Mayenite (12 $CaO{\cdot}7Al_2O_3$, $K7_4$, C12A7) Structure: A7B12C19_cI152_220_ac_2d_bce-001

This structure originally had the label `A7B12C19_cI152_220_bc_2d_ace`. Calls to that address will be redirected here.

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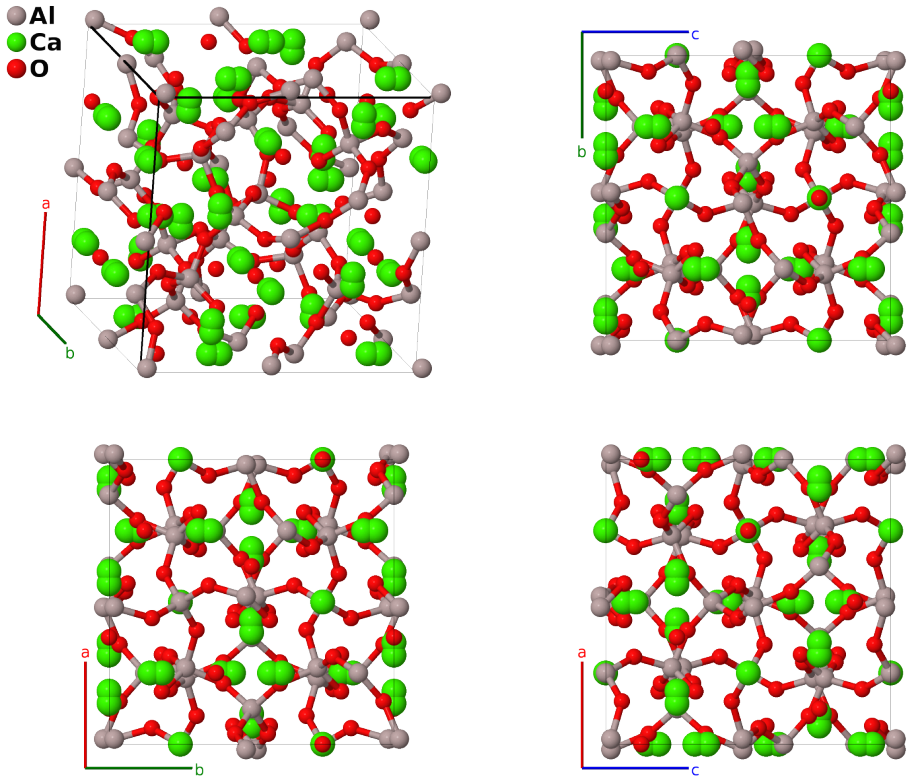
https://aflow.org/p/L8NP

https://aflow.org/p/A7B12C19_cI152_220_ac_2d_bce-001

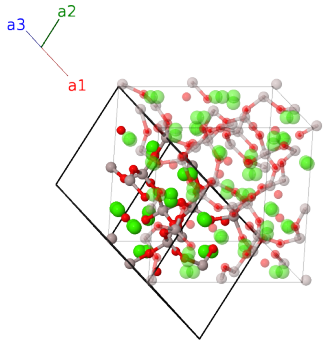


Prototype	$Al_{14}Ca_{12}O_{33}$
AFLOW prototype label	A7B12C19_cI152_220_ac_2d_bce-001
***Strukturbericht* designation**	$K7_4$
Mineral name	mayenite
ICSD	24100
Pearson symbol	cI152
Space group number	220
Space group symbol	$I\bar{4}3d$
AFLOW prototype command	`aflow --proto=A7B12C19_cI152_220_ac_2d_bce-001 --params=`$a, x_3, x_4, x_5, x_6, x_7, y_7, z_7$

- We present the structure determined by (Boysen, 2007) with data taken at 293K. This slightly differs from the original determination of (Büssem, 1936), which was given the $K7_4$ designation by (Gottfried, 1938). In the original work, the calcium atoms were thought to be located at a single (24d) site. Newer findings show that calcium is split between two (24d) sites, with the site we have labeled Ca-I having 87.5% of the atoms and Ca-II the remainder, although presumably only one of the two sites is occupied in any pair.
- All studies show that the O-I (12a) site is only partially occupied: if this is occupied 1/6 of the time we get the proper stoichiometry, though (Boysen, 2007) found the occupation was 0.251 at 293K, dropping as the temperature decreased.
- This structure is often referred to in the literature as C12A7 to distinguish it from other CaO/Al_2O_3 compounds.

Body-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \frac{3}{8}\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(12a)	Al I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(12a)	Al I
$\mathbf{B_3}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{5}{8}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}}$	(12a)	Al I
$\mathbf{B_4}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}}$	(12a)	Al I
$\mathbf{B_5}$	=	$\frac{5}{8}\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(12a)	Al I
$\mathbf{B_6}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(12a)	Al I
$\mathbf{B_7}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - \frac{1}{4}a\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_8}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 + \frac{5}{8}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_9}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{10}}$	=	$\frac{5}{8}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{8}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{11}}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{12}}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{13}}$	=	$2x_3\,\mathbf{a}_1 + 2x_3\,\mathbf{a}_2 + 2x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(16c)	Al II
$\mathbf{B_{14}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(2x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(16c)	Al II
$\mathbf{B_{15}}$	=	$-\left(2x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(16c)	Al II
$\mathbf{B_{16}}$	=	$-\left(2x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16c)	Al II
$\mathbf{B_{17}}$	=	$\left(2x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(2x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(2x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	Al II
$\mathbf{B_{18}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - 2x_3\,\mathbf{a}_3$	=	$-a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	Al II
$\mathbf{B_{19}}$	=	$-2x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	Al II

$\mathbf{B_{20}}$	$=$	$-2x_3\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	$=$	$-a\left(x_3-\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	Al II
$\mathbf{B_{21}}$	$=$	$2x_4\,\mathbf{a}_1+2x_4\,\mathbf{a}_2+2x_4\,\mathbf{a}_3$	$=$	$ax_4\,\hat{\mathbf{x}}+ax_4\,\hat{\mathbf{y}}+ax_4\,\hat{\mathbf{z}}$	(16c)	O II
$\mathbf{B_{22}}$	$=$	$\frac{1}{2}\,\mathbf{a}_1-\left(2x_4-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ax_4\,\hat{\mathbf{x}}-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{y}}+ax_4\,\hat{\mathbf{z}}$	(16c)	O II
$\mathbf{B_{23}}$	$=$	$-\left(2x_4-\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	$=$	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}}+ax_4\,\hat{\mathbf{y}}-ax_4\,\hat{\mathbf{z}}$	(16c)	O II
$\mathbf{B_{24}}$	$=$	$-\left(2x_4-\frac{1}{2}\right)\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2$	$=$	$ax_4\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16c)	O II
$\mathbf{B_{25}}$	$=$	$\left(2x_4+\frac{1}{2}\right)\,\mathbf{a}_1+\left(2x_4+\frac{1}{2}\right)\,\mathbf{a}_2+\left(2x_4+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	O II
$\mathbf{B_{26}}$	$=$	$\frac{1}{2}\,\mathbf{a}_1-2x_4\,\mathbf{a}_3$	$=$	$-a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(x_4-\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	O II
$\mathbf{B_{27}}$	$=$	$-2x_4\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2$	$=$	$a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(x_4-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	O II
$\mathbf{B_{28}}$	$=$	$-2x_4\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	$=$	$-a\left(x_4-\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	O II
$\mathbf{B_{29}}$	$=$	$\frac{1}{4}\,\mathbf{a}_1+\left(x_5+\frac{1}{4}\right)\,\mathbf{a}_2+x_5\,\mathbf{a}_3$	$=$	$ax_5\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Ca I
$\mathbf{B_{30}}$	$=$	$\frac{3}{4}\,\mathbf{a}_1-\left(x_5-\frac{1}{4}\right)\,\mathbf{a}_2-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ax_5\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}+\frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Ca I
$\mathbf{B_{31}}$	$=$	$x_5\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2+\left(x_5+\frac{1}{4}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}$	(24d)	Ca I
$\mathbf{B_{32}}$	$=$	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2-\left(x_5-\frac{1}{4}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}+\frac{1}{2}a\,\hat{\mathbf{z}}$	(24d)	Ca I
$\mathbf{B_{33}}$	$=$	$\left(x_5+\frac{1}{4}\right)\,\mathbf{a}_1+x_5\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\hat{\mathbf{y}}+ax_5\,\hat{\mathbf{z}}$	(24d)	Ca I
$\mathbf{B_{34}}$	$=$	$-\left(x_5-\frac{1}{4}\right)\,\mathbf{a}_1-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}-ax_5\,\hat{\mathbf{z}}$	(24d)	Ca I
$\mathbf{B_{35}}$	$=$	$\left(x_5+\frac{3}{4}\right)\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2+\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\hat{\mathbf{x}}+a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{1}{2}a\,\hat{\mathbf{z}}$	(24d)	Ca I
$\mathbf{B_{36}}$	$=$	$-\left(x_5-\frac{3}{4}\right)\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2-x_5\,\mathbf{a}_3$	$=$	$-\frac{1}{4}a\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{1}{2}a\,\hat{\mathbf{z}}$	(24d)	Ca I
$\mathbf{B_{37}}$	$=$	$\frac{3}{4}\,\mathbf{a}_1+\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_5+\frac{3}{4}\right)\,\mathbf{a}_3$	$=$	$a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}+\frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Ca I
$\mathbf{B_{38}}$	$=$	$\frac{1}{4}\,\mathbf{a}_1-x_5\,\mathbf{a}_2-\left(x_5-\frac{3}{4}\right)\,\mathbf{a}_3$	$=$	$-a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}-\frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Ca I
$\mathbf{B_{39}}$	$=$	$\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_5+\frac{3}{4}\right)\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}+a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(24d)	Ca I
$\mathbf{B_{40}}$	$=$	$-x_5\,\mathbf{a}_1-\left(x_5-\frac{3}{4}\right)\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{1}{4}a\,\hat{\mathbf{y}}-a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(24d)	Ca I
$\mathbf{B_{41}}$	$=$	$\frac{1}{4}\,\mathbf{a}_1+\left(x_6+\frac{1}{4}\right)\,\mathbf{a}_2+x_6\,\mathbf{a}_3$	$=$	$ax_6\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Ca II
$\mathbf{B_{42}}$	$=$	$\frac{3}{4}\,\mathbf{a}_1-\left(x_6-\frac{1}{4}\right)\,\mathbf{a}_2-\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ax_6\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}+\frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Ca II
$\mathbf{B_{43}}$	$=$	$x_6\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2+\left(x_6+\frac{1}{4}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\hat{\mathbf{x}}+ax_6\,\hat{\mathbf{y}}$	(24d)	Ca II
$\mathbf{B_{44}}$	$=$	$-\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2-\left(x_6-\frac{1}{4}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\hat{\mathbf{x}}-ax_6\,\hat{\mathbf{y}}+\frac{1}{2}a\,\hat{\mathbf{z}}$	(24d)	Ca II
$\mathbf{B_{45}}$	$=$	$\left(x_6+\frac{1}{4}\right)\,\mathbf{a}_1+x_6\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\hat{\mathbf{y}}+ax_6\,\hat{\mathbf{z}}$	(24d)	Ca II
$\mathbf{B_{46}}$	$=$	$-\left(x_6-\frac{1}{4}\right)\,\mathbf{a}_1-\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}-ax_6\,\hat{\mathbf{z}}$	(24d)	Ca II
$\mathbf{B_{47}}$	$=$	$\left(x_6+\frac{3}{4}\right)\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2+\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\hat{\mathbf{x}}+a\left(x_6+\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{1}{2}a\,\hat{\mathbf{z}}$	(24d)	Ca II
$\mathbf{B_{48}}$	$=$	$-\left(x_6-\frac{3}{4}\right)\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2-x_6\,\mathbf{a}_3$	$=$	$-\frac{1}{4}a\,\hat{\mathbf{x}}-a\left(x_6-\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{1}{2}a\,\hat{\mathbf{z}}$	(24d)	Ca II
$\mathbf{B_{49}}$	$=$	$\frac{3}{4}\,\mathbf{a}_1+\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_6+\frac{3}{4}\right)\,\mathbf{a}_3$	$=$	$a\left(x_6+\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}+\frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Ca II
$\mathbf{B_{50}}$	$=$	$\frac{1}{4}\,\mathbf{a}_1-x_6\,\mathbf{a}_2-\left(x_6-\frac{3}{4}\right)\,\mathbf{a}_3$	$=$	$-a\left(x_6-\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}-\frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Ca II
$\mathbf{B_{51}}$	$=$	$\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_6+\frac{3}{4}\right)\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}+a\left(x_6+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(24d)	Ca II
$\mathbf{B_{52}}$	$=$	$-x_6\,\mathbf{a}_1-\left(x_6-\frac{3}{4}\right)\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{1}{4}a\,\hat{\mathbf{y}}-a\left(x_6-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(24d)	Ca II
$\mathbf{B_{53}}$	$=$	$(y_7+z_7)\,\mathbf{a}_1+(x_7+z_7)\,\mathbf{a}_2+(x_7+y_7)\,\mathbf{a}_3$	$=$	$ax_7\,\hat{\mathbf{x}}+ay_7\,\hat{\mathbf{y}}+az_7\,\hat{\mathbf{z}}$	(48e)	O III

$$\mathbf{B_{54}} = \begin{array}{c}\left(-y_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_1- \\ (x_7-z_7)\,\mathbf{a}_2-\left(x_7+y_7-\frac{1}{2}\right)\,\mathbf{a}_3\end{array} = -ax_7\,\hat{\mathbf{x}}-a\left(y_7-\tfrac{1}{2}\right)\,\hat{\mathbf{y}}+az_7\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$$\mathbf{B_{55}} = \begin{array}{c}(y_7-z_7)\,\mathbf{a}_1-\left(x_7+z_7-\frac{1}{2}\right)\,\mathbf{a}_2+ \\ \left(-x_7+y_7+\frac{1}{2}\right)\,\mathbf{a}_3\end{array} = -a\left(x_7-\tfrac{1}{2}\right)\,\hat{\mathbf{x}}+ay_7\,\hat{\mathbf{y}}-az_7\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$$\mathbf{B_{56}} = \begin{array}{c}-\left(y_7+z_7-\frac{1}{2}\right)\,\mathbf{a}_1+ \\ \left(x_7-z_7+\frac{1}{2}\right)\,\mathbf{a}_2+(x_7-y_7)\,\mathbf{a}_3\end{array} = ax_7\,\hat{\mathbf{x}}-ay_7\,\hat{\mathbf{y}}-a\left(z_7-\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$$\mathbf{B_{57}} = \begin{array}{c}(x_7+y_7)\,\mathbf{a}_1+(y_7+z_7)\,\mathbf{a}_2+ \\ (x_7+z_7)\,\mathbf{a}_3\end{array} = az_7\,\hat{\mathbf{x}}+ax_7\,\hat{\mathbf{y}}+ay_7\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$$\mathbf{B_{58}} = \begin{array}{c}-\left(x_7+y_7-\frac{1}{2}\right)\,\mathbf{a}_1+ \\ \left(-y_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_2-(x_7-z_7)\,\mathbf{a}_3\end{array} = az_7\,\hat{\mathbf{x}}-ax_7\,\hat{\mathbf{y}}-a\left(y_7-\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$$\mathbf{B_{59}} = \begin{array}{c}\left(-x_7+y_7+\frac{1}{2}\right)\,\mathbf{a}_1+ \\ (y_7-z_7)\,\mathbf{a}_2-\left(x_7+z_7-\frac{1}{2}\right)\,\mathbf{a}_3\end{array} = -az_7\,\hat{\mathbf{x}}-a\left(x_7-\tfrac{1}{2}\right)\,\hat{\mathbf{y}}+ay_7\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$$\mathbf{B_{60}} = \begin{array}{c}(x_7-y_7)\,\mathbf{a}_1-\left(y_7+z_7-\frac{1}{2}\right)\,\mathbf{a}_2+ \\ \left(x_7-z_7+\frac{1}{2}\right)\,\mathbf{a}_3\end{array} = -a\left(z_7-\tfrac{1}{2}\right)\,\hat{\mathbf{x}}+ax_7\,\hat{\mathbf{y}}-ay_7\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$$\mathbf{B_{61}} = \begin{array}{c}(x_7+z_7)\,\mathbf{a}_1+(x_7+y_7)\,\mathbf{a}_2+ \\ (y_7+z_7)\,\mathbf{a}_3\end{array} = ay_7\,\hat{\mathbf{x}}+az_7\,\hat{\mathbf{y}}+ax_7\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$$\mathbf{B_{62}} = \begin{array}{c}-(x_7-z_7)\,\mathbf{a}_1- \\ \left(x_7+y_7-\frac{1}{2}\right)\,\mathbf{a}_2+ \\ \left(-y_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_3\end{array} = -a\left(y_7-\tfrac{1}{2}\right)\,\hat{\mathbf{x}}+az_7\,\hat{\mathbf{y}}-ax_7\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$$\mathbf{B_{63}} = \begin{array}{c}-\left(x_7+z_7-\frac{1}{2}\right)\,\mathbf{a}_1+ \\ \left(-x_7+y_7+\frac{1}{2}\right)\,\mathbf{a}_2+(y_7-z_7)\,\mathbf{a}_3\end{array} = ay_7\,\hat{\mathbf{x}}-az_7\,\hat{\mathbf{y}}-a\left(x_7-\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$$\mathbf{B_{64}} = \begin{array}{c}\left(x_7-z_7+\frac{1}{2}\right)\,\mathbf{a}_1+ \\ (x_7-y_7)\,\mathbf{a}_2-\left(y_7+z_7-\frac{1}{2}\right)\,\mathbf{a}_3\end{array} = -ay_7\,\hat{\mathbf{x}}-a\left(z_7-\tfrac{1}{2}\right)\,\hat{\mathbf{y}}+ax_7\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$$\mathbf{B_{65}} = \begin{array}{c}\left(x_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_1+ \\ \left(y_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_2+ \\ \left(x_7+y_7+\frac{1}{2}\right)\,\mathbf{a}_3\end{array} = a\left(y_7+\tfrac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(x_7+\tfrac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(z_7+\tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$$\mathbf{B_{66}} = \begin{array}{c}\left(-x_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_1- \\ (y_7-z_7)\,\mathbf{a}_2-(x_7+y_7)\,\mathbf{a}_3\end{array} = -a\left(y_7+\tfrac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(x_7-\tfrac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(z_7+\tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$$\mathbf{B_{67}} = \begin{array}{c}-(x_7+z_7)\,\mathbf{a}_1+ \\ \left(y_7-z_7+\frac{1}{2}\right)\,\mathbf{a}_2-(x_7-y_7)\,\mathbf{a}_3\end{array} = a\left(y_7+\tfrac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(x_7+\tfrac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(z_7-\tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$$\mathbf{B_{68}} = \begin{array}{c}(x_7-z_7)\,\mathbf{a}_1-(y_7+z_7)\,\mathbf{a}_2+ \\ \left(x_7-y_7+\frac{1}{2}\right)\,\mathbf{a}_3\end{array} = -a\left(y_7-\tfrac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(x_7+\tfrac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(z_7+\tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$$\mathbf{B_{69}} = \begin{array}{c}\left(y_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_1+ \\ \left(x_7+y_7+\frac{1}{2}\right)\,\mathbf{a}_2+ \\ \left(x_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_3\end{array} = a\left(x_7+\tfrac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(z_7+\tfrac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(y_7+\tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$$\mathbf{B_{70}} = \begin{array}{c}-(y_7-z_7)\,\mathbf{a}_1-(x_7+y_7)\,\mathbf{a}_2+ \\ \left(-x_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_3\end{array} = -a\left(x_7-\tfrac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(z_7+\tfrac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(y_7+\tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$$\mathbf{B_{71}} = \begin{array}{c}\left(y_7-z_7+\frac{1}{2}\right)\,\mathbf{a}_1- \\ (x_7-y_7)\,\mathbf{a}_2-(x_7+z_7)\,\mathbf{a}_3\end{array} = -a\left(x_7+\tfrac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(z_7-\tfrac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(y_7+\tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$$\mathbf{B_{72}} = \begin{array}{c}-(y_7+z_7)\,\mathbf{a}_1+ \\ \left(x_7-y_7+\frac{1}{2}\right)\,\mathbf{a}_2+(x_7-z_7)\,\mathbf{a}_3\end{array} = a\left(x_7+\tfrac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(z_7+\tfrac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(y_7-\tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$$\mathbf{B_{73}} = \begin{array}{c}\left(x_7+y_7+\frac{1}{2}\right)\,\mathbf{a}_1+ \\ \left(x_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_2+ \\ \left(y_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_3\end{array} = a\left(z_7+\tfrac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(y_7+\tfrac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(x_7+\tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$$\mathbf{B_{74}} = \begin{array}{c}-(x_7+y_7)\,\mathbf{a}_1+ \\ \left(-x_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_2-(y_7-z_7)\,\mathbf{a}_3\end{array} = a\left(z_7+\tfrac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(y_7+\tfrac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(x_7-\tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$$\mathbf{B_{75}} = \begin{array}{c}-(x_7-y_7)\,\mathbf{a}_1-(x_7+z_7)\,\mathbf{a}_2+ \\ \left(y_7-z_7+\frac{1}{2}\right)\,\mathbf{a}_3\end{array} = -a\left(z_7-\tfrac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(y_7+\tfrac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(x_7+\tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (48e) \quad \text{O III}$$

$\mathbf{B_{76}}$ = $\left(x_7 - y_7 + \frac{1}{2}\right)\,\mathbf{a}_1 + (x_7 - z_7)\,\mathbf{a}_2 - (y_7 + z_7)\,\mathbf{a}_3$ = $-a\left(z_7 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(y_7 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_7 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$ (48e) O III

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