Chabazite ($Ca_{1.4}Sr_{0.3}Al_{3.8}Si_{8.3}O_{24}{\cdot}13H_2O$, $S3_4$ (I)) Structure: A5B21C24D12_hR62_166_a2c_ehi_fg2h_i-001

This structure previously used the label(s) `A5B21C24D12_hR62_166_a2c_ehi_fg2h_i`. Calls to these addresses will be redirected here.

Cite this page as:

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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.

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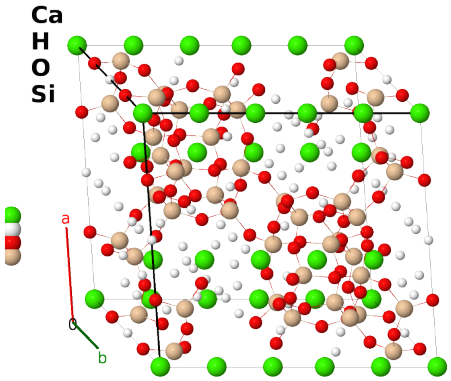
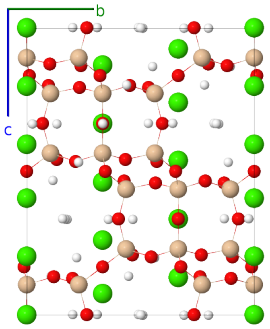
https://aflow.org/prototype-encyclopedia/2K92

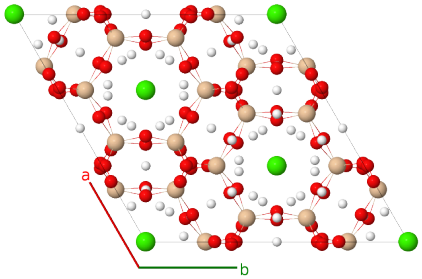
https://aflow.org/prototype-encyclopedia/A5B21C24D12_hR62_166_a2c_ehi_fg2h_i-001

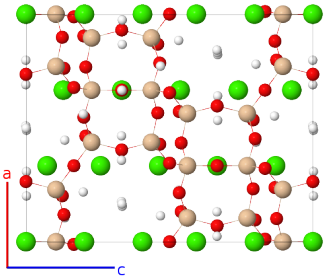
Prototype	$Al_{3.8}Ca_{1.4}H_{26}O_{37}Si_{8.3}Sr_{0.3}$
AFLOW prototype label	A5B21C24D12_hR62_166_a2c_ehi_fg2h_i-001
***Strukturbericht* designation**	$S3_4$(I)
Mineral name	chabazite
ICSD	32553
CCDC	1606019
Pearson symbol	hR62
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A5B21C24D12_hR62_166_a2c_ehi_fg2h_i-001 --params=`$a, c/a, x_2, x_3, x_5, x_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}$

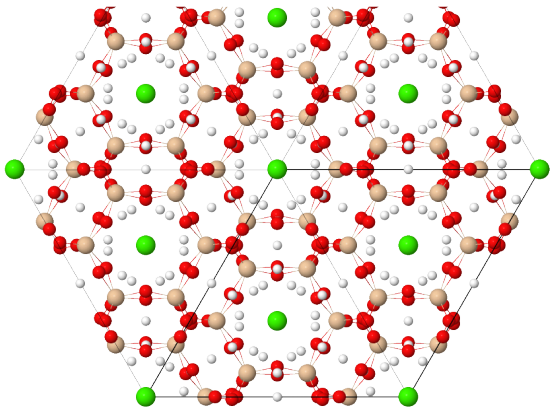
- The structure given here, from (Calligaris, 1982), has substantially the same Wyckoff positions as the structure designated $S3_4$ by (Gottfried, 1937). The largest change is the splitting of the calcium site from one stoichiometric (2c) site to three partially filled sites, one (1a) and two (2c).
- (Calligaris, 1982) did not give the exact positions of the water molecules, so we use the positions given by (Downs, 2003). However, this leaves us with only 7.7 water molecules per formula unit, rather than the 13 claimed by (Calligaris, 1982).
- Only the oxygen sites are fully occupied. For the remaining sites, according to (Downs, 2003),
  - The (1a) site is 9.06% Ca and 1.94% Sr, with the remaining sites vacant.
  - The first (2c) site is 43.65% Ca and 9.35% Sr.
  - The second (2c) site is 19.76% Ca and 4.24% Sr.
  - The (3e) H_2O site is only occupied by a water molecule 50% of the time.
  - The (6h) H_2O site is only occupied 57% of the time.
  - The (12h) H_2O site is only occupied 23% of the time.
  - The remaining (12h) site is 69% Si and 31% Al.
- (Gottfried, 1937) gave chabazite the *Strukturbericht* designation $S3_4$. However, (Gottfried, 1940) designated catapleiite, $Na_2ZrSi_3O_9{\cdot}2H_2O$ as *Strukturbericht* $S3_4$. We distinguish between the two cases by using $S3_4$(I) to designate chabazite and $S3_4$(II) to designate catapleiite.

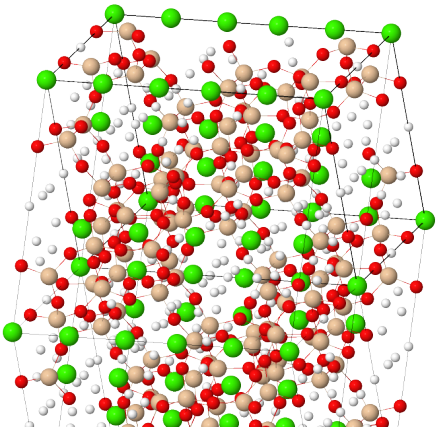

Ca
H
O
Si
a
c
b


b
c


a
b

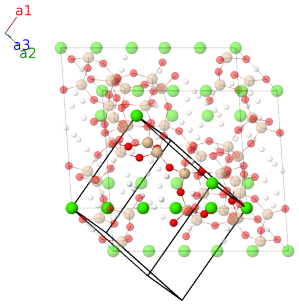

a
c





Rhombohedral primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Ca I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(2c)	Ca II
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(2c)	Ca II
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	Ca III
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	Ca III
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$	(3e)	H I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$	(3e)	H I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$	(3e)	H I
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2$	=	$\frac{1}{2}ax_5\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}$	(6f)	O I
$\mathbf{B_{10}}$	=	$x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$\frac{1}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}$	(6f)	O I
$\mathbf{B_{11}}$	=	$-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}$	(6f)	O I
$\mathbf{B_{12}}$	=	$-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2$	=	$-\frac{1}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}$	(6f)	O I
$\mathbf{B_{13}}$	=	$-x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_5\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}$	(6f)	O I
$\mathbf{B_{14}}$	=	$x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}$	(6f)	O I
$\mathbf{B_{15}}$	=	$x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,(2x_6 - 1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a\,(6x_6 + 1)\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{16}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$\frac{1}{4}a\,(2x_6 + 1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a\,(6x_6 - 1)\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{17}}$	=	$-x_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{18}}$	=	$-x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,(2x_6 + 1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a\,(6x_6 - 1)\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{19}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,(2x_6 - 1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a\,(6x_6 + 1)\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{20}}$	=	$x_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{21}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_7 - z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	H II
$\mathbf{B_{22}}$	=	$z_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_7 - z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	H II
$\mathbf{B_{23}}$	=	$x_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_7 - z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	H II
$\mathbf{B_{24}}$	=	$-z_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_7 - z_7)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	H II
$\mathbf{B_{25}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_7 - z_7)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	H II

$\mathbf{B_{26}}$	$=$	$-x_7\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	$=$	$\frac{1}{\sqrt{3}}a\,(x_7 - z_7)\;\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_7 + z_7)\;\hat{\mathbf{z}}$	(6h)	H II
$\mathbf{B_{27}}$	$=$	$x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_8 - z_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_8 - z_8)\;\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_8 + z_8)\;\hat{\mathbf{z}}$	(6h)	O III
$\mathbf{B_{28}}$	$=$	$z_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_8 - z_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_8 - z_8)\;\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_8 + z_8)\;\hat{\mathbf{z}}$	(6h)	O III
$\mathbf{B_{29}}$	$=$	$x_8\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a\,(x_8 - z_8)\;\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_8 + z_8)\;\hat{\mathbf{z}}$	(6h)	O III
$\mathbf{B_{30}}$	$=$	$-z_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_8 - z_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_8 - z_8)\;\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_8 + z_8)\;\hat{\mathbf{z}}$	(6h)	O III
$\mathbf{B_{31}}$	$=$	$-x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_8 - z_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_8 - z_8)\;\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_8 + z_8)\;\hat{\mathbf{z}}$	(6h)	O III
$\mathbf{B_{32}}$	$=$	$-x_8\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3$	$=$	$\frac{1}{\sqrt{3}}a\,(x_8 - z_8)\;\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_8 + z_8)\;\hat{\mathbf{z}}$	(6h)	O III
$\mathbf{B_{33}}$	$=$	$x_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_9 - z_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_9 - z_9)\;\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_9 + z_9)\;\hat{\mathbf{z}}$	(6h)	O IV
$\mathbf{B_{34}}$	$=$	$z_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + x_9\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_9 - z_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_9 - z_9)\;\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_9 + z_9)\;\hat{\mathbf{z}}$	(6h)	O IV
$\mathbf{B_{35}}$	$=$	$x_9\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 + x_9\,\mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a\,(x_9 - z_9)\;\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_9 + z_9)\;\hat{\mathbf{z}}$	(6h)	O IV
$\mathbf{B_{36}}$	$=$	$-z_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 - x_9\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_9 - z_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_9 - z_9)\;\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_9 + z_9)\;\hat{\mathbf{z}}$	(6h)	O IV
$\mathbf{B_{37}}$	$=$	$-x_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_9 - z_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_9 - z_9)\;\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_9 + z_9)\;\hat{\mathbf{z}}$	(6h)	O IV
$\mathbf{B_{38}}$	$=$	$-x_9\,\mathbf{a}_1 - z_9\,\mathbf{a}_2 - x_9\,\mathbf{a}_3$	$=$	$\frac{1}{\sqrt{3}}a\,(x_9 - z_9)\;\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_9 + z_9)\;\hat{\mathbf{z}}$	(6h)	O IV
$\mathbf{B_{39}}$	$=$	$x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_{10} - z_{10})\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_{10} - 2y_{10} + z_{10})\;\hat{\mathbf{y}} + \frac{1}{3}c\,(x_{10} + y_{10} + z_{10})\;\hat{\mathbf{z}}$	(12i)	H III
$\mathbf{B_{40}}$	$=$	$z_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + y_{10}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(y_{10} - z_{10})\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_{10} - y_{10} - z_{10})\;\hat{\mathbf{y}} + \frac{1}{3}c\,(x_{10} + y_{10} + z_{10})\;\hat{\mathbf{z}}$	(12i)	H III
$\mathbf{B_{41}}$	$=$	$y_{10}\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_2 + x_{10}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_{10} - y_{10})\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_{10} + y_{10} - 2z_{10})\;\hat{\mathbf{y}} + \frac{1}{3}c\,(x_{10} + y_{10} + z_{10})\;\hat{\mathbf{z}}$	(12i)	H III
$\mathbf{B_{42}}$	$=$	$-z_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 - x_{10}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_{10} - z_{10})\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_{10} - 2y_{10} + z_{10})\;\hat{\mathbf{y}} - \frac{1}{3}c\,(x_{10} + y_{10} + z_{10})\;\hat{\mathbf{z}}$	(12i)	H III
$\mathbf{B_{43}}$	$=$	$-y_{10}\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(y_{10} - z_{10})\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_{10} - y_{10} - z_{10})\;\hat{\mathbf{y}} - \frac{1}{3}c\,(x_{10} + y_{10} + z_{10})\;\hat{\mathbf{z}}$	(12i)	H III
$\mathbf{B_{44}}$	$=$	$-x_{10}\,\mathbf{a}_1 - z_{10}\,\mathbf{a}_2 - y_{10}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_{10} - y_{10})\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_{10} + y_{10} - 2z_{10})\;\hat{\mathbf{y}} - \frac{1}{3}c\,(x_{10} + y_{10} + z_{10})\;\hat{\mathbf{z}}$	(12i)	H III
$\mathbf{B_{45}}$	$=$	$-x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_{10} - z_{10})\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_{10} - 2y_{10} + z_{10})\;\hat{\mathbf{y}} - \frac{1}{3}c\,(x_{10} + y_{10} + z_{10})\;\hat{\mathbf{z}}$	(12i)	H III
$\mathbf{B_{46}}$	$=$	$-z_{10}\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 - y_{10}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(y_{10} - z_{10})\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_{10} - y_{10} - z_{10})\;\hat{\mathbf{y}} - \frac{1}{3}c\,(x_{10} + y_{10} + z_{10})\;\hat{\mathbf{z}}$	(12i)	H III

$$\mathbf{B_{47}} = -y_{10}\,\mathbf{a}_1 - z_{10}\,\mathbf{a}_2 - x_{10}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{10}-y_{10})\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_{10}+y_{10}-2z_{10})\;\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_{10}+y_{10}+z_{10})\;\hat{\mathbf{z}} \quad (12\text{i}) \quad \text{H III}$$

$$\mathbf{B_{48}} = z_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + x_{10}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{10}-z_{10})\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_{10}-2y_{10}+z_{10})\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{10}+y_{10}+z_{10})\;\hat{\mathbf{z}} \quad (12\text{i}) \quad \text{H III}$$

$$\mathbf{B_{49}} = y_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(y_{10}-z_{10})\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_{10}-y_{10}-z_{10})\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{10}+y_{10}+z_{10})\;\hat{\mathbf{z}} \quad (12\text{i}) \quad \text{H III}$$

$$\mathbf{B_{50}} = x_{10}\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_2 + y_{10}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{10}-y_{10})\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_{10}+y_{10}-2z_{10})\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{10}+y_{10}+z_{10})\;\hat{\mathbf{z}} \quad (12\text{i}) \quad \text{H III}$$

$$\mathbf{B_{51}} = x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{11}-z_{11})\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_{11}-2y_{11}+z_{11})\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{11}+y_{11}+z_{11})\;\hat{\mathbf{z}} \quad (12\text{i}) \quad \text{Si I}$$

$$\mathbf{B_{52}} = z_{11}\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + y_{11}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_{11}-z_{11})\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_{11}-y_{11}-z_{11})\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{11}+y_{11}+z_{11})\;\hat{\mathbf{z}} \quad (12\text{i}) \quad \text{Si I}$$

$$\mathbf{B_{53}} = y_{11}\,\mathbf{a}_1 + z_{11}\,\mathbf{a}_2 + x_{11}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{11}-y_{11})\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_{11}+y_{11}-2z_{11})\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{11}+y_{11}+z_{11})\;\hat{\mathbf{z}} \quad (12\text{i}) \quad \text{Si I}$$

$$\mathbf{B_{54}} = -z_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 - x_{11}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{11}-z_{11})\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_{11}-2y_{11}+z_{11})\;\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_{11}+y_{11}+z_{11})\;\hat{\mathbf{z}} \quad (12\text{i}) \quad \text{Si I}$$

$$\mathbf{B_{55}} = -y_{11}\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_{11}-z_{11})\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(2x_{11}-y_{11}-z_{11})\;\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_{11}+y_{11}+z_{11})\;\hat{\mathbf{z}} \quad (12\text{i}) \quad \text{Si I}$$

$$\mathbf{B_{56}} = -x_{11}\,\mathbf{a}_1 - z_{11}\,\mathbf{a}_2 - y_{11}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{11}-y_{11})\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_{11}+y_{11}-2z_{11})\;\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_{11}+y_{11}+z_{11})\;\hat{\mathbf{z}} \quad (12\text{i}) \quad \text{Si I}$$

$$\mathbf{B_{57}} = -x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{11}-z_{11})\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_{11}-2y_{11}+z_{11})\;\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_{11}+y_{11}+z_{11})\;\hat{\mathbf{z}} \quad (12\text{i}) \quad \text{Si I}$$

$$\mathbf{B_{58}} = -z_{11}\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 - y_{11}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(y_{11}-z_{11})\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(2x_{11}-y_{11}-z_{11})\;\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_{11}+y_{11}+z_{11})\;\hat{\mathbf{z}} \quad (12\text{i}) \quad \text{Si I}$$

$$\mathbf{B_{59}} = -y_{11}\,\mathbf{a}_1 - z_{11}\,\mathbf{a}_2 - x_{11}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{11}-y_{11})\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_{11}+y_{11}-2z_{11})\;\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_{11}+y_{11}+z_{11})\;\hat{\mathbf{z}} \quad (12\text{i}) \quad \text{Si I}$$

$$\mathbf{B_{60}} = z_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + x_{11}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{11}-z_{11})\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_{11}-2y_{11}+z_{11})\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{11}+y_{11}+z_{11})\;\hat{\mathbf{z}} \quad (12\text{i}) \quad \text{Si I}$$

$$\mathbf{B_{61}} = y_{11}\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(y_{11}-z_{11})\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_{11}-y_{11}-z_{11})\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{11}+y_{11}+z_{11})\;\hat{\mathbf{z}} \quad (12\text{i}) \quad \text{Si I}$$

$$\mathbf{B_{62}} = x_{11}\,\mathbf{a}_1 + z_{11}\,\mathbf{a}_2 + y_{11}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{11}-y_{11})\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_{11}+y_{11}-2z_{11})\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{11}+y_{11}+z_{11})\;\hat{\mathbf{z}} \quad (12\text{i}) \quad \text{Si I}$$

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