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

This structure previously used the label(s) `A7B12C19_cI152_220_bc_2d_ace`. Calls to these addresses will be redirected here.

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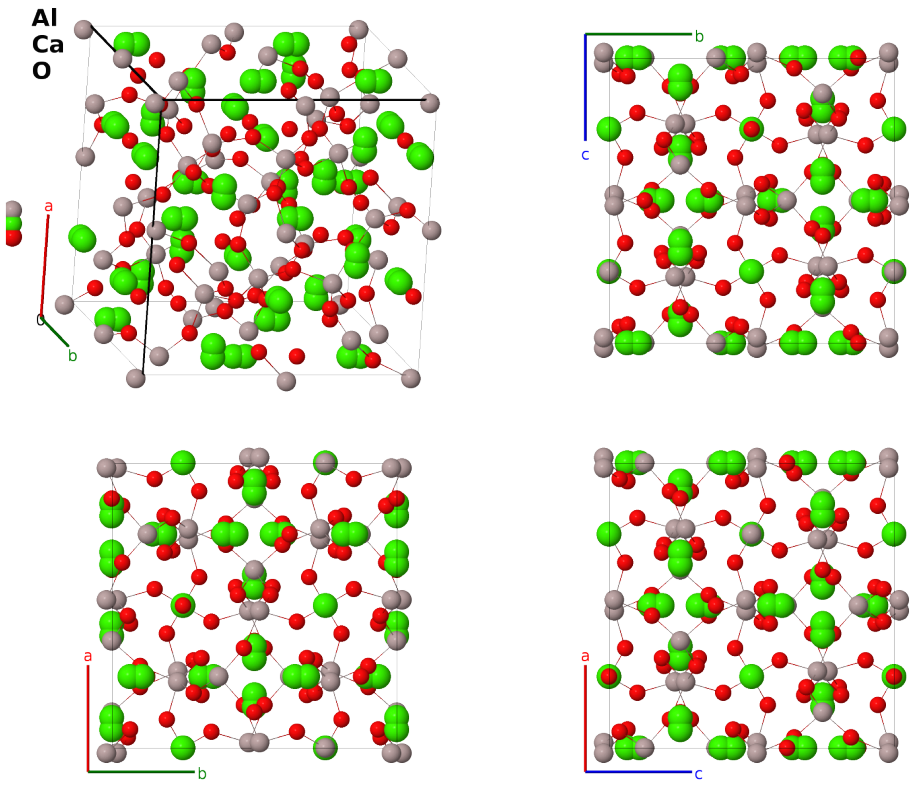
https://aflow.org/prototype-encyclopedia/L8NP

https://aflow.org/prototype-encyclopedia/A7B12C19_cI152_220_ac_2d_bce-001



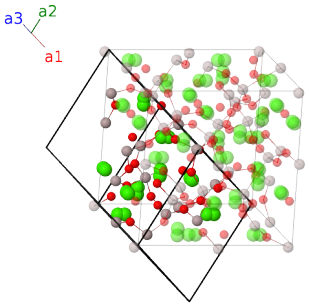
Prototype	$Al_{14}Ca_{12}O_{33}$
AFLOW prototype label	A7B12C19_cI152_220_ac_2d_bce-001
***Strukturbericht* designation**	$K7_4$
Mineral name	mayenite
ICSD	24100
CCDC	1600150
Pearson symbol	cI152
Space group number	220
Space group symbol	$I\bar{4}3d$

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

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\begin{array}{lcccccc}
\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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{Ca II}
\end{array}
$$

$\mathbf{B_{52}}$	$=$	$-x_6\,\mathbf{a}_1-\left(x_6-\frac{3}{4}\right)\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{1}{4}a\,\hat{\mathbf{y}}-a\left(x_6-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{54}}$	$=$	$\left(-y_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_1-(x_7-z_7)\,\mathbf{a}_2-\left(x_7+y_7-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ax_7\,\hat{\mathbf{x}}-a\left(y_7-\frac{1}{2}\right)\,\hat{\mathbf{y}}+az_7\,\hat{\mathbf{z}}$	(48e)	O III
$\mathbf{B_{55}}$	$=$	$(y_7-z_7)\,\mathbf{a}_1-\left(x_7+z_7-\frac{1}{2}\right)\,\mathbf{a}_2+\left(-x_7+y_7+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(x_7-\frac{1}{2}\right)\,\hat{\mathbf{x}}+ay_7\,\hat{\mathbf{y}}-az_7\,\hat{\mathbf{z}}$	(48e)	O III
$\mathbf{B_{56}}$	$=$	$-\left(y_7+z_7-\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_7-z_7+\frac{1}{2}\right)\,\mathbf{a}_2+(x_7-y_7)\,\mathbf{a}_3$	$=$	$ax_7\,\hat{\mathbf{x}}-ay_7\,\hat{\mathbf{y}}-a\left(z_7-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(48e)	O III
$\mathbf{B_{57}}$	$=$	$(x_7+y_7)\,\mathbf{a}_1+(y_7+z_7)\,\mathbf{a}_2+(x_7+z_7)\,\mathbf{a}_3$	$=$	$az_7\,\hat{\mathbf{x}}+ax_7\,\hat{\mathbf{y}}+ay_7\,\hat{\mathbf{z}}$	(48e)	O III
$\mathbf{B_{58}}$	$=$	$-\left(x_7+y_7-\frac{1}{2}\right)\,\mathbf{a}_1+\left(-y_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_2-(x_7-z_7)\,\mathbf{a}_3$	$=$	$az_7\,\hat{\mathbf{x}}-ax_7\,\hat{\mathbf{y}}-a\left(y_7-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(48e)	O III
$\mathbf{B_{59}}$	$=$	$\left(-x_7+y_7+\frac{1}{2}\right)\,\mathbf{a}_1+(y_7-z_7)\,\mathbf{a}_2-\left(x_7+z_7-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-az_7\,\hat{\mathbf{x}}-a\left(x_7-\frac{1}{2}\right)\,\hat{\mathbf{y}}+ay_7\,\hat{\mathbf{z}}$	(48e)	O III
$\mathbf{B_{60}}$	$=$	$(x_7-y_7)\,\mathbf{a}_1-\left(y_7+z_7-\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_7-z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(z_7-\frac{1}{2}\right)\,\hat{\mathbf{x}}+ax_7\,\hat{\mathbf{y}}-ay_7\,\hat{\mathbf{z}}$	(48e)	O III
$\mathbf{B_{61}}$	$=$	$(x_7+z_7)\,\mathbf{a}_1+(x_7+y_7)\,\mathbf{a}_2+(y_7+z_7)\,\mathbf{a}_3$	$=$	$ay_7\,\hat{\mathbf{x}}+az_7\,\hat{\mathbf{y}}+ax_7\,\hat{\mathbf{z}}$	(48e)	O III
$\mathbf{B_{62}}$	$=$	$-(x_7-z_7)\,\mathbf{a}_1-\left(x_7+y_7-\frac{1}{2}\right)\,\mathbf{a}_2+\left(-y_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(y_7-\frac{1}{2}\right)\,\hat{\mathbf{x}}+az_7\,\hat{\mathbf{y}}-ax_7\,\hat{\mathbf{z}}$	(48e)	O III
$\mathbf{B_{63}}$	$=$	$-\left(x_7+z_7-\frac{1}{2}\right)\,\mathbf{a}_1+\left(-x_7+y_7+\frac{1}{2}\right)\,\mathbf{a}_2+(y_7-z_7)\,\mathbf{a}_3$	$=$	$ay_7\,\hat{\mathbf{x}}-az_7\,\hat{\mathbf{y}}-a\left(x_7-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(48e)	O III
$\mathbf{B_{64}}$	$=$	$\left(x_7-z_7+\frac{1}{2}\right)\,\mathbf{a}_1+(x_7-y_7)\,\mathbf{a}_2-\left(y_7+z_7-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ay_7\,\hat{\mathbf{x}}-a\left(z_7-\frac{1}{2}\right)\,\hat{\mathbf{y}}+ax_7\,\hat{\mathbf{z}}$	(48e)	O III
$\mathbf{B_{65}}$	$=$	$\left(x_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_7+y_7+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(y_7+\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(x_7+\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(z_7+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48e)	O III
$\mathbf{B_{66}}$	$=$	$\left(-x_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_1-(y_7-z_7)\,\mathbf{a}_2-(x_7+y_7)\,\mathbf{a}_3$	$=$	$-a\left(y_7+\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(x_7-\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(z_7+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48e)	O III
$\mathbf{B_{67}}$	$=$	$-(x_7+z_7)\,\mathbf{a}_1+\left(y_7-z_7+\frac{1}{2}\right)\,\mathbf{a}_2-(x_7-y_7)\,\mathbf{a}_3$	$=$	$a\left(y_7+\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(x_7+\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(z_7-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48e)	O III
$\mathbf{B_{68}}$	$=$	$(x_7-z_7)\,\mathbf{a}_1-(y_7+z_7)\,\mathbf{a}_2+\left(x_7-y_7+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(y_7-\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(x_7+\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(z_7+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48e)	O III
$\mathbf{B_{69}}$	$=$	$\left(y_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_7+y_7+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(x_7+\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(z_7+\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(y_7+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48e)	O III
$\mathbf{B_{70}}$	$=$	$-(y_7-z_7)\,\mathbf{a}_1-(x_7+y_7)\,\mathbf{a}_2+\left(-x_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(x_7-\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(z_7+\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(y_7+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48e)	O III
$\mathbf{B_{71}}$	$=$	$\left(y_7-z_7+\frac{1}{2}\right)\,\mathbf{a}_1-(x_7-y_7)\,\mathbf{a}_2-(x_7+z_7)\,\mathbf{a}_3$	$=$	$-a\left(x_7+\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(z_7-\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(y_7+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48e)	O III
$\mathbf{B_{72}}$	$=$	$-(y_7+z_7)\,\mathbf{a}_1+\left(x_7-y_7+\frac{1}{2}\right)\,\mathbf{a}_2+(x_7-z_7)\,\mathbf{a}_3$	$=$	$a\left(x_7+\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(z_7+\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(y_7-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48e)	O III
$\mathbf{B_{73}}$	$=$	$\left(x_7+y_7+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(z_7+\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(y_7+\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(x_7+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48e)	O III

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

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

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

References

[1] H. Boysen, M. Lerch, A. Stys, and A. Senyshyn, *Structure and oxygen mobility in mayenite ($Ca_{12}Al_{14}O_{33}$): a high-temperature neutron powder diffraction study*, Acta Crystallogr. Sect. B **63**, 675–682 (2007), doi:10.1107/S0108768107030005.

[2] W. Büssem and A. Eitel, *Die Struktur des Pentacalciumtrialuminats*, Zeitschrift für Kristallographie **95**, 175–188 (1936).

[3] C. Gottfried, ed., *Strukturbericht Band IV 1936* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1938).

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

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.