α'_H-Ca_2SiO_4 Structure: A4B8C_oP52_62_2d_4d_c-001

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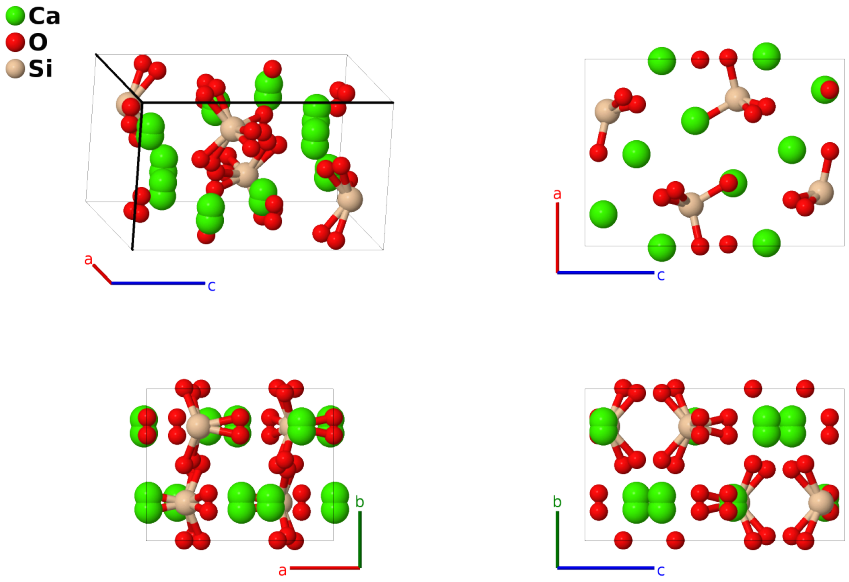
https://aflow.org/p/1R45

https://aflow.org/p/A4B8C_oP52_62_2d_4d_c-001



Prototype	Ca_2O_4Si
AFLOW prototype label	A4B8C_oP52_62_2d_4d_c-001
ICSD	82997
Pearson symbol	oP52
Space group number	62
Space group symbol	*Pnma*
AFLOW prototype command	`aflow --proto=A4B8C_oP52_62_2d_4d_c-001 --params=`$a, b/a, c/a, x_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

Other compounds with this structure
Sr_2SiO_4

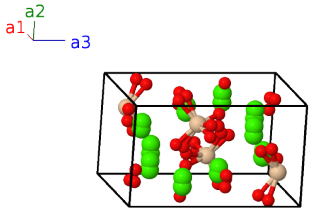
- Ca_2SiO_4 exists in a variety of structures (Mumme, 1996; Yamnova, 2011):
  - hexagonal α-Ca_2SiO_4, stable above 1445°C. There is some dispute as to whether this occurs in a
    - trigonal, space group $P\bar{3}m1$ #164 structure or a
    - disordered hexagonal, space group $P6_3/mmc$ #194 structure.
  - orthorhombic α_H'-Ca_2SiO_4 (this structure), stable in the range 1160 – 1425°C,

– orthorhombic α_L'-Ca_2SiO_4, stable in the range $690 - 1160$°C,
– monoclinic β-Ca_2SiO_4, stable in the range $500 - 690$°C and found in nature as the metastable mineral larnite, and
– γ-Ca_2SiO_4, stable below 500°C, in the olivine ($S1_2$) structure.

- We use the neutron scattering data of (Mumme, 1996) taken at 1250°C. Their refinement of the data requires that all of the calcium and oxygen sites are only half filled, *i.e.*, only site of each Ca-Ca and O-O pair in the diagram is filled at any given time.

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8d)	Ca I
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Ca I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8d)	Ca I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Ca I
$\mathbf{B_9}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8d)	Ca I
$\mathbf{B_{10}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Ca I
$\mathbf{B_{11}}$	=	$x_2\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8d)	Ca I
$\mathbf{B_{12}}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Ca I
$\mathbf{B_{13}}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8d)	Ca II
$\mathbf{B_{14}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Ca II
$\mathbf{B_{15}}$	=	$-x_3\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8d)	Ca II
$\mathbf{B_{16}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Ca II
$\mathbf{B_{17}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8d)	Ca II
$\mathbf{B_{18}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Ca II
$\mathbf{B_{19}}$	=	$x_3\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8d)	Ca II

$$
\begin{array}{lcccccc}
\mathbf{B_{20}} & = & -\left(x_3-\frac{1}{2}\right)\mathbf{a}_1+\left(y_3+\frac{1}{2}\right)\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\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}}+c\left(z_3+\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(8d)} & \text{Ca II} \\
\mathbf{B_{21}} & = & 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}} & \text{(8d)} & \text{O I} \\
\mathbf{B_{22}} & = & -\left(x_4-\frac{1}{2}\right)\mathbf{a}_1-y_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\mathbf{a}_3 & = & -a\left(x_4-\frac{1}{2}\right)\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(8d)} & \text{O I} \\
\mathbf{B_{23}} & = & -x_4\,\mathbf{a}_1+\left(y_4+\frac{1}{2}\right)\mathbf{a}_2-z_4\,\mathbf{a}_3 & = & -ax_4\,\hat{\mathbf{x}}+b\left(y_4+\frac{1}{2}\right)\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}} & \text{(8d)} & \text{O I} \\
\mathbf{B_{24}} & = & \left(x_4+\frac{1}{2}\right)\mathbf{a}_1-\left(y_4-\frac{1}{2}\right)\mathbf{a}_2-\left(z_4-\frac{1}{2}\right)\mathbf{a}_3 & = & a\left(x_4+\frac{1}{2}\right)\hat{\mathbf{x}}-b\left(y_4-\frac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_4-\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(8d)} & \text{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}} & \text{(8d)} & \text{O I} \\
\mathbf{B_{26}} & = & \left(x_4+\frac{1}{2}\right)\mathbf{a}_1+y_4\,\mathbf{a}_2-\left(z_4-\frac{1}{2}\right)\mathbf{a}_3 & = & a\left(x_4+\frac{1}{2}\right)\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(8d)} & \text{O I} \\
\mathbf{B_{27}} & = & x_4\,\mathbf{a}_1-\left(y_4-\frac{1}{2}\right)\mathbf{a}_2+z_4\,\mathbf{a}_3 & = & ax_4\,\hat{\mathbf{x}}-b\left(y_4-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}} & \text{(8d)} & \text{O I} \\
\mathbf{B_{28}} & = & -\left(x_4-\frac{1}{2}\right)\mathbf{a}_1+\left(y_4+\frac{1}{2}\right)\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\mathbf{a}_3 & = & -a\left(x_4-\frac{1}{2}\right)\hat{\mathbf{x}}+b\left(y_4+\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(8d)} & \text{O I} \\
\mathbf{B_{29}} & = & 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}} & \text{(8d)} & \text{O II} \\
\mathbf{B_{30}} & = & -\left(x_5-\frac{1}{2}\right)\mathbf{a}_1-y_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\mathbf{a}_3 & = & -a\left(x_5-\frac{1}{2}\right)\hat{\mathbf{x}}-by_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(8d)} & \text{O II} \\
\mathbf{B_{31}} & = & -x_5\,\mathbf{a}_1+\left(y_5+\frac{1}{2}\right)\mathbf{a}_2-z_5\,\mathbf{a}_3 & = & -ax_5\,\hat{\mathbf{x}}+b\left(y_5+\frac{1}{2}\right)\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}} & \text{(8d)} & \text{O II} \\
\mathbf{B_{32}} & = & \left(x_5+\frac{1}{2}\right)\mathbf{a}_1-\left(y_5-\frac{1}{2}\right)\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\mathbf{a}_3 & = & a\left(x_5+\frac{1}{2}\right)\hat{\mathbf{x}}-b\left(y_5-\frac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_5-\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(8d)} & \text{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}} & \text{(8d)} & \text{O II} \\
\mathbf{B_{34}} & = & \left(x_5+\frac{1}{2}\right)\mathbf{a}_1+y_5\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\mathbf{a}_3 & = & a\left(x_5+\frac{1}{2}\right)\hat{\mathbf{x}}+by_5\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(8d)} & \text{O II} \\
\mathbf{B_{35}} & = & x_5\,\mathbf{a}_1-\left(y_5-\frac{1}{2}\right)\mathbf{a}_2+z_5\,\mathbf{a}_3 & = & ax_5\,\hat{\mathbf{x}}-b\left(y_5-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}} & \text{(8d)} & \text{O II} \\
\mathbf{B_{36}} & = & -\left(x_5-\frac{1}{2}\right)\mathbf{a}_1+\left(y_5+\frac{1}{2}\right)\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\mathbf{a}_3 & = & -a\left(x_5-\frac{1}{2}\right)\hat{\mathbf{x}}+b\left(y_5+\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(8d)} & \text{O II} \\
\mathbf{B_{37}} & = & 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}} & \text{(8d)} & \text{O III} \\
\mathbf{B_{38}} & = & -\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}} & \text{(8d)} & \text{O III} \\
\mathbf{B_{39}} & = & -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}} & \text{(8d)} & \text{O III} \\
\mathbf{B_{40}} & = & \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 & = & 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}} & \text{(8d)} & \text{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}} & \text{(8d)} & \text{O III} \\
\mathbf{B_{42}} & = & \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}} & \text{(8d)} & \text{O III} \\
\mathbf{B_{43}} & = & 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}} & \text{(8d)} & \text{O III} \\
\mathbf{B_{44}} & = & -\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 & = & -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}} & \text{(8d)} & \text{O III} \\
\mathbf{B_{45}} & = & 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}} & \text{(8d)} & \text{O IV} \\
\mathbf{B_{46}} & = & -\left(x_7-\frac{1}{2}\right)\mathbf{a}_1-y_7\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\mathbf{a}_3 & = & -a\left(x_7-\frac{1}{2}\right)\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(8d)} & \text{O IV} \\
\mathbf{B_{47}} & = & -x_7\,\mathbf{a}_1+\left(y_7+\frac{1}{2}\right)\mathbf{a}_2-z_7\,\mathbf{a}_3 & = & -ax_7\,\hat{\mathbf{x}}+b\left(y_7+\frac{1}{2}\right)\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}} & \text{(8d)} & \text{O IV} \\
\mathbf{B_{48}} & = & \left(x_7+\frac{1}{2}\right)\mathbf{a}_1-\left(y_7-\frac{1}{2}\right)\mathbf{a}_2-\left(z_7-\frac{1}{2}\right)\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}}-c\left(z_7-\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(8d)} & \text{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}} & \text{(8d)} & \text{O IV} \\
\mathbf{B_{50}} & = & \left(x_7+\frac{1}{2}\right)\mathbf{a}_1+y_7\,\mathbf{a}_2-\left(z_7-\frac{1}{2}\right)\mathbf{a}_3 & = & a\left(x_7+\frac{1}{2}\right)\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}-c\left(z_7-\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(8d)} & \text{O IV} \\
\mathbf{B_{51}} & = & x_7\,\mathbf{a}_1-\left(y_7-\frac{1}{2}\right)\mathbf{a}_2+z_7\,\mathbf{a}_3 & = & ax_7\,\hat{\mathbf{x}}-b\left(y_7-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}} & \text{(8d)} & \text{O IV}
\end{array}
$$

$$\mathbf{B_{52}} = -\left(x_7 - \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_7 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_7 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_7 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{O IV}$$

References

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[2] N. A. Yamnova, N. V. Zubkova, N. N. Eremin, A. E. Zadov, and V. M. Gazeev, *Crystal structure of larnite β-Ca_2SiO_4 and specific features of polymorphic transitions in dicalcium orthosilicate*, Crystallogr. Rep. **56**, 210–220 (2011), doi:10.1134/S1063774511020209.