

AlPO₄-54 Structure:

AB2_hP108_193_kl_fg2ijl-001

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<https://aflow.org/prototype-encyclopedia/UU4R>

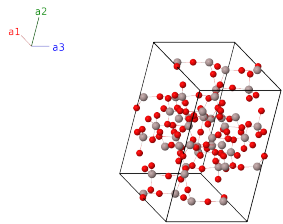
https://aflow.org/prototype-encyclopedia/AB2_hP108_193_kl_fg2ijl-001

Prototype	AlO ₄ P
AFLOW prototype label	AB2_hP108_193_kl_fg2ijl-001
ICSD	40272
CCDC	1610141
Pearson symbol	hP108
Space group number	193
Space group symbol	$P6_3/mcm$
AFLOW prototype command	<pre>aflow --proto=AB2_hP108_193_kl_fg2ijl-001 --params=a,c/a,x2,x3,x4,x5,y5,x6,z6,x7,y7,z7,x8,y8,z8</pre>

- We take the label AlPO₄-54 from (Withers, 2005).
- Related structures can be found on the silica and aluminum phosphate page.
- The (12k) and (24l) sites are a 50-50 mixture of aluminium and phosphorous. We arbitrarily label them as aluminum.

Hexagonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}}$	(6f)	O I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a \hat{\mathbf{y}}$	(6f)	O I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}}$	(6f)	O I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6f)	O I

$$\begin{aligned}
\mathbf{B}_{81} &= x_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(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}} & (241) & \text{Al II} \\
\mathbf{B}_{82} &= y_7 \mathbf{a}_1 + x_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}} & (241) & \text{Al II} \\
\mathbf{B}_{83} &= (x_7 - y_7) \mathbf{a}_1 - 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}} & (241) & \text{Al II} \\
\mathbf{B}_{84} &= -x_7 \mathbf{a}_1 - (x_7 - y_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}} & (241) & \text{Al II} \\
\mathbf{B}_{85} &= 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}} & (241) & \text{O VI} \\
\mathbf{B}_{86} &= -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}} & (241) & \text{O VI} \\
\mathbf{B}_{87} &= -(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}} & (241) & \text{O VI} \\
\mathbf{B}_{88} &= -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}} & (241) & \text{O VI} \\
\mathbf{B}_{89} &= 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}} & (241) & \text{O VI} \\
\mathbf{B}_{90} &= (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}} & (241) & \text{O VI} \\
\mathbf{B}_{91} &= y_8 \mathbf{a}_1 + x_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}} & (241) & \text{O VI} \\
\mathbf{B}_{92} &= (x_8 - y_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 - 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}} & (241) & \text{O VI} \\
\mathbf{B}_{93} &= -x_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(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}} & (241) & \text{O VI} \\
\mathbf{B}_{94} &= -y_8 \mathbf{a}_1 - x_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}} & (241) & \text{O VI} \\
\mathbf{B}_{95} &= -(x_8 - y_8) \mathbf{a}_1 + 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}} & (241) & \text{O VI} \\
\mathbf{B}_{96} &= x_8 \mathbf{a}_1 + (x_8 - y_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}} & (241) & \text{O VI} \\
\mathbf{B}_{97} &= -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}} & (241) & \text{O VI} \\
\mathbf{B}_{98} &= 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}} & (241) & \text{O VI} \\
\mathbf{B}_{99} &= (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}} & (241) & \text{O VI} \\
\mathbf{B}_{100} &= 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}} & (241) & \text{O VI} \\
\mathbf{B}_{101} &= -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}} & (241) & \text{O VI} \\
\mathbf{B}_{102} &= -(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}} & (241) & \text{O VI} \\
\mathbf{B}_{103} &= -y_8 \mathbf{a}_1 - x_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}} & (241) & \text{O VI} \\
\mathbf{B}_{104} &= -(x_8 - y_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 + 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}} & (241) & \text{O VI} \\
\mathbf{B}_{105} &= x_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(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}} & (241) & \text{O VI} \\
\mathbf{B}_{106} &= y_8 \mathbf{a}_1 + x_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}} & (241) & \text{O VI} \\
\mathbf{B}_{107} &= (x_8 - y_8) \mathbf{a}_1 - 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}} & (241) & \text{O VI} \\
\mathbf{B}_{108} &= -x_8 \mathbf{a}_1 - (x_8 - y_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}} & (241) & \text{O VI}
\end{aligned}$$

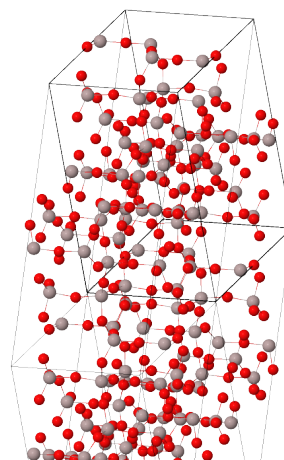
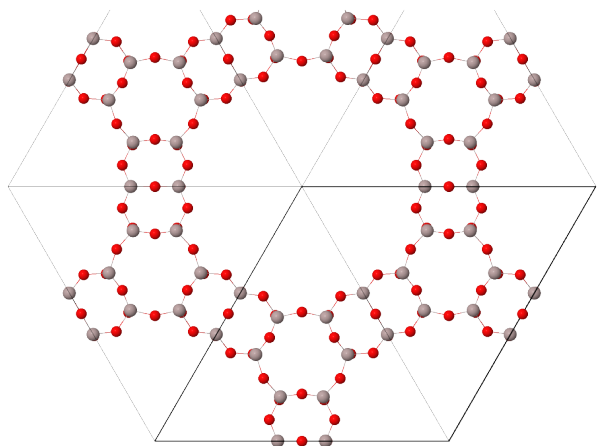
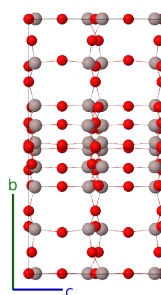
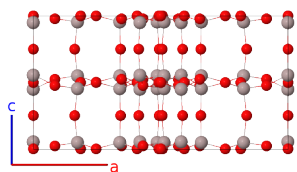
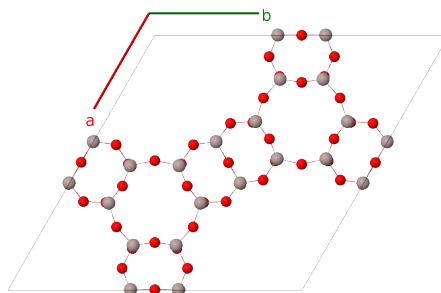
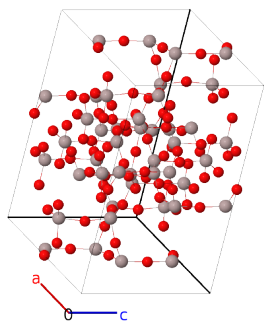
References

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Found in

- [1] R. L. Withers and Y. Lin, *A coupled electron diffraction and rigid unit mode (RUM) study of the crystal chemistry of some zeotypic AlPO_4 compounds*, J. Solid State Chem. **178**, 2647–2657 (2005), doi:10.1016/j.jssc.2005.06.003.

Al
O



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