y_{10} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 &= ax_{10} \hat{\mathbf{x}} - b \left(y_{10} - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}} &(8c) & \text{Si II} \\
\mathbf{B}_{80} &= -\left(x_{10} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= -a \left(x_{10} - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_{10} + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} &(8c) & \text{Si II}
\end{aligned}$$

## References

- [1] B. E. Warren and D. I. Modell, *The Structure of Enstatite MgSiO<sub>3</sub>*, *Z. Kristallogr.* **75**, 1–14 (1930), doi:10.1515/zkri-1930-0102.
- [2] A. Byström, *Roentgenuntersuchung des Systems MgO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub>*, *Berichte Deutsch. Keram. G.* **24**, 2–15 (1943).