PdAl Structure: AB_hR26_148_a2f_b2f-001

This structure originally had the label `AB_hR26_148_b2f_a2f`. Calls to that address will be redirected here.

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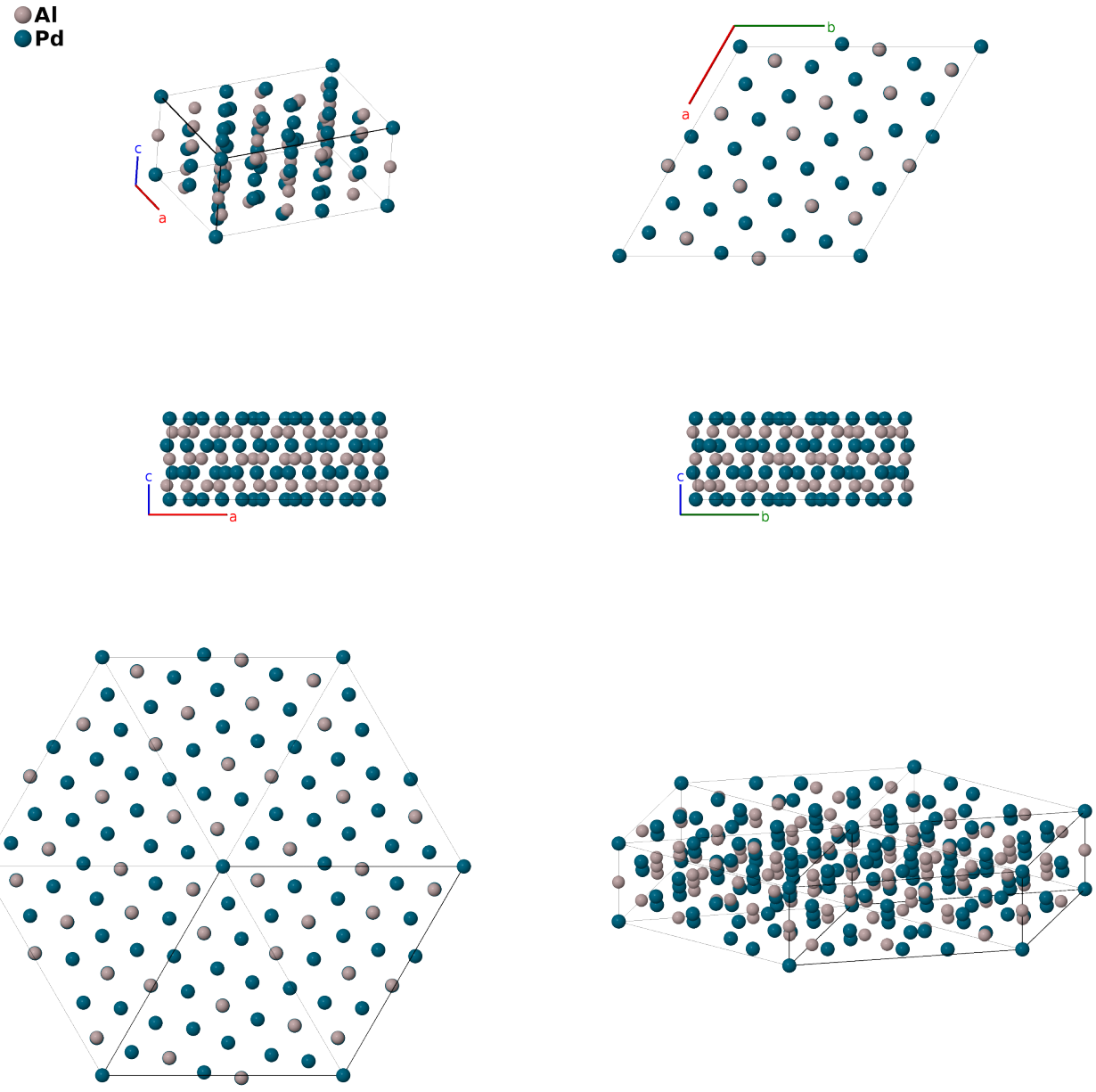
https://aflow.org/p/5EQ4

https://aflow.org/p/AB_hR26_148_a2f_b2f-001



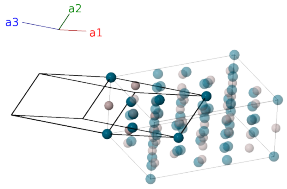
Prototype	AlPd
AFLOW prototype label	AB_hR26_148_a2f_b2f-001

ICSD	58112
Pearson symbol	hR26
Space group number	148
Space group symbol	$R\bar{3}$
AFLOW prototype command	`aflow --proto=AB_hR26_148_a2f_b2f-001 --params=`$a, c/a, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Pd I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_3 - 2y_3 + z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	Al II
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_3 - y_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	Al II
$\mathbf{B_5}$	=	$y_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3 - y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_3 + y_3 - 2z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	Al II
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - 2y_3 + z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	Al II
$\mathbf{B_7}$	=	$-z_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_3 - z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_3 - y_3 - z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	Al II
$\mathbf{B_8}$	=	$-y_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 + y_3 - 2z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	Al II
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - z_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_4 - 2y_4 + z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(6f)	Al III
$\mathbf{B_{10}}$	=	$z_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_4 - z_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_4 - y_4 - z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(6f)	Al III
$\mathbf{B_{11}}$	=	$y_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_4 - y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_4 + y_4 - 2z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(6f)	Al III
$\mathbf{B_{12}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_4 - z_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_4 - 2y_4 + z_4)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(6f)	Al III
$\mathbf{B_{13}}$	=	$-z_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_4 - z_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_4 - y_4 - z_4)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(6f)	Al III

$$\mathbf{B_{14}} = -y_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_4 - y_4)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_4 + y_4 - 2z_4)\,\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Al III}$$

$$\mathbf{B_{15}} = x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_5 - z_5)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_5 - 2y_5 + z_5)\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Pd II}$$

$$\mathbf{B_{16}} = z_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + y_5\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_5 - z_5)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_5 - y_5 - z_5)\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Pd II}$$

$$\mathbf{B_{17}} = y_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_5 - y_5)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_5 + y_5 - 2z_5)\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Pd II}$$

$$\mathbf{B_{18}} = -x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_5 - z_5)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_5 - 2y_5 + z_5)\,\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Pd II}$$

$$\mathbf{B_{19}} = -z_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - y_5\,\mathbf{a}_3 = \tfrac{1}{2}a\,(y_5 - z_5)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(2x_5 - y_5 - z_5)\,\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Pd II}$$

$$\mathbf{B_{20}} = -y_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_5 - y_5)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_5 + y_5 - 2z_5)\,\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Pd II}$$

$$\mathbf{B_{21}} = x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Pd III}$$

$$\mathbf{B_{22}} = z_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + y_6\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_6 - z_6)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Pd III}$$

$$\mathbf{B_{23}} = y_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_6 - y_6)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Pd III}$$

$$\mathbf{B_{24}} = -x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\,\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Pd III}$$

$$\mathbf{B_{25}} = -z_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - y_6\,\mathbf{a}_3 = \tfrac{1}{2}a\,(y_6 - z_6)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\,\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Pd III}$$

$$\mathbf{B_{26}} = -y_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_6 - y_6)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\,\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Pd III}$$

References

[1] T. Matković and K. Schubert, *Kristallstruktur vo PdAl.r*, J. Less-Common Met. **55**, 45–52 (1977), doi:10.1016/0022-5088(77)90258-2.

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[1] P. Villars, K. Cenzual, J. Daams, R. Gladyshevskii, O. Shcherban, V. Dubenskyy, V. Kuprysyuk, and I. Savesyuk, *Landolt–Börnstein – Group III Condensed Matter* (Springer–Verlag GmbH, Heidelberg, 2010), chap. Structure Types. Part 8: Space Groups (156)P3m1 – (148)R-3 · PdAl rt, doi:10.1007/978-3-540-70892-6_476. Part 8.