

$(\text{AlPO}_4)_9(\text{O}_2)_9\text{O}$ [AlPO₄-17 Framework] Structure: A9B55C9_hP146_176_hi_a2h8i_hi-001

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<https://aflow.org/prototype-encyclopedia/UE8N>

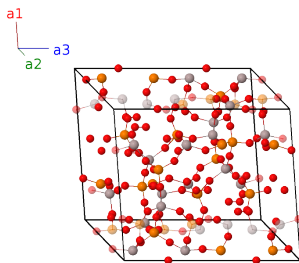
https://aflow.org/prototype-encyclopedia/A9B55C9_hP146_176_hi_a2h8i_hi-001

Prototype	$\text{Al}_9\text{O}_{55}\text{P}_9$
AFLOW prototype label	A9B55C9_hP146_176_hi_a2h8i_hi-001
ICSD	139992
CCDC	2211251
Pearson symbol	hP146
Space group number	176
Space group symbol	$P6_3/m$
AFLOW prototype command	<pre>aflow --proto=A9B55C9_hP146_176_hi_a2h8i_hi-001 --params=a, c/a, x₂, y₂, x₃, y₃, x₄, y₄, x₅, y₅, x₆, y₆, z₆, x₇, y₇, z₇, x₈, y₈, z₈, x₉, y₉, z₉, x₁₀, y₁₀, z₁₀, x₁₁, y₁₁, z₁₁, x₁₂, y₁₂, z₁₂, x₁₃, y₁₃, z₁₃, x₁₄, y₁₄, z₁₄, x₁₅, y₁₅, z₁₅</pre>

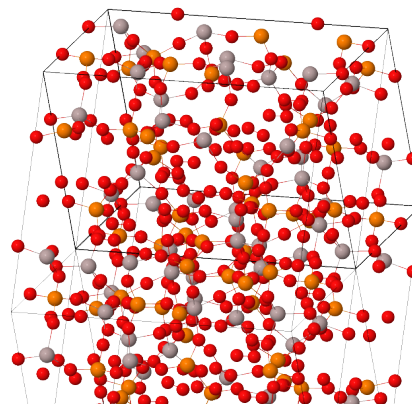
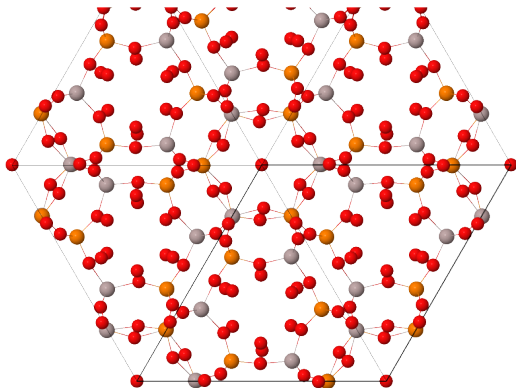
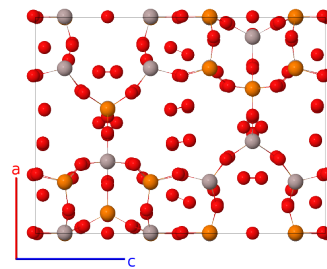
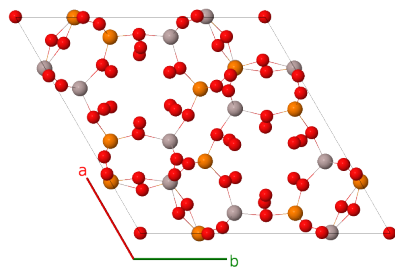
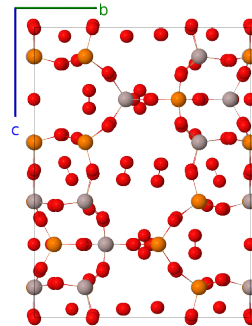
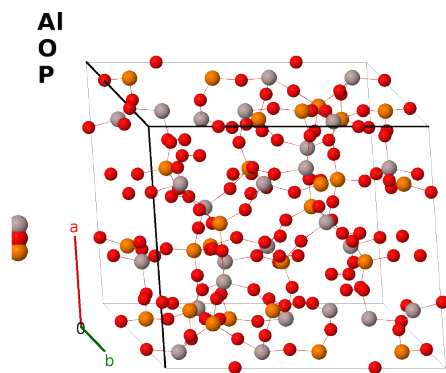
- This is another AlPO_4 framework with embedded O_2 molecules and free oxygens. It is remarkable because it exhibits negative thermal conductivity below 300K.
- (Attfield, 1998) give two versions of this structure: one in space group $P6_3/m$ #176, with one set of extra oxygens. The second version is in space group $P6_3/mmc$ #194, and only gives the bare framework. Neither set of coordinates agrees exactly with the data filed in ICSD 139992/CCDC 2211251, which includes all of the interstitial oxygen. We use the structure filed with the ICSD and the CCDC, taken at 298K. The AlPO_4 -17 framework can be recovered by removing the O I, O V, O IX, O X, and O XI atoms.

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



$\mathbf{B}_{72}$	$=$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_9 + y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_9 - y_9) \hat{\mathbf{y}} - c\left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	O VI
$\mathbf{B}_{73}$	$=$	$-y_9 \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_9 - 2y_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9 \hat{\mathbf{y}} - c\left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	O VI
$\mathbf{B}_{74}$	$=$	$-(x_9 - y_9) \mathbf{a}_1 - x_9 \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_9 - y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_9 \hat{\mathbf{y}} - c\left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	O VI
$\mathbf{B}_{75}$	$=$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{10} + y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{10} - y_{10}) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(12i)	O VII
$\mathbf{B}_{76}$	$=$	$-y_{10} \mathbf{a}_1 + (x_{10} - y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{10} - 2y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(12i)	O VII
$\mathbf{B}_{77}$	$=$	$-(x_{10} - y_{10}) \mathbf{a}_1 - x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{10} - y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(12i)	O VII
$\mathbf{B}_{78}$	$=$	$-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_{10} + y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{10} - y_{10}) \hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	O VII
$\mathbf{B}_{79}$	$=$	$y_{10} \mathbf{a}_1 - (x_{10} - y_{10}) \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_{10} + 2y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	O VII
$\mathbf{B}_{80}$	$=$	$(x_{10} - y_{10}) \mathbf{a}_1 + x_{10} \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_{10} - y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{10} \hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	O VII
$\mathbf{B}_{81}$	$=$	$-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_{10} + y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{10} - y_{10}) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(12i)	O VII
$\mathbf{B}_{82}$	$=$	$y_{10} \mathbf{a}_1 - (x_{10} - y_{10}) \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_{10} + 2y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(12i)	O VII
$\mathbf{B}_{83}$	$=$	$(x_{10} - y_{10}) \mathbf{a}_1 + x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_{10} - y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(12i)	O VII
$\mathbf{B}_{84}$	$=$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{10} + y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{10} - y_{10}) \hat{\mathbf{y}} - c\left(z_{10} - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	O VII
$\mathbf{B}_{85}$	$=$	$-y_{10} \mathbf{a}_1 + (x_{10} - y_{10}) \mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{10} - 2y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} - c\left(z_{10} - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	O VII
$\mathbf{B}_{86}$	$=$	$-(x_{10} - y_{10}) \mathbf{a}_1 - x_{10} \mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{10} - y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{10} \hat{\mathbf{y}} - c\left(z_{10} - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	O VII
$\mathbf{B}_{87}$	$=$	$x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{11} + y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{11} - y_{11}) \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(12i)	O VIII
$\mathbf{B}_{88}$	$=$	$-y_{11} \mathbf{a}_1 + (x_{11} - y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{11} - 2y_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(12i)	O VIII
$\mathbf{B}_{89}$	$=$	$-(x_{11} - y_{11}) \mathbf{a}_1 - x_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{11} - y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(12i)	O VIII
$\mathbf{B}_{90}$	$=$	$-x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_{11} + y_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{11} - y_{11}) \hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	O VIII
$\mathbf{B}_{91}$	$=$	$y_{11} \mathbf{a}_1 - (x_{11} - y_{11}) \mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_{11} + 2y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{11} \hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	O VIII
$\mathbf{B}_{92}$	$=$	$(x_{11} - y_{11}) \mathbf{a}_1 + x_{11} \mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_{11} - y_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{11} \hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	O VIII
$\mathbf{B}_{93}$	$=$	$-x_{11} \mathbf{a}_1 -$				

$$\begin{aligned}
\mathbf{B}_{127} &= y_{14} \mathbf{a}_1 - (x_{14} - y_{14}) \mathbf{a}_2 + (z_{14} + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_{14} + 2y_{14}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{14} \hat{\mathbf{y}} + c(z_{14} + \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{O XI} \\
\mathbf{B}_{128} &= (x_{14} - y_{14}) \mathbf{a}_1 + x_{14} \mathbf{a}_2 + (z_{14} + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(2x_{14} - y_{14}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{14} \hat{\mathbf{y}} + c(z_{14} + \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{O XI} \\
\mathbf{B}_{129} &= -x_{14} \mathbf{a}_1 - y_{14} \mathbf{a}_2 - z_{14} \mathbf{a}_3 = -\frac{1}{2}a(x_{14} + y_{14}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{14} - y_{14}) \hat{\mathbf{y}} - cz_{14} \hat{\mathbf{z}} & (12i) & \text{O XI} \\
\mathbf{B}_{130} &= y_{14} \mathbf{a}_1 - (x_{14} - y_{14}) \mathbf{a}_2 - z_{14} \mathbf{a}_3 = \frac{1}{2}a(-x_{14} + 2y_{14}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{14} \hat{\mathbf{y}} - cz_{14} \hat{\mathbf{z}} & (12i) & \text{O XI} \\
\mathbf{B}_{131} &= (x_{14} - y_{14}) \mathbf{a}_1 + x_{14} \mathbf{a}_2 - z_{14} \mathbf{a}_3 = \frac{1}{2}a(2x_{14} - y_{14}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{14} \hat{\mathbf{y}} - cz_{14} \hat{\mathbf{z}} & (12i) & \text{O XI} \\
\mathbf{B}_{132} &= x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 - (z_{14} - \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(x_{14} + y_{14}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{14} - y_{14}) \hat{\mathbf{y}} - c(z_{14} - \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{O XI} \\
\mathbf{B}_{133} &= -y_{14} \mathbf{a}_1 + (x_{14} - y_{14}) \mathbf{a}_2 - (z_{14} - \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(x_{14} - 2y_{14}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{14} \hat{\mathbf{y}} - c(z_{14} - \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{O XI} \\
\mathbf{B}_{134} &= -(x_{14} - y_{14}) \mathbf{a}_1 - x_{14} \mathbf{a}_2 - (z_{14} - \frac{1}{2}) \mathbf{a}_3 = -\frac{1}{2}a(2x_{14} - y_{14}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{14} \hat{\mathbf{y}} - c(z_{14} - \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{O XI} \\
\mathbf{B}_{135} &= x_{15} \mathbf{a}_1 + y_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3 = \frac{1}{2}a(x_{15} + y_{15}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{15} - y_{15}) \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}} & (12i) & \text{P II} \\
\mathbf{B}_{136} &= -y_{15} \mathbf{a}_1 + (x_{15} - y_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3 = \frac{1}{2}a(x_{15} - 2y_{15}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}} & (12i) & \text{P II} \\
\mathbf{B}_{137} &= -(x_{15} - y_{15}) \mathbf{a}_1 - x_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3 = -\frac{1}{2}a(2x_{15} - y_{15}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}} & (12i) & \text{P II} \\
\mathbf{B}_{138} &= -x_{15} \mathbf{a}_1 - y_{15} \mathbf{a}_2 + (z_{15} + \frac{1}{2}) \mathbf{a}_3 = -\frac{1}{2}a(x_{15} + y_{15}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{15} - y_{15}) \hat{\mathbf{y}} + c(z_{15} + \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{P II} \\
\mathbf{B}_{139} &= y_{15} \mathbf{a}_1 - (x_{15} - y_{15}) \mathbf{a}_2 + (z_{15} + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_{15} + 2y_{15}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{15} \hat{\mathbf{y}} + c(z_{15} + \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{P II} \\
\mathbf{B}_{140} &= (x_{15} - y_{15}) \mathbf{a}_1 + x_{15} \mathbf{a}_2 + (z_{15} + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(2x_{15} - y_{15}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{15} \hat{\mathbf{y}} + c(z_{15} + \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{P II} \\
\mathbf{B}_{141} &= -x_{15} \mathbf{a}_1 - y_{15} \mathbf{a}_2 - z_{15} \mathbf{a}_3 = -\frac{1}{2}a(x_{15} + y_{15}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{15} - y_{15}) \hat{\mathbf{y}} - cz_{15} \hat{\mathbf{z}} & (12i) & \text{P II} \\
\mathbf{B}_{142} &= y_{15} \mathbf{a}_1 - (x_{15} - y_{15}) \mathbf{a}_2 - z_{15} \mathbf{a}_3 = \frac{1}{2}a(-x_{15} + 2y_{15}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{15} \hat{\mathbf{y}} - cz_{15} \hat{\mathbf{z}} & (12i) & \text{P II} \\
\mathbf{B}_{143} &= (x_{15} - y_{15}) \mathbf{a}_1 + x_{15} \mathbf{a}_2 - z_{15} \mathbf{a}_3 = \frac{1}{2}a(2x_{15} - y_{15}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{15} \hat{\mathbf{y}} - cz_{15} \hat{\mathbf{z}} & (12i) & \text{P II} \\
\mathbf{B}_{144} &= x_{15} \mathbf{a}_1 + y_{15} \mathbf{a}_2 - (z_{15} - \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(x_{15} + y_{15}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{15} - y_{15}) \hat{\mathbf{y}} - c(z_{15} - \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{P II} \\
\mathbf{B}_{145} &= -y_{15} \mathbf{a}_1 + (x_{15} - y_{15}) \mathbf{a}_2 - (z_{15} - \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(x_{15} - 2y_{15}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{15} \hat{\mathbf{y}} - c(z_{15} - \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{P II} \\
\mathbf{B}_{146} &= -(x_{15} - y_{15}) \mathbf{a}_1 - x_{15} \mathbf{a}_2 - (z_{15} - \frac{1}{2}) \mathbf{a}_3 = -\frac{1}{2}a(2x_{15} - y_{15}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{15} \hat{\mathbf{y}} - c(z_{15} - \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{P II}
\end{aligned}$$

References

- [1] M. P. Attfield and A. W. Sleight, *Exceptional Negative Thermal Expansion in AlPO_417* , Chem. Mater. **10**, 2013–2019 (1998), doi:10.1021/acs.jpcclett.2c02718.

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