Sodium nepheline ($Na_{8-x}Al_{8-x}Si_{8+x}O_{32}$) Structure: A2B3C9D2_hP64_173_bc_2c_6c_bc-001

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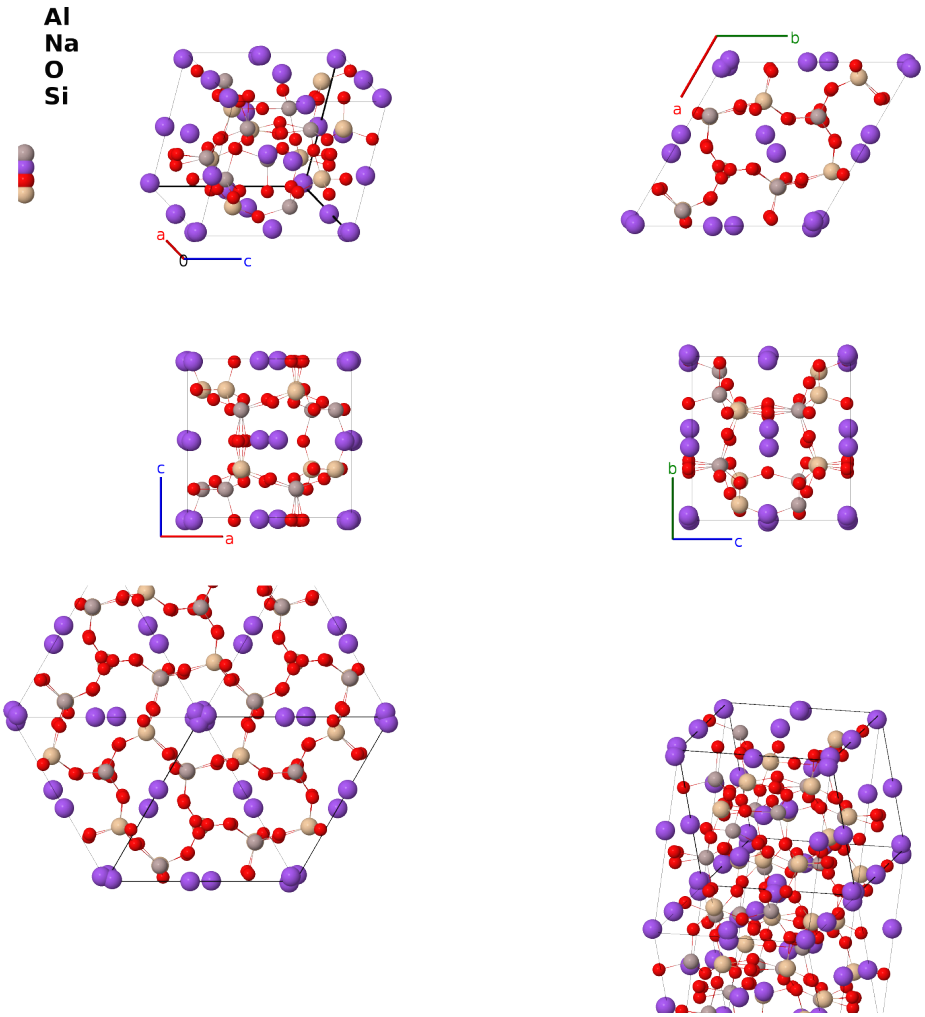
https://aflow.org/prototype-encyclopedia/2KJL

https://aflow.org/prototype-encyclopedia/A2B3C9D2_hP64_173_bc_2c_6c_bc-001



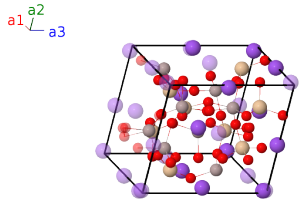
Prototype	$Al_{8-x}Na_{8-x}O_{32}Si_{8+x}$
AFLOW prototype label	A2B3C9D2_hP64_173_bc_2c_6c_bc-001
Mineral name	nepheline
ICSD	65958
CCDC	1628058
Pearson symbol	hP64

Space group number	173
Space group symbol	$P6_3$
AFLOW prototype command	`aflow --proto=A2B3C9D2_hP64_173_bc_2c_6c_bc-001 --params=`$a, c/a, z_1, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}$

- $NaAlSiO_4$ can be found in a variety of structures, depending upon the conditions of its formation.
- Hexagonal forms include:
  - trinepheline and
  - sodium-nepheline (this structure).
- There is considerable disorder in this structure, controlled by the sodium vacancy parameter x, which can take values on the interval [0,2]. Here we use the data from (Hippler, 1989) for what they call $x = 0.8$.
- The Na-II (6c) site has an occupation of 0.185, which actually corresponds to $x = 0.89$. This site can be seen as the doubled sodium atoms at the corner of the unit cell. This could be approximated removing the doublets and placing the sodium atom on a (2b) site.
- The O-I (6c) site is 1/3 occupied. Thus only one of the three oxygen sites in the triplet sites on the crystal is occupied at any time. This could be approximated by removing the triplets and placing an oxygen atom on a (2a) site.
- There is a complete mixture of aluminum and silicon on the (2b) and (2c) sites, with next concentration $Al_{8-x}Si_{8+x}$. For illustrative purposes we arbitrarily designate one (2b) site and one (2c) site to be occupied by each species.

Hexagonal primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(2b)	Al I
$\mathbf{B_2}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Al I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2b)	Si I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Si I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 + y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_3 - y_3)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6c)	Al II
$\mathbf{B_6}$	=	$-y_3\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - 2y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6c)	Al II
$\mathbf{B_7}$	=	$-(x_3 - y_3)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6c)	Al II
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3 + y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_3 - y_3)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Al II
$\mathbf{B_9}$	=	$y_3\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_3 + 2y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Al II
$\mathbf{B_{10}}$	=	$(x_3 - y_3)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Al II

$$
\begin{array}{lcccccl}
\mathbf{B_{11}} & = & x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_4+y_4)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_4-y_4)\;\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}} & \text{(6c)} & \text{Na I} \\
\mathbf{B_{12}} & = & -y_4\,\mathbf{a}_1 + (x_4-y_4)\;\mathbf{a}_2 + z_4\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_4-2y_4)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}} & \text{(6c)} & \text{Na I} \\
\mathbf{B_{13}} & = & -(x_4-y_4)\;\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_4-y_4)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}} & \text{(6c)} & \text{Na I} \\
\mathbf{B_{14}} & = & -x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4+\frac{1}{2}\right)\;\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_4+y_4)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_4-y_4)\;\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\;\hat{\mathbf{z}} & \text{(6c)} & \text{Na I} \\
\mathbf{B_{15}} & = & y_4\,\mathbf{a}_1 - (x_4-y_4)\;\mathbf{a}_2 + \left(z_4+\frac{1}{2}\right)\;\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_4+2y_4)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\;\hat{\mathbf{z}} & \text{(6c)} & \text{Na I} \\
\mathbf{B_{16}} & = & (x_4-y_4)\;\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(z_4+\frac{1}{2}\right)\;\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_4-y_4)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\;\hat{\mathbf{z}} & \text{(6c)} & \text{Na I} \\
\mathbf{B_{17}} & = & x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_5+y_5)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_5-y_5)\;\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}} & \text{(6c)} & \text{Na II} \\
\mathbf{B_{18}} & = & -y_5\,\mathbf{a}_1 + (x_5-y_5)\;\mathbf{a}_2 + z_5\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_5-2y_5)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}} & \text{(6c)} & \text{Na II} \\
\mathbf{B_{19}} & = & -(x_5-y_5)\;\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_5-y_5)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}} & \text{(6c)} & \text{Na II} \\
\mathbf{B_{20}} & = & -x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5+\frac{1}{2}\right)\;\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_5+y_5)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_5-y_5)\;\hat{\mathbf{y}} + c\left(z_5+\frac{1}{2}\right)\;\hat{\mathbf{z}} & \text{(6c)} & \text{Na II} \\
\mathbf{B_{21}} & = & y_5\,\mathbf{a}_1 - (x_5-y_5)\;\mathbf{a}_2 + \left(z_5+\frac{1}{2}\right)\;\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_5+2y_5)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + c\left(z_5+\frac{1}{2}\right)\;\hat{\mathbf{z}} & \text{(6c)} & \text{Na II} \\
\mathbf{B_{22}} & = & (x_5-y_5)\;\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \left(z_5+\frac{1}{2}\right)\;\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_5-y_5)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + c\left(z_5+\frac{1}{2}\right)\;\hat{\mathbf{z}} & \text{(6c)} & \text{Na II} \\
\mathbf{B_{23}} & = & x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_6+y_6)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6-y_6)\;\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} & \text{(6c)} & \text{O I} \\
\mathbf{B_{24}} & = & -y_6\,\mathbf{a}_1 + (x_6-y_6)\;\mathbf{a}_2 + z_6\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_6-2y_6)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} & \text{(6c)} & \text{O I} \\
\mathbf{B_{25}} & = & -(x_6-y_6)\;\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_6-y_6)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} & \text{(6c)} & \text{O I} \\
\mathbf{B_{26}} & = & -x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6+\frac{1}{2}\right)\;\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_6+y_6)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_6-y_6)\;\hat{\mathbf{y}} + c\left(z_6+\frac{1}{2}\right)\;\hat{\mathbf{z}} & \text{(6c)} & \text{O I} \\
\mathbf{B_{27}} & = & y_6\,\mathbf{a}_1 - (x_6-y_6)\;\mathbf{a}_2 + \left(z_6+\frac{1}{2}\right)\;\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_6+2y_6)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + c\left(z_6+\frac{1}{2}\right)\;\hat{\mathbf{z}} & \text{(6c)} & \text{O I} \\
\mathbf{B_{28}} & = & (x_6-y_6)\;\mathbf{a}_1 + x_6\,\mathbf{a}_2 + \left(z_6+\frac{1}{2}\right)\;\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_6-y_6)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + c\left(z_6+\frac{1}{2}\right)\;\hat{\mathbf{z}} & \text{(6c)} & \text{O I} \\
\mathbf{B_{29}} & = & x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_7+y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_7-y_7)\;\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} & \text{(6c)} & \text{O II} \\
\mathbf{B_{30}} & = & -y_7\,\mathbf{a}_1 + (x_7-y_7)\;\mathbf{a}_2 + z_7\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_7-2y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} & \text{(6c)} & \text{O II} \\
\mathbf{B_{31}} & = & -(x_7-y_7)\;\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_7-y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} & \text{(6c)} & \text{O II} \\
\mathbf{B_{32}} & = & -x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7+\frac{1}{2}\right)\;\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_7+y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_7-y_7)\;\hat{\mathbf{y}} + c\left(z_7+\frac{1}{2}\right)\;\hat{\mathbf{z}} & \text{(6c)} & \text{O II} \\
\mathbf{B_{33}} & = & y_7\,\mathbf{a}_1 - (x_7-y_7)\;\mathbf{a}_2 + \left(z_7+\frac{1}{2}\right)\;\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_7+2y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + c\left(z_7+\frac{1}{2}\right)\;\hat{\mathbf{z}} & \text{(6c)} & \text{O II} \\
\mathbf{B_{34}} & = & (x_7-y_7)\;\mathbf{a}_1 + x_7\,\mathbf{a}_2 + \left(z_7+\frac{1}{2}\right)\;\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_7-y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + c\left(z_7+\frac{1}{2}\right)\;\hat{\mathbf{z}} & \text{(6c)} & \text{O II} \\
\mathbf{B_{35}} & = & x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_8+y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_8-y_8)\;\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} & \text{(6c)} & \text{O III} \\
\mathbf{B_{36}} & = & -y_8\,\mathbf{a}_1 + (x_8-y_8)\;\mathbf{a}_2 + z_8\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_8-2y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} & \text{(6c)} & \text{O III} \\
\mathbf{B_{37}} & = & -(x_8-y_8)\;\mathbf{a}_1 - x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_8-y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} & \text{(6c)} & \text{O III} \\
\mathbf{B_{38}} & = & -x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + \left(z_8+\frac{1}{2}\right)\;\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_8+y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_8-y_8)\;\hat{\mathbf{y}} + c\left(z_8+\frac{1}{2}\right)\;\hat{\mathbf{z}} & \text{(6c)} & \text{O III} \\
\mathbf{B_{39}} & = & y_8\,\mathbf{a}_1 - (x_8-y_8)\;\mathbf{a}_2 + \left(z_8+\frac{1}{2}\right)\;\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_8+2y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + c\left(z_8+\frac{1}{2}\right)\;\hat{\mathbf{z}} & \text{(6c)} & \text{O III} \\
\mathbf{B_{40}} & = & (x_8-y_8)\;\mathbf{a}_1 + x_8\,\mathbf{a}_2 + \left(z_8+\frac{1}{2}\right)\;\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_8-y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} + c\left(z_8+\frac{1}{2}\right)\;\hat{\mathbf{z}} & \text{(6c)} & \text{O III} \\
\mathbf{B_{41}} & = & x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_9+y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_9-y_9)\;\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} & \text{(6c)} & \text{O IV} \\
\mathbf{B_{42}} & = & -y_9\,\mathbf{a}_1 + (x_9-y_9)\;\mathbf{a}_2 + z_9\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_9-2y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} & \text{(6c)} & \text{O IV} \\
\mathbf{B_{43}} & = & -(x_9-y_9)\;\mathbf{a}_1 - x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_9-y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} & \text{(6c)} & \text{O IV} \\
\mathbf{B_{44}} & = & -x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + \left(z_9+\frac{1}{2}\right)\;\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_9+y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_9-y_9)\;\hat{\mathbf{y}} + c\left(z_9+\frac{1}{2}\right)\;\hat{\mathbf{z}} & \text{(6c)} & \text{O IV} \\
\mathbf{B_{45}} & = & y_9\,\mathbf{a}_1 - (x_9-y_9)\;\mathbf{a}_2 + \left(z_9+\frac{1}{2}\right)\;\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_9+2y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + c\left(z_9+\frac{1}{2}\right)\;\hat{\mathbf{z}} & \text{(6c)} & \text{O IV} \\
\mathbf{B_{46}} & = & (x_9-y_9)\;\mathbf{a}_1 + x_9\,\mathbf{a}_2 + \left(z_9+\frac{1}{2}\right)\;\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_9-y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}} + c\left(z_9+\frac{1}{2}\right)\;\hat{\mathbf{z}} & \text{(6c)} & \text{O IV}
\end{array}
$$

$$\mathbf{B_{47}} = x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{10}+y_{10})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{10}-y_{10})\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$$ (6c) O V

$$\mathbf{B_{48}} = -y_{10}\,\mathbf{a}_1 + (x_{10}-y_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{10}-2y_{10})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$$ (6c) O V

$$\mathbf{B_{49}} = -(x_{10}-y_{10})\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{10}-y_{10})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$$ (6c) O V

$$\mathbf{B_{50}} = -x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 + \left(z_{10}+\tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{10}+y_{10})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_{10}-y_{10})\,\hat{\mathbf{y}} + c\left(z_{10}+\tfrac{1}{2}\right)\hat{\mathbf{z}}$$ (6c) O V

$$\mathbf{B_{51}} = y_{10}\,\mathbf{a}_1 - (x_{10}-y_{10})\,\mathbf{a}_2 + \left(z_{10}+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_{10}+2y_{10})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + c\left(z_{10}+\tfrac{1}{2}\right)\hat{\mathbf{z}}$$ (6c) O V

$$\mathbf{B_{52}} = (x_{10}-y_{10})\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + \left(z_{10}+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_{10}-y_{10})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_{10}\,\hat{\mathbf{y}} + c\left(z_{10}+\tfrac{1}{2}\right)\hat{\mathbf{z}}$$ (6c) O V

$$\mathbf{B_{53}} = x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{11}+y_{11})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{11}-y_{11})\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$$ (6c) O VI

$$\mathbf{B_{54}} = -y_{11}\,\mathbf{a}_1 + (x_{11}-y_{11})\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{11}-2y_{11})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$$ (6c) O VI

$$\mathbf{B_{55}} = -(x_{11}-y_{11})\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{11}-y_{11})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$$ (6c) O VI

$$\mathbf{B_{56}} = -x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 + \left(z_{11}+\tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{11}+y_{11})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_{11}-y_{11})\,\hat{\mathbf{y}} + c\left(z_{11}+\tfrac{1}{2}\right)\hat{\mathbf{z}}$$ (6c) O VI

$$\mathbf{B_{57}} = y_{11}\,\mathbf{a}_1 - (x_{11}-y_{11})\,\mathbf{a}_2 + \left(z_{11}+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_{11}+2y_{11})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{11}\,\hat{\mathbf{y}} + c\left(z_{11}+\tfrac{1}{2}\right)\hat{\mathbf{z}}$$ (6c) O VI

$$\mathbf{B_{58}} = (x_{11}-y_{11})\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + \left(z_{11}+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_{11}-y_{11})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_{11}\,\hat{\mathbf{y}} + c\left(z_{11}+\tfrac{1}{2}\right)\hat{\mathbf{z}}$$ (6c) O VI

$$\mathbf{B_{59}} = x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{12}+y_{12})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{12}-y_{12})\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$$ (6c) Si II

$$\mathbf{B_{60}} = -y_{12}\,\mathbf{a}_1 + (x_{12}-y_{12})\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{12}-2y_{12})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$$ (6c) Si II

$$\mathbf{B_{61}} = -(x_{12}-y_{12})\,\mathbf{a}_1 - x_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{12}-y_{12})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$$ (6c) Si II

$$\mathbf{B_{62}} = -x_{12}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 + \left(z_{12}+\tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{12}+y_{12})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_{12}-y_{12})\,\hat{\mathbf{y}} + c\left(z_{12}+\tfrac{1}{2}\right)\hat{\mathbf{z}}$$ (6c) Si II

$$\mathbf{B_{63}} = y_{12}\,\mathbf{a}_1 - (x_{12}-y_{12})\,\mathbf{a}_2 + \left(z_{12}+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_{12}+2y_{12})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{12}\,\hat{\mathbf{y}} + c\left(z_{12}+\tfrac{1}{2}\right)\hat{\mathbf{z}}$$ (6c) Si II

$$\mathbf{B_{64}} = (x_{12}-y_{12})\,\mathbf{a}_1 + x_{12}\,\mathbf{a}_2 + \left(z_{12}+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_{12}-y_{12})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_{12}\,\hat{\mathbf{y}} + c\left(z_{12}+\tfrac{1}{2}\right)\hat{\mathbf{z}}$$ (6c) Si II

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