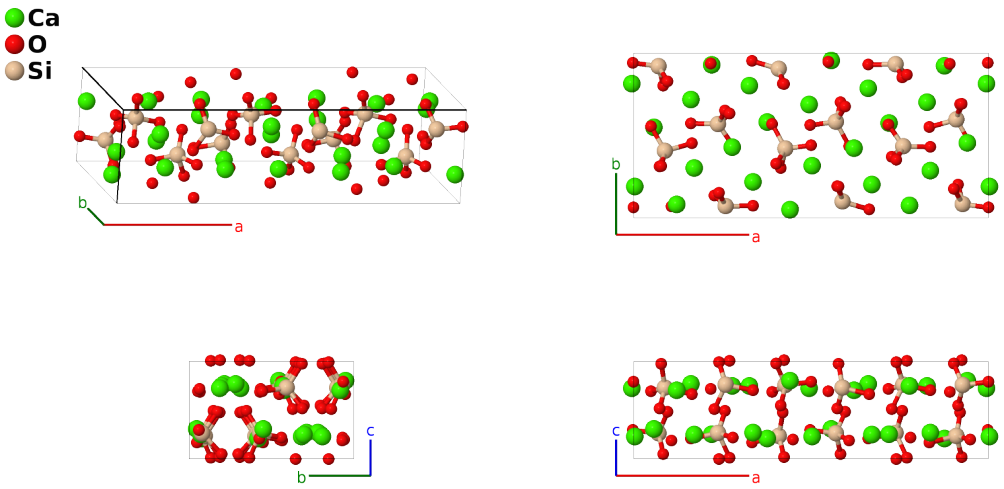
α'_L-Ca_2SiO_4 Structure: A2B4C_oP84_33_6a_12a_3a-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/2RUZ

https://aflow.org/p/A2B4C_oP84_33_6a_12a_3a-001



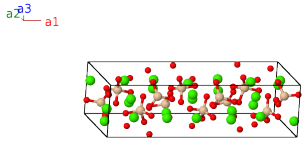
Prototype	Ca_2O_4Si
AFLOW prototype label	A2B4C_oP84_33_6a_12a_3a-001
ICSD	82996
Pearson symbol	oP84
Space group number	33
Space group symbol	$Pna2_1$
AFLOW prototype command	`aflow --proto=A2B4C_oP84_33_6a_12a_3a-001 --params=`$a, b/a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}, x_{20}, y_{20}, z_{20}, x_{21}, y_{21}, z_{21}$

- 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, stable in the range 1160 – 1425°C,
  - orthorhombic α_L'-Ca_2SiO_4 (this structure), 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 1250°C neutron scattering data from (Mumme, 1996).

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	Ca I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Ca I
$\mathbf{B_3}$	=	$\left(x_1+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_1-\frac{1}{2}\right)\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_1-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	Ca I
$\mathbf{B_4}$	=	$-\left(x_1-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_1+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_1+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Ca I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	Ca II
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Ca II
$\mathbf{B_7}$	=	$\left(x_2+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2-\frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	Ca II
$\mathbf{B_8}$	=	$-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Ca II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4a)	Ca III
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Ca III
$\mathbf{B_{11}}$	=	$\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3-\frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4a)	Ca III
$\mathbf{B_{12}}$	=	$-\left(x_3-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Ca III
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4a)	Ca IV
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Ca IV
$\mathbf{B_{15}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4-\frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4a)	Ca IV
$\mathbf{B_{16}}$	=	$-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Ca IV
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4a)	Ca V
$\mathbf{B_{18}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Ca V
$\mathbf{B_{19}}$	=	$\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5-\frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4a)	Ca V
$\mathbf{B_{20}}$	=	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Ca V
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4a)	Ca VI
$\mathbf{B_{22}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Ca VI
$\mathbf{B_{23}}$	=	$\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_6-\frac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4a)	Ca VI
$\mathbf{B_{24}}$	=	$-\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Ca VI
$\mathbf{B_{25}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4a)	O I

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\begin{array}{lcccccc}
\mathbf{B_{26}} & = & -x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}} & (4a) & \text{O I} \\
\mathbf{B_{27}} & = & \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}} & (4a) & \text{O I} \\
\mathbf{B_{28}} & = & -\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}} & (4a) & \text{O I} \\
\mathbf{B_{29}} & = & 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}} & (4a) & \text{O II} \\
\mathbf{B_{30}} & = & -x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + \left(z_8+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + c\left(z_8+\frac{1}{2}\right)\,\hat{\mathbf{z}} & (4a) & \text{O II} \\
\mathbf{B_{31}} & = & \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}} & (4a) & \text{O II} \\
\mathbf{B_{32}} & = & -\left(x_8-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_8+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_8+\frac{1}{2}\right)\,\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}} + c\left(z_8+\frac{1}{2}\right)\,\hat{\mathbf{z}} & (4a) & \text{O II} \\
\mathbf{B_{33}} & = & 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}} & (4a) & \text{O III} \\
\mathbf{B_{34}} & = & -x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + \left(z_9+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + c\left(z_9+\frac{1}{2}\right)\,\hat{\mathbf{z}} & (4a) & \text{O III} \\
\mathbf{B_{35}} & = & \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}} & (4a) & \text{O III} \\
\mathbf{B_{36}} & = & -\left(x_9-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_9+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_9+\frac{1}{2}\right)\,\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}} + c\left(z_9+\frac{1}{2}\right)\,\hat{\mathbf{z}} & (4a) & \text{O III} \\
\mathbf{B_{37}} & = & 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}} & (4a) & \text{O IV} \\
\mathbf{B_{38}} & = & -x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 + \left(z_{10}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + c\left(z_{10}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & (4a) & \text{O IV} \\
\mathbf{B_{39}} & = & \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}} & (4a) & \text{O IV} \\
\mathbf{B_{40}} & = & -\left(x_{10}-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_{10}+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{10}+\frac{1}{2}\right)\,\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}} + c\left(z_{10}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & (4a) & \text{O IV} \\
\mathbf{B_{41}} & = & x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 & = & ax_{11}\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} & (4a) & \text{O V} \\
\mathbf{B_{42}} & = & -x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 + \left(z_{11}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_{11}\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + c\left(z_{11}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & (4a) & \text{O V} \\
\mathbf{B_{43}} & = & \left(x_{11}+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_{11}-\frac{1}{2}\right)\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 & = & a\left(x_{11}+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_{11}-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} & (4a) & \text{O V} \\
\mathbf{B_{44}} & = & -\left(x_{11}-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_{11}+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{11}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_{11}-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_{11}+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{11}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & (4a) & \text{O V} \\
\mathbf{B_{45}} & = & x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 & = & ax_{12}\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B_{46}} & = & -x_{12}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 + \left(z_{12}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_{12}\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} + c\left(z_{12}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B_{47}} & = & \left(x_{12}+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_{12}-\frac{1}{2}\right)\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 & = & a\left(x_{12}+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_{12}-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B_{48}} & = & -\left(x_{12}-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_{12}+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{12}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_{12}-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_{12}+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{12}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B_{49}} & = & x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3 & = & ax_{13}\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}} & (4a) & \text{O VII} \\
\mathbf{B_{50}} & = & -x_{13}\,\mathbf{a}_1 - y_{13}\,\mathbf{a}_2 + \left(z_{13}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_{13}\,\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} + c\left(z_{13}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & (4a) & \text{O VII} \\
\mathbf{B_{51}} & = & \left(x_{13}+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_{13}-\frac{1}{2}\right)\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3 & = & a\left(x_{13}+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_{13}-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}} & (4a) & \text{O VII} \\
\mathbf{B_{52}} & = & -\left(x_{13}-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_{13}+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{13}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_{13}-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_{13}+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{13}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & (4a) & \text{O VII} \\
\mathbf{B_{53}} & = & x_{14}\,\mathbf{a}_1 + y_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3 & = & ax_{14}\,\hat{\mathbf{x}} + by_{14}\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}} & (4a) & \text{O VIII} \\
\mathbf{B_{54}} & = & -x_{14}\,\mathbf{a}_1 - y_{14}\,\mathbf{a}_2 + \left(z_{14}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_{14}\,\hat{\mathbf{x}} - by_{14}\,\hat{\mathbf{y}} + c\left(z_{14}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & (4a) & \text{O VIII} \\
\mathbf{B_{55}} & = & \left(x_{14}+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_{14}-\frac{1}{2}\right)\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3 & = & a\left(x_{14}+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_{14}-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}} & (4a) & \text{O VIII} \\
\mathbf{B_{56}} & = & -\left(x_{14}-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_{14}+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{14}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_{14}-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_{14}+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{14}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & (4a) & \text{O VIII}
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\begin{array}{lcccccc}
\mathbf{B_{57}} & = & x_{15}\,\mathbf{a}_1 + y_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3 & = & a x_{15}\,\hat{\mathbf{x}} + b y_{15}\,\hat{\mathbf{y}} + c z_{15}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O IX} \\
\mathbf{B_{58}} & = & -x_{15}\,\mathbf{a}_1 - y_{15}\,\mathbf{a}_2 + \left(z_{15}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a x_{15}\,\hat{\mathbf{x}} - b y_{15}\,\hat{\mathbf{y}} + c\left(z_{15}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O IX} \\
\mathbf{B_{59}} & = & \left(x_{15}+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_{15}-\frac{1}{2}\right)\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3 & = & a\left(x_{15}+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_{15}-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c z_{15}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O IX} \\
\mathbf{B_{60}} & = & -\left(x_{15}-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_{15}+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{15}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_{15}-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_{15}+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{15}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O IX} \\
\mathbf{B_{61}} & = & x_{16}\,\mathbf{a}_1 + y_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3 & = & a x_{16}\,\hat{\mathbf{x}} + b y_{16}\,\hat{\mathbf{y}} + c z_{16}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O X} \\
\mathbf{B_{62}} & = & -x_{16}\,\mathbf{a}_1 - y_{16}\,\mathbf{a}_2 + \left(z_{16}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a x_{16}\,\hat{\mathbf{x}} - b y_{16}\,\hat{\mathbf{y}} + c\left(z_{16}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O X} \\
\mathbf{B_{63}} & = & \left(x_{16}+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_{16}-\frac{1}{2}\right)\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3 & = & a\left(x_{16}+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_{16}-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c z_{16}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O X} \\
\mathbf{B_{64}} & = & -\left(x_{16}-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_{16}+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{16}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_{16}-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_{16}+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{16}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O X} \\
\mathbf{B_{65}} & = & x_{17}\,\mathbf{a}_1 + y_{17}\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3 & = & a x_{17}\,\hat{\mathbf{x}} + b y_{17}\,\hat{\mathbf{y}} + c z_{17}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XI} \\
\mathbf{B_{66}} & = & -x_{17}\,\mathbf{a}_1 - y_{17}\,\mathbf{a}_2 + \left(z_{17}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a x_{17}\,\hat{\mathbf{x}} - b y_{17}\,\hat{\mathbf{y}} + c\left(z_{17}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XI} \\
\mathbf{B_{67}} & = & \left(x_{17}+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_{17}-\frac{1}{2}\right)\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3 & = & a\left(x_{17}+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_{17}-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c z_{17}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XI} \\
\mathbf{B_{68}} & = & -\left(x_{17}-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_{17}+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{17}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_{17}-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_{17}+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{17}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XI} \\
\mathbf{B_{69}} & = & x_{18}\,\mathbf{a}_1 + y_{18}\,\mathbf{a}_2 + z_{18}\,\mathbf{a}_3 & = & a x_{18}\,\hat{\mathbf{x}} + b y_{18}\,\hat{\mathbf{y}} + c z_{18}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XII} \\
\mathbf{B_{70}} & = & -x_{18}\,\mathbf{a}_1 - y_{18}\,\mathbf{a}_2 + \left(z_{18}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a x_{18}\,\hat{\mathbf{x}} - b y_{18}\,\hat{\mathbf{y}} + c\left(z_{18}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XII} \\
\mathbf{B_{71}} & = & \left(x_{18}+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_{18}-\frac{1}{2}\right)\,\mathbf{a}_2 + z_{18}\,\mathbf{a}_3 & = & a\left(x_{18}+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_{18}-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c z_{18}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XII} \\
\mathbf{B_{72}} & = & -\left(x_{18}-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_{18}+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{18}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_{18}-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_{18}+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{18}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XII} \\
\mathbf{B_{73}} & = & x_{19}\,\mathbf{a}_1 + y_{19}\,\mathbf{a}_2 + z_{19}\,\mathbf{a}_3 & = & a x_{19}\,\hat{\mathbf{x}} + b y_{19}\,\hat{\mathbf{y}} + c z_{19}\,\hat{\mathbf{z}} & \text{(4a)} & \text{Si I} \\
\mathbf{B_{74}} & = & -x_{19}\,\mathbf{a}_1 - y_{19}\,\mathbf{a}_2 + \left(z_{19}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a x_{19}\,\hat{\mathbf{x}} - b y_{19}\,\hat{\mathbf{y}} + c\left(z_{19}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{Si I} \\
\mathbf{B_{75}} & = & \left(x_{19}+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_{19}-\frac{1}{2}\right)\,\mathbf{a}_2 + z_{19}\,\mathbf{a}_3 & = & a\left(x_{19}+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_{19}-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c z_{19}\,\hat{\mathbf{z}} & \text{(4a)} & \text{Si I} \\
\mathbf{B_{76}} & = & -\left(x_{19}-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_{19}+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{19}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_{19}-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_{19}+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{19}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{Si I} \\
\mathbf{B_{77}} & = & x_{20}\,\mathbf{a}_1 + y_{20}\,\mathbf{a}_2 + z_{20}\,\mathbf{a}_3 & = & a x_{20}\,\hat{\mathbf{x}} + b y_{20}\,\hat{\mathbf{y}} + c z_{20}\,\hat{\mathbf{z}} & \text{(4a)} & \text{Si II} \\
\mathbf{B_{78}} & = & -x_{20}\,\mathbf{a}_1 - y_{20}\,\mathbf{a}_2 + \left(z_{20}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a x_{20}\,\hat{\mathbf{x}} - b y_{20}\,\hat{\mathbf{y}} + c\left(z_{20}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{Si II} \\
\mathbf{B_{79}} & = & \left(x_{20}+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_{20}-\frac{1}{2}\right)\,\mathbf{a}_2 + z_{20}\,\mathbf{a}_3 & = & a\left(x_{20}+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_{20}-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c z_{20}\,\hat{\mathbf{z}} & \text{(4a)} & \text{Si II} \\
\mathbf{B_{80}} & = & -\left(x_{20}-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_{20}+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{20}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_{20}-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_{20}+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{20}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{Si II} \\
\mathbf{B_{81}} & = & x_{21}\,\mathbf{a}_1 + y_{21}\,\mathbf{a}_2 + z_{21}\,\mathbf{a}_3 & = & a x_{21}\,\hat{\mathbf{x}} + b y_{21}\,\hat{\mathbf{y}} + c z_{21}\,\hat{\mathbf{z}} & \text{(4a)} & \text{Si III} \\
\mathbf{B_{82}} & = & -x_{21}\,\mathbf{a}_1 - y_{21}\,\mathbf{a}_2 + \left(z_{21}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a x_{21}\,\hat{\mathbf{x}} - b y_{21}\,\hat{\mathbf{y}} + c\left(z_{21}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{Si III} \\
\mathbf{B_{83}} & = & \left(x_{21}+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_{21}-\frac{1}{2}\right)\,\mathbf{a}_2 + z_{21}\,\mathbf{a}_3 & = & a\left(x_{21}+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_{21}-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c z_{21}\,\hat{\mathbf{z}} & \text{(4a)} & \text{Si III} \\
\mathbf{B_{84}} & = & -\left(x_{21}-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_{21}+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{21}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_{21}-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_{21}+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{21}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{Si III}
\end{array}
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