

PtAl₄ Structure:

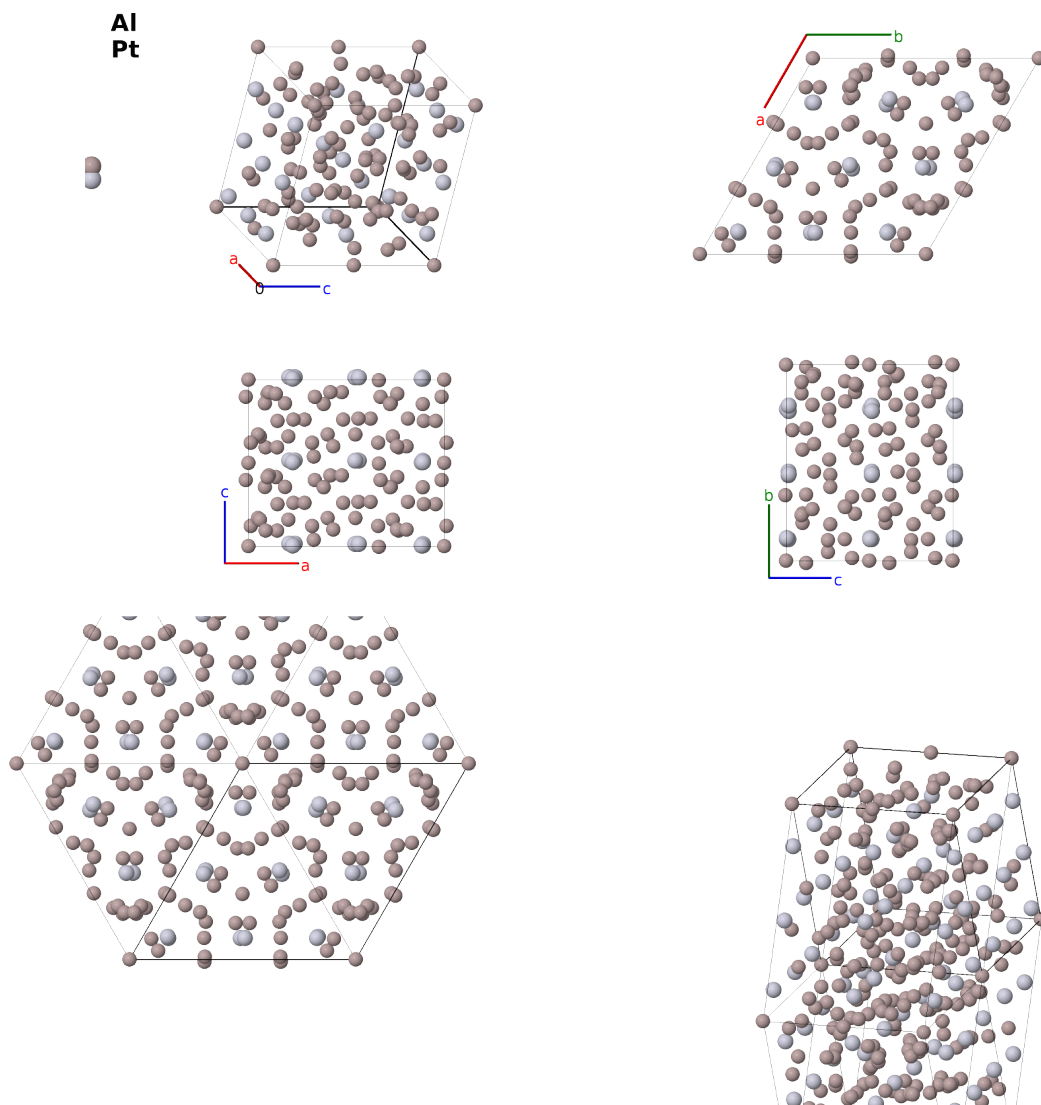
A14B3_hP102_158_abc13d_3d-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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.

<https://aflow.org/prototype-encyclopedia/05TH>

https://aflow.org/prototype-encyclopedia/A14B3_hP102_158_abc13d_3d-001



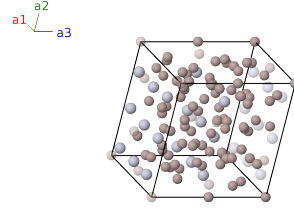
Prototype	Al ₄ Pt
AFLOW prototype label	A14B3_hP102_158_abc13d_3d-001
ICSD	417146
CCDC	1730613

Pearson symbol	hP102
Space group number	158
Space group symbol	$P3c1$
AFLOW prototype command	<pre>aflow --proto=A14B3_hP102_158_abc13d_3d-001 --params=a,c/a,z1,z2,z3,x4,y4,z4,x5,y5,z5,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,x16,y16,z16,x17, y17,z17,x18,y18,z18,x19,y19,z19</pre>

- (Wörle, 2008) found that the Al-V/Al-VI pair of sites was only occupied 57% and 33% of the time, respectively, with no more than one atom of pair of neighbors occupied. Similarly the Al-VII/Al-VIII occupation is 60% and 30%. All the other Wyckoff positions are fully occupied. The actual stoichiometry is thus $\text{PtAl}_{3.933}$.

Trigonal (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
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(2a)	Al I
$\mathbf{B}_2$	$= (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c (z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Al I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(2b)	Al II
$\mathbf{B}_4$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Al II
$\mathbf{B}_5$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(2c)	Al III
$\mathbf{B}_6$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(2c)	Al III
$\mathbf{B}_7$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_4 - y_4) \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(6d)	Al IV
$\mathbf{B}_8$	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(6d)	Al IV
$\mathbf{B}_9$	$= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(6d)	Al IV
$\mathbf{B}_{10}$	$= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_4 - y_4) \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(6d)	Al IV
$\mathbf{B}_{11}$	$= -(x_4 - y_4) \mathbf{a}_1 + y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_4 + 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_4 \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(6d)	Al IV
$\mathbf{B}_{12}$	$= x_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_4 \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(6d)	Al IV
$\mathbf{B}_{13}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_5 - y_5) \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(6d)	Al V
$\mathbf{B}_{14}$	$= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(6d)	Al V
$\mathbf{B}_{15}$	$= -(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(6d)	Al V
$\mathbf{B}_{16}$	$= -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_5 - y_5) \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(6d)	Al V

$$\begin{aligned}
\mathbf{B}_{17} &= -(x_5 - y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}} & (6d) & \text{Al V} \\
\mathbf{B}_{18} &= x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}} & (6d) & \text{Al V} \\
\mathbf{B}_{19} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = \frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (6d) & \text{Al VI} \\
\mathbf{B}_{20} &= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3 = \frac{1}{2}a(x_6 - 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (6d) & \text{Al VI} \\
\mathbf{B}_{21} &= -(x_6 - y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = -\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (6d) & \text{Al VI} \\
\mathbf{B}_{22} &= -y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 = -\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}} & (6d) & \text{Al VI} \\
\mathbf{B}_{23} &= -(x_6 - y_6) \mathbf{a}_1 + y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_6 + 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}} & (6d) & \text{Al VI} \\
\mathbf{B}_{24} &= x_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}} & (6d) & \text{Al VI} \\
\mathbf{B}_{25} &= x_7 \mathbf{a}_1 + y_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}} & (6d) & \text{Al VII} \\
\mathbf{B}_{26} &= -y_7 \mathbf{a}_1 + (x_7 - 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}} & (6d) & \text{Al VII} \\
\mathbf{B}_{27} &= -(x_7 - y_7) \mathbf{a}_1 - x_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}} & (6d) & \text{Al VII} \\
\mathbf{B}_{28} &= -y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \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}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} & (6d) & \text{Al VII} \\
\mathbf{B}_{29} &= -(x_7 - y_7) \mathbf{a}_1 + y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_7 + 2y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} & (6d) & \text{Al VII} \\
\mathbf{B}_{30} &= x_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} & (6d) & \text{Al VII} \\
\mathbf{B}_{31} &= 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}} & (6d) & \text{Al VIII} \\
\mathbf{B}_{32} &= -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}} & (6d) & \text{Al VIII} \\
\mathbf{B}_{33} &= -(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}} & (6d) & \text{Al VIII} \\
\mathbf{B}_{34} &= -y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \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(z_8 + \frac{1}{2}) \hat{\mathbf{z}} & (6d) & \text{Al VIII} \\
\mathbf{B}_{35} &= -(x_8 - y_8) \mathbf{a}_1 + y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_8 + 2y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}} & (6d) & \text{Al VIII} \\
\mathbf{B}_{36} &= x_8 \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(2x_8 - y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}} & (6d) & \text{Al VIII} \\
\mathbf{B}_{37} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \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}} + cz_9 \hat{\mathbf{z}} & (6d) & \text{Al IX} \\
\mathbf{B}_{38} &= -y_9 \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3 = \frac{1}{2}a(x_9 - 2y_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (6d) & \text{Al IX} \\
\mathbf{B}_{39} &= -(x_9 - y_9) \mathbf{a}_1 - x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = -\frac{1}{2}a(2x_9 - y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (6d) & \text{Al IX} \\
\mathbf{B}_{40} &= -y_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \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(z_9 + \frac{1}{2}) \hat{\mathbf{z}} & (6d) & \text{Al IX} \\
\mathbf{B}_{41} &= -(x_9 - y_9) \mathbf{a}_1 + y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_9 + 2y_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}} & (6d) & \text{Al IX} \\
\mathbf{B}_{42} &= x_9 \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(2x_9 - y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}} & (6d) & \text{Al IX} \\
\mathbf{B}_{43} &= 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}} & (6d) & \text{Al X} \\
\mathbf{B}_{44} &= -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}} & (6d) & \text{Al X} \\
\mathbf{B}_{45} &= -(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}} & (6d) & \text{Al X} \\
\mathbf{B}_{46} &= -y_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \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(z_{10} + \frac{1}{2}) \hat{\mathbf{z}} & (6d) & \text{Al X} \\
\mathbf{B}_{47} &= -(x_{10} - y_{10}) \mathbf{a}_1 + y_{10} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_{10} + 2y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}} & (6d) & \text{Al X} \\
\mathbf{B}_{48} &= x_{10} \mathbf{a}_1 + (x_{10} - y_{10}) \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(2x_{10} - y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}} & (6d) & \text{Al X}
\end{aligned}$$

$\mathbf{B}_{49} =$	$x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{11} + y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{11} - y_{11}) \hat{\mathbf{y}} +$ $cz_{11} \hat{\mathbf{z}}$	$(6d)$	Al XI
$\mathbf{B}_{50} =$	$-y_{11} \mathbf{a}_1 + (x_{11} - y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{11} - 2y_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	$(6d)$	Al XI
$\mathbf{B}_{51} =$	$-(x_{11} - y_{11}) \mathbf{a}_1 - x_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{11} - y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	$(6d)$	Al XI
$\mathbf{B}_{52} =$	$-y_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_{11} + y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{11} - y_{11}) \hat{\mathbf{y}} +$ $c(z_{11} + \frac{1}{2}) \hat{\mathbf{z}}$	$(6d)$	Al XI
$\mathbf{B}_{53} =$	$-(x_{11} - y_{11}) \mathbf{a}_1 + y_{11} \mathbf{a}_2 +$ $(z_{11} + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_{11} + 2y_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{11} \hat{\mathbf{y}} +$ $c(z_{11} + \frac{1}{2}) \hat{\mathbf{z}}$	$(6d)$	Al XI
$\mathbf{B}_{54} =$	$x_{11} \mathbf{a}_1 + (x_{11} - y_{11}) \mathbf{a}_2 +$ $(z_{11} + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_{11} - y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{11} \hat{\mathbf{y}} +$ $c(z_{11} + \frac{1}{2}) \hat{\mathbf{z}}$	$(6d)$	Al XI
$\mathbf{B}_{55} =$	$x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{12} + y_{12}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{12} - y_{12}) \hat{\mathbf{y}} +$ $cz_{12} \hat{\mathbf{z}}$	$(6d)$	Al XII
$\mathbf{B}_{56} =$	$-y_{12} \mathbf{a}_1 + (x_{12} - y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{12} - 2y_{12}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}}$	$(6d)$	Al XII
$\mathbf{B}_{57} =$	$-(x_{12} - y_{12}) \mathbf{a}_1 - x_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{12} - y_{12}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}}$	$(6d)$	Al XII
$\mathbf{B}_{58} =$	$-y_{12} \mathbf{a}_1 - x_{12} \mathbf{a}_2 + (z_{12} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_{12} + y_{12}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{12} - y_{12}) \hat{\mathbf{y}} +$ $c(z_{12} + \frac{1}{2}) \hat{\mathbf{z}}$	$(6d)$	Al XII
$\mathbf{B}_{59} =$	$-(x_{12} - y_{12}) \mathbf{a}_1 + y_{12} \mathbf{a}_2 +$ $(z_{12} + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_{12} + 2y_{12}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{12} \hat{\mathbf{y}} +$ $c(z_{12} + \frac{1}{2}) \hat{\mathbf{z}}$	$(6d)$	Al XII
$\mathbf{B}_{60} =$	$x_{12} \mathbf{a}_1 + (x_{12} - y_{12}) \mathbf{a}_2 +$ $(z_{12} + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_{12} - y_{12}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{12} \hat{\mathbf{y}} +$ $c(z_{12} + \frac{1}{2}) \hat{\mathbf{z}}$	$(6d)$	Al XII
$\mathbf{B}_{61} =$	$x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{13} + y_{13}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{13} - y_{13}) \hat{\mathbf{y}} +$ $cz_{13} \hat{\mathbf{z}}$	$(6d)$	Al XIII
$\mathbf{B}_{62} =$	$-y_{13} \mathbf{a}_1 + (x_{13} - y_{13}) \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{13} - 2y_{13}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}}$	$(6d)$	Al XIII
$\mathbf{B}_{63} =$	$-(x_{13} - y_{13}) \mathbf{a}_1 - x_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{13} - y_{13}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}}$	$(6d)$	Al XIII
$\mathbf{B}_{64} =$	$-y_{13} \mathbf{a}_1 - x_{13} \mathbf{a}_2 + (z_{13} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_{13} + y_{13}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{13} - y_{13}) \hat{\mathbf{y}} +$ $c(z_{13} + \frac{1}{2}) \hat{\mathbf{z}}$	$(6d)$	Al XIII
$\mathbf{B}_{65} =$	$-(x_{13} - y_{13}) \mathbf{a}_1 + y_{13} \mathbf{a}_2 +$ $(z_{13} + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_{13} + 2y_{13}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{13} \hat{\mathbf{y}} +$ $c(z_{13} + \frac{1}{2}) \hat{\mathbf{z}}$	$(6d)$	Al XIII
$\mathbf{B}_{66} =$	$x_{13} \mathbf{a}_1 + (x_{13} - y_{13}) \mathbf{a}_2 +$ $(z_{13} + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_{13} - y_{13}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{13} \hat{\mathbf{y}} +$ $c(z_{13} + \frac{1}{2}) \hat{\mathbf{z}}$	$(6d)$	Al XIII
$\mathbf{B}_{67} =$	$x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{14} + y_{14}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{14} - y_{14}) \hat{\mathbf{y}} +$ $cz_{14} \hat{\mathbf{z}}$	$(6d)$	Al XIV
$\mathbf{B}_{68} =$	$-y_{14} \mathbf{a}_1 + (x_{14} - y_{14}) \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{14} - 2y_{14}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}}$	$(6d)$	Al XIV
$\mathbf{B}_{69} =$	$-(x_{14} - y_{14}) \mathbf{a}_1 - x_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{14} - y_{14}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}}$	$(6d)$	Al XIV
$\mathbf{B}_{70} =$	$-y_{14} \mathbf{a}_1 - x_{14} \mathbf{a}_2 + (z_{14} + \frac{1}{2}) \mathbf{a}_3$	$=$			

References

- [1] M. Wörle, F. Krumeich, T. Chatterji, S. Kek, and R. Nesper, *On the structure and twinning of PtAl₄*, J. Alloys Compd. **455**, 130–136 (2008), doi:10.1016/j.jallcom.2007.01.161.

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