# Disordered Calcined $AlPO_4$-11 Structure: AB2_oI120_74_h2j_aef2i3j-001

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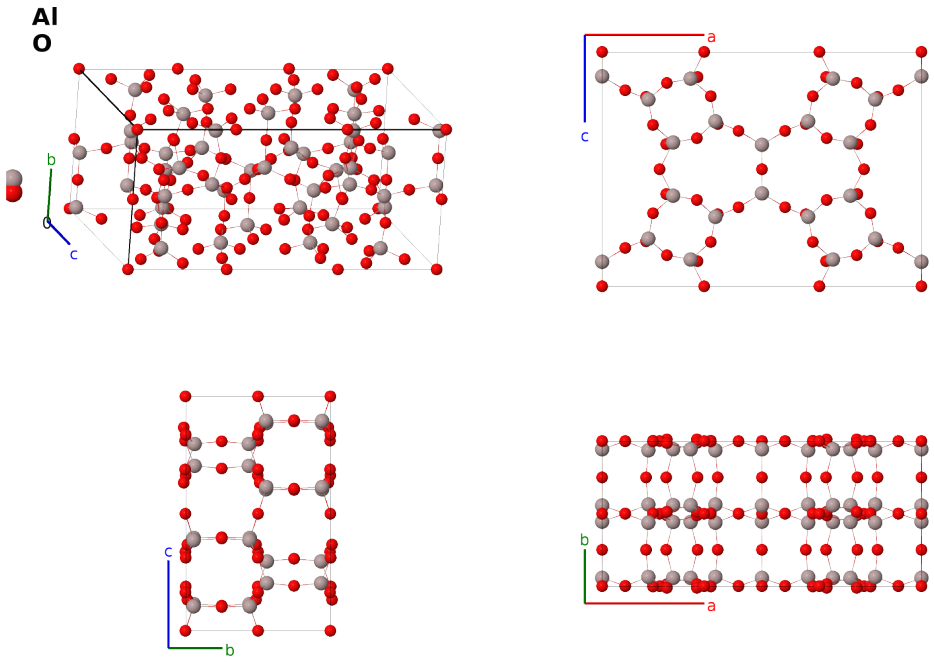
https://aflow.org/prototype-encyclopedia/VR57

https://aflow.org/prototype-encyclopedia/AB2_oI120_74_h2j_aef2i3j-001




| | |
|---|---|
| **Prototype** | $AlO_4P$ |
| **AFLOW prototype label** | AB2_oI120_74_h2j_aef2i3j-001 |
| **ICSD** | 63665 |
| **CCDC** | 1626746 |
| **Pearson symbol** | oI120 |
| **Space group number** | 74 |
| **Space group symbol** | $Imma$ |
| **AFLOW prototype command** | `aflow --proto=AB2_oI120_74_h2j_aef2i3j-001 --params=`$a, b/a, c/a, z_2, x_3, y_4, z_4, x_5, z_5, x_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}$ |

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- Samples of $AlPO_4$-11 were calcined at 873K to remove impurities and then dehydrated at 573K. Data was collected at 295K.

- (Richardson, 1988) found an ordered structure, but also found a good fit to the data by assuming this disordered phase where the aluminum and phosphorous atoms are randomly distributed. We arbitrarily label these mixed Al/P sites as aluminum. This randomization changes the space group from polar $Ima2$ #46 to centrosymmetric $Imma$ #74.
- More information about $AlPO_4$ structures can be found on the $SiO_2$ and $AlPO_4$ page.
- (Richardson, 1988) give the data for this structure in the $Icmm$ setting of space group #74. We used AFLOW to transform it into the standard $Imma$ setting.

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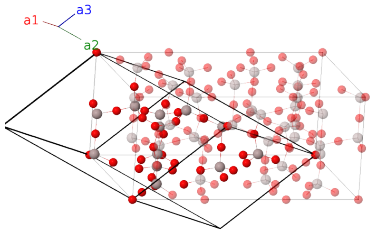
**Body-centered Orthorhombic primitive vectors**

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

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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (4a) | O I |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}b\,\hat{\mathbf{y}}$ | (4a) | O I |
| $\mathbf{B_3}$ | = | $\left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $\frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (4e) | O II |
| $\mathbf{B_4}$ | = | $-\left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $\frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$ | (4e) | O II |
| $\mathbf{B_5}$ | = | $x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$ | = | $ax_3\,\hat{\mathbf{x}}$ | (8f) | O III |
| $\mathbf{B_6}$ | = | $\frac{1}{2}\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$ | (8f) | O III |
| $\mathbf{B_7}$ | = | $-x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$ | = | $-ax_3\,\hat{\mathbf{x}}$ | (8f) | O III |
| $\mathbf{B_8}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $ax_3\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$ | (8f) | O III |
| $\mathbf{B_9}$ | = | $(y_4 + z_4)\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$ | = | $by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (8h) | Al I |
| $\mathbf{B_{10}}$ | = | $\left(-y_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (8h) | Al I |
| $\mathbf{B_{11}}$ | = | $\left(y_4 - z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$ | (8h) | Al I |
| $\mathbf{B_{12}}$ | = | $-(y_4 + z_4)\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$ | = | $-by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$ | (8h) | Al I |
| $\mathbf{B_{13}}$ | = | $\left(z_5 + \frac{1}{4}\right)\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + \left(x_5 + \frac{1}{4}\right)\,\mathbf{a}_3$ | = | $ax_5\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$ | (8i) | O IV |
| $\mathbf{B_{14}}$ | = | $\left(z_5 + \frac{1}{4}\right)\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - \left(x_5 - \frac{1}{4}\right)\,\mathbf{a}_3$ | = | $-ax_5\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$ | (8i) | O IV |
| $\mathbf{B_{15}}$ | = | $-\left(z_5 - \frac{3}{4}\right)\,\mathbf{a}_1 - (x_5 + z_5)\,\mathbf{a}_2 - \left(x_5 - \frac{3}{4}\right)\,\mathbf{a}_3$ | = | $-ax_5\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$ | (8i) | O IV |
| $\mathbf{B_{16}}$ | = | $-\left(z_5 - \frac{3}{4}\right)\,\mathbf{a}_1 + (x_5 - z_5)\,\mathbf{a}_2 + \left(x_5 + \frac{3}{4}\right)\,\mathbf{a}_3$ | = | $ax_5\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$ | (8i) | O IV |
| $\mathbf{B_{17}}$ | = | $\left(z_6 + \frac{1}{4}\right)\,\mathbf{a}_1 + (x_6 + z_6)\,\mathbf{a}_2 + \left(x_6 + \frac{1}{4}\right)\,\mathbf{a}_3$ | = | $ax_6\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (8i) | O V |

| | | | | | | |
|---|---|---|---|---|---|---|
| $\mathbf{B_{18}}$ | = | $\left(z_6+\frac{1}{4}\right)\mathbf{a}_1-(x_6-z_6)\,\mathbf{a}_2-\left(x_6-\frac{1}{4}\right)\mathbf{a}_3$ | = | $-ax_6\,\hat{\mathbf{x}}+\frac{1}{4}b\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$ | (8i) | O V |
| $\mathbf{B_{19}}$ | = | $-\left(z_6-\frac{3}{4}\right)\mathbf{a}_1-(x_6+z_6)\,\mathbf{a}_2-\left(x_6-\frac{3}{4}\right)\mathbf{a}_3$ | = | $-ax_6\,\hat{\mathbf{x}}+\frac{3}{4}b\,\hat{\mathbf{y}}-cz_6\,\hat{\mathbf{z}}$ | (8i) | O V |
| $\mathbf{B_{20}}$ | = | $-\left(z_6-\frac{3}{4}\right)\mathbf{a}_1+(x_6-z_6)\,\mathbf{a}_2+\left(x_6+\frac{3}{4}\right)\mathbf{a}_3$ | = | $ax_6\,\hat{\mathbf{x}}+\frac{3}{4}b\,\hat{\mathbf{y}}-cz_6\,\hat{\mathbf{z}}$ | (8i) | O V |
| $\mathbf{B_{21}}$ | = | $(y_7+z_7)\,\mathbf{a}_1+(x_7+z_7)\,\mathbf{a}_2+(x_7+y_7)\,\mathbf{a}_3$ | = | $ax_7\,\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$ | (16j) | Al II |
| $\mathbf{B_{22}}$ | = | $\left(-y_7+z_7+\frac{1}{2}\right)\mathbf{a}_1-(x_7-z_7)\,\mathbf{a}_2-\left(x_7+y_7-\frac{1}{2}\right)\mathbf{a}_3$ | = | $-ax_7\,\hat{\mathbf{x}}-b\left(y_7-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$ | (16j) | Al II |
| $\mathbf{B_{23}}$ | = | $\left(y_7-z_7+\frac{1}{2}\right)\mathbf{a}_1-(x_7+z_7)\,\mathbf{a}_2+\left(-x_7+y_7+\frac{1}{2}\right)\mathbf{a}_3$ | = | $-ax_7\,\hat{\mathbf{x}}+b\left(y_7+\frac{1}{2}\right)\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}}$ | (16j) | Al II |
| $\mathbf{B_{24}}$ | = | $-(y_7+z_7)\,\mathbf{a}_1+(x_7-z_7)\,\mathbf{a}_2+(x_7-y_7)\,\mathbf{a}_3$ | = | $ax_7\,\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}}$ | (16j) | Al II |
| $\mathbf{B_{25}}$ | = | $-(y_7+z_7)\,\mathbf{a}_1-(x_7+z_7)\,\mathbf{a}_2-(x_7+y_7)\,\mathbf{a}_3$ | = | $-ax_7\,\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}}$ | (16j) | Al II |
| $\mathbf{B_{26}}$ | = | $\left(y_7-z_7+\frac{1}{2}\right)\mathbf{a}_1+(x_7-z_7)\,\mathbf{a}_2+\left(x_7+y_7+\frac{1}{2}\right)\mathbf{a}_3$ | = | $ax_7\,\hat{\mathbf{x}}+b\left(y_7+\frac{1}{2}\right)\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}}$ | (16j) | Al II |
| $\mathbf{B_{27}}$ | = | $\left(-y_7+z_7+\frac{1}{2}\right)\mathbf{a}_1+(x_7+z_7)\,\mathbf{a}_2+\left(x_7-y_7+\frac{1}{2}\right)\mathbf{a}_3$ | = | $ax_7\,\hat{\mathbf{x}}-b\left(y_7-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$ | (16j) | Al II |
| $\mathbf{B_{28}}$ | = | $(y_7+z_7)\,\mathbf{a}_1-(x_7-z_7)\,\mathbf{a}_2-(x_7-y_7)\,\mathbf{a}_3$ | = | $-ax_7\,\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$ | (16j) | Al II |
| $\mathbf{B_{29}}$ | = | $(y_8+z_8)\,\mathbf{a}_1+(x_8+z_8)\,\mathbf{a}_2+(x_8+y_8)\,\mathbf{a}_3$ | = | $ax_8\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$ | (16j) | Al III |
| $\mathbf{B_{30}}$ | = | $\left(-y_8+z_8+\frac{1}{2}\right)\mathbf{a}_1-(x_8-z_8)\,\mathbf{a}_2-\left(x_8+y_8-\frac{1}{2}\right)\mathbf{a}_3$ | = | $-ax_8\,\hat{\mathbf{x}}-b\left(y_8-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$ | (16j) | Al III |
| $\mathbf{B_{31}}$ | = | $\left(y_8-z_8+\frac{1}{2}\right)\mathbf{a}_1-(x_8+z_8)\,\mathbf{a}_2+\left(-x_8+y_8+\frac{1}{2}\right)\mathbf{a}_3$ | = | $-ax_8\,\hat{\mathbf{x}}+b\left(y_8+\frac{1}{2}\right)\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$ | (16j) | Al III |
| $\mathbf{B_{32}}$ | = | $-(y_8+z_8)\,\mathbf{a}_1+(x_8-z_8)\,\mathbf{a}_2+(x_8-y_8)\,\mathbf{a}_3$ | = | $ax_8\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$ | (16j) | Al III |
| $\mathbf{B_{33}}$ | = | $-(y_8+z_8)\,\mathbf{a}_1-(x_8+z_8)\,\mathbf{a}_2-(x_8+y_8)\,\mathbf{a}_3$ | = | $-ax_8\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$ | (16j) | Al III |
| $\mathbf{B_{34}}$ | = | $\left(y_8-z_8+\frac{1}{2}\right)\mathbf{a}_1+(x_8-z_8)\,\mathbf{a}_2+\left(x_8+y_8+\frac{1}{2}\right)\mathbf{a}_3$ | = | $ax_8\,\hat{\mathbf{x}}+b\left(y_8+\frac{1}{2}\right)\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$ | (16j) | Al III |
| $\mathbf{B_{35}}$ | = | $\left(-y_8+z_8+\frac{1}{2}\right)\mathbf{a}_1+(x_8+z_8)\,\mathbf{a}_2+\left(x_8-y_8+\frac{1}{2}\right)\mathbf{a}_3$ | = | $ax_8\,\hat{\mathbf{x}}-b\left(y_8-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$ | (16j) | Al III |
| $\mathbf{B_{36}}$ | = | $(y_8+z_8)\,\mathbf{a}_1-(x_8-z_8)\,\mathbf{a}_2-(x_8-y_8)\,\mathbf{a}_3$ | = | $-ax_8\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$ | (16j) | Al III |
| $\mathbf{B_{37}}$ | = | $(y_9+z_9)\,\mathbf{a}_1+(x_9+z_9)\,\mathbf{a}_2+(x_9+y_9)\,\mathbf{a}_3$ | = | $ax_9\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$ | (16j) | O VI |
| $\mathbf{B_{38}}$ | = | $\left(-y_9+z_9+\frac{1}{2}\right)\mathbf{a}_1-(x_9-z_9)\,\mathbf{a}_2-\left(x_9+y_9-\frac{1}{2}\right)\mathbf{a}_3$ | = | $-ax_9\,\hat{\mathbf{x}}-b\left(y_9-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$ | (16j) | O VI |
| $\mathbf{B_{39}}$ | = | $\left(y_9-z_9+\frac{1}{2}\right)\mathbf{a}_1-(x_9+z_9)\,\mathbf{a}_2+\left(-x_9+y_9+\frac{1}{2}\right)\mathbf{a}_3$ | = | $-ax_9\,\hat{\mathbf{x}}+b\left(y_9+\frac{1}{2}\right)\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}}$ | (16j) | O VI |
| $\mathbf{B_{40}}$ | = | $-(y_9+z_9)\,\mathbf{a}_1+(x_9-z_9)\,\mathbf{a}_2+(x_9-y_9)\,\mathbf{a}_3$ | = | $ax_9\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}}$ | (16j) | O VI |

$$\mathbf{B_{41}} = -(y_9+z_9)\,\mathbf{a}_1-(x_9+z_9)\,\mathbf{a}_2-(x_9+y_9)\,\mathbf{a}_3 = -ax_9\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}} \quad (16j) \quad \text{O VI}$$

$$\mathbf{B_{42}} = \left(y_9-z_9+\tfrac{1}{2}\right)\mathbf{a}_1+(x_9-z_9)\,\mathbf{a}_2+\left(x_9+y_9+\tfrac{1}{2}\right)\mathbf{a}_3 = ax_9\,\hat{\mathbf{x}}+b\left(y_9+\tfrac{1}{2}\right)\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}} \quad (16j) \quad \text{O VI}$$

$$\mathbf{B_{43}} = \left(-y_9+z_9+\tfrac{1}{2}\right)\mathbf{a}_1+(x_9+z_9)\,\mathbf{a}_2+\left(x_9-y_9+\tfrac{1}{2}\right)\mathbf{a}_3 = ax_9\,\hat{\mathbf{x}}-b\left(y_9-\tfrac{1}{2}\right)\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}} \quad (16j) \quad \text{O VI}$$

$$\mathbf{B_{44}} = (y_9+z_9)\,\mathbf{a}_1-(x_9-z_9)\,\mathbf{a}_2-(x_9-y_9)\,\mathbf{a}_3 = -ax_9\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}} \quad (16j) \quad \text{O VI}$$

$$\mathbf{B_{45}} = (y_{10}+z_{10})\,\mathbf{a}_1+(x_{10}+z_{10})\,\mathbf{a}_2+(x_{10}+y_{10})\,\mathbf{a}_3 = ax_{10}\,\hat{\mathbf{x}}+by_{10}\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}} \quad (16j) \quad \text{O VII}$$

$$\mathbf{B_{46}} = \left(-y_{10}+z_{10}+\tfrac{1}{2}\right)\mathbf{a}_1-(x_{10}-z_{10})\,\mathbf{a}_2-\left(x_{10}+y_{10}-\tfrac{1}{2}\right)\mathbf{a}_3 = -ax_{10}\,\hat{\mathbf{x}}-b\left(y_{10}-\tfrac{1}{2}\right)\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}} \quad (16j) \quad \text{O VII}$$

$$\mathbf{B_{47}} = \left(y_{10}-z_{10}+\tfrac{1}{2}\right)\mathbf{a}_1-(x_{10}+z_{10})\,\mathbf{a}_2+\left(-x_{10}+y_{10}+\tfrac{1}{2}\right)\mathbf{a}_3 = -ax_{10}\,\hat{\mathbf{x}}+b\left(y_{10}+\tfrac{1}{2}\right)\,\hat{\mathbf{y}}-cz_{10}\,\hat{\mathbf{z}} \quad (16j) \quad \text{O VII}$$

$$\mathbf{B_{48}} = -(y_{10}+z_{10})\,\mathbf{a}_1+(x_{10}-z_{10})\,\mathbf{a}_2+(x_{10}-y_{10})\,\mathbf{a}_3 = ax_{10}\,\hat{\mathbf{x}}-by_{10}\,\hat{\mathbf{y}}-cz_{10}\,\hat{\mathbf{z}} \quad (16j) \quad \text{O VII}$$

$$\mathbf{B_{49}} = -(y_{10}+z_{10})\,\mathbf{a}_1-(x_{10}+z_{10})\,\mathbf{a}_2-(x_{10}+y_{10})\,\mathbf{a}_3 = -ax_{10}\,\hat{\mathbf{x}}-by_{10}\,\hat{\mathbf{y}}-cz_{10}\,\hat{\mathbf{z}} \quad (16j) \quad \text{O VII}$$

$$\mathbf{B_{50}} = \left(y_{10}-z_{10}+\tfrac{1}{2}\right)\mathbf{a}_1+(x_{10}-z_{10})\,\mathbf{a}_2+\left(x_{10}+y_{10}+\tfrac{1}{2}\right)\mathbf{a}_3 = ax_{10}\,\hat{\mathbf{x}}+b\left(y_{10}+\tfrac{1}{2}\right)\,\hat{\mathbf{y}}-cz_{10}\,\hat{\mathbf{z}} \quad (16j) \quad \text{O VII}$$

$$\mathbf{B_{51}} = \left(-y_{10}+z_{10}+\tfrac{1}{2}\right)\mathbf{a}_1+(x_{10}+z_{10})\,\mathbf{a}_2+\left(x_{10}-y_{10}+\tfrac{1}{2}\right)\mathbf{a}_3 = ax_{10}\,\hat{\mathbf{x}}-b\left(y_{10}-\tfrac{1}{2}\right)\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}} \quad (16j) \quad \text{O VII}$$

$$\mathbf{B_{52}} = (y_{10}+z_{10})\,\mathbf{a}_1-(x_{10}-z_{10})\,\mathbf{a}_2-(x_{10}-y_{10})\,\mathbf{a}_3 = -ax_{10}\,\hat{\mathbf{x}}+by_{10}\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}} \quad (16j) \quad \text{O VII}$$

$$\mathbf{B_{53}} = (y_{11}+z_{11})\,\mathbf{a}_1+(x_{11}+z_{11})\,\mathbf{a}_2+(x_{11}+y_{11})\,\mathbf{a}_3 = ax_{11}\,\hat{\mathbf{x}}+by_{11}\,\hat{\mathbf{y}}+cz_{11}\,\hat{\mathbf{z}} \quad (16j) \quad \text{O VIII}$$

$$\mathbf{B_{54}} = \left(-y_{11}+z_{11}+\tfrac{1}{2}\right)\mathbf{a}_1-(x_{11}-z_{11})\,\mathbf{a}_2-\left(x_{11}+y_{11}-\tfrac{1}{2}\right)\mathbf{a}_3 = -ax_{11}\,\hat{\mathbf{x}}-b\left(y_{11}-\tfrac{1}{2}\right)\,\hat{\mathbf{y}}+cz_{11}\,\hat{\mathbf{z}} \quad (16j) \quad \text{O VIII}$$

$$\mathbf{B_{55}} = \left(y_{11}-z_{11}+\tfrac{1}{2}\right)\mathbf{a}_1-(x_{11}+z_{11})\,\mathbf{a}_2+\left(-x_{11}+y_{11}+\tfrac{1}{2}\right)\mathbf{a}_3 = -ax_{11}\,\hat{\mathbf{x}}+b\left(y_{11}+\tfrac{1}{2}\right)\,\hat{\mathbf{y}}-cz_{11}\,\hat{\mathbf{z}} \quad (16j) \quad \text{O VIII}$$

$$\mathbf{B_{56}} = -(y_{11}+z_{11})\,\mathbf{a}_1+(x_{11}-z_{11})\,\mathbf{a}_2+(x_{11}-y_{11})\,\mathbf{a}_3 = ax_{11}\,\hat{\mathbf{x}}-by_{11}\,\hat{\mathbf{y}}-cz_{11}\,\hat{\mathbf{z}} \quad (16j) \quad \text{O VIII}$$

$$\mathbf{B_{57}} = -(y_{11}+z_{11})\,\mathbf{a}_1-(x_{11}+z_{11})\,\mathbf{a}_2-(x_{11}+y_{11})\,\mathbf{a}_3 = -ax_{11}\,\hat{\mathbf{x}}-by_{11}\,\hat{\mathbf{y}}-cz_{11}\,\hat{\mathbf{z}} \quad (16j) \quad \text{O VIII}$$

$$\mathbf{B_{58}} = \left(y_{11}-z_{11}+\tfrac{1}{2}\right)\mathbf{a}_1+(x_{11}-z_{11})\,\mathbf{a}_2+\left(x_{11}+y_{11}+\tfrac{1}{2}\right)\mathbf{a}_3 = ax_{11}\,\hat{\mathbf{x}}+b\left(y_{11}+\tfrac{1}{2}\right)\,\hat{\mathbf{y}}-cz_{11}\,\hat{\mathbf{z}} \quad (16j) \quad \text{O VIII}$$

$$\mathbf{B_{59}} = \left(-y_{11}+z_{11}+\tfrac{1}{2}\right)\mathbf{a}_1+(x_{11}+z_{11})\,\mathbf{a}_2+\left(x_{11}-y_{11}+\tfrac{1}{2}\right)\mathbf{a}_3 = ax_{11}\,\hat{\mathbf{x}}-b\left(y_{11}-\tfrac{1}{2}\right)\,\hat{\mathbf{y}}+cz_{11}\,\hat{\mathbf{z}} \quad (16j) \quad \text{O VIII}$$

$$\mathbf{B_{60}} = (y_{11}+z_{11})\,\mathbf{a}_1-(x_{11}-z_{11})\,\mathbf{a}_2-(x_{11}-y_{11})\,\mathbf{a}_3 = -ax_{11}\,\hat{\mathbf{x}}+by_{11}\,\hat{\mathbf{y}}+cz_{11}\,\hat{\mathbf{z}} \quad (16j) \quad \text{O VIII}$$

## References

[1] J. R. Richardson, Jr., J. J. Pluth, and J. V. Smith, *Rietveld profile analysis of calcined $AlPO_4$-11 using pulsed neutron powder diffraction*, Acta Crystallographica B **44**, 367–373 (1988), doi:10.1107/S0108768188003076.

## Found in

[1] M. Fischer, *Revisiting the Structure of Calcined and Hydrated AlPO-11 with DFT-Based Molecular Dynamics Simulations*, ChemPhysChem **22**, 2063–2077 (2021), doi:10.1002/cphc.202100486.

## First cited in

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