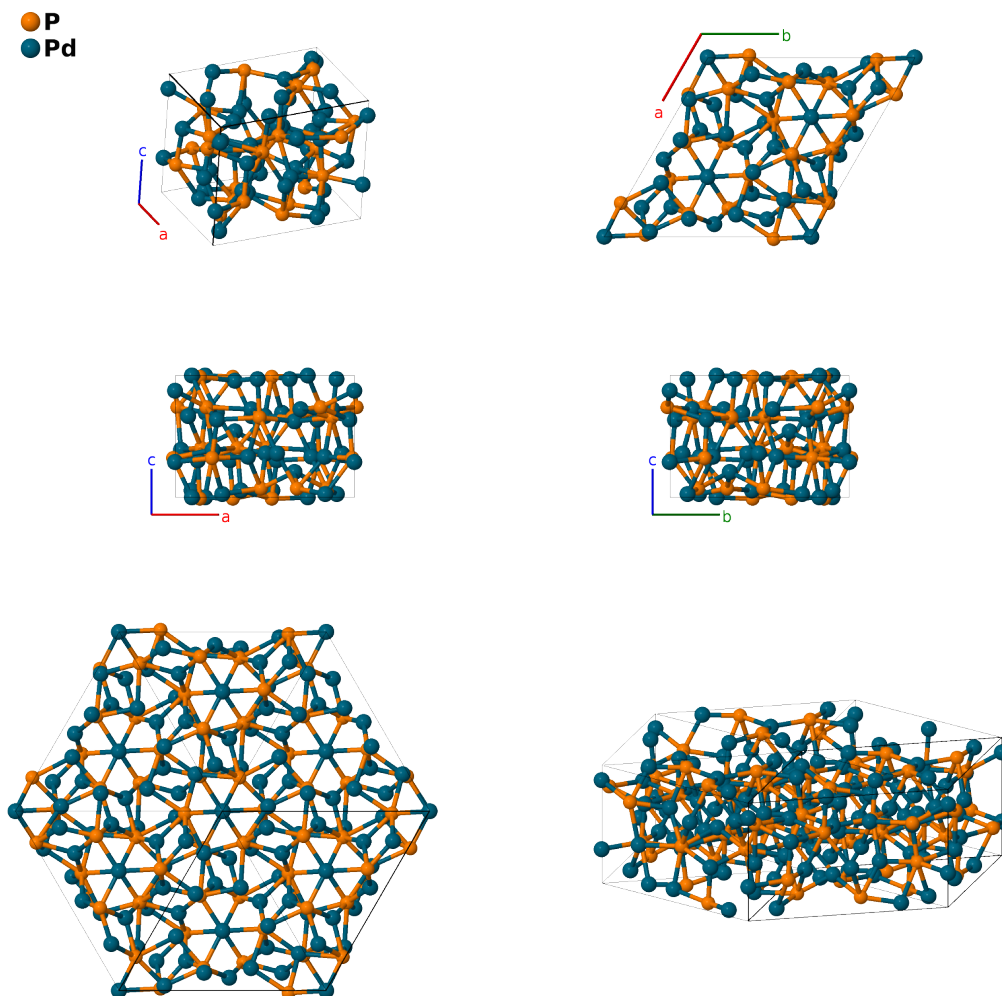


Pd₇P₃ Structure: A3B7_hR20_146_2b_2a4b-001

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<https://aflow.org/p/35AG>

https://aflow.org/p/A3B7_hR20_146_2b_2a4b-001

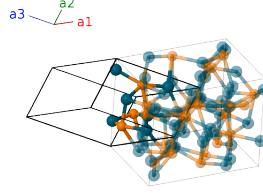


| | |
|-------------------------|--|
| Prototype | P ₃ Pd ₇ |
| AFLOW prototype label | A3B7_hR20_146_2b_2a4b-001 |
| ICSD | 200055 |
| Pearson symbol | hR20 |
| Space group number | 146 |
| Space group symbol | <i>R</i> 3 |
| AFLOW prototype command | <code>aflow --proto=A3B7_hR20_146_2b_2a4b-001</code> <code>--params=a, c/a, x₁, x₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆, x₇, y₇, z₇, x₈, y₈, z₈</code> |

- Space group $R3$ #146 allows an arbitrary choice of the origin of the z -axis. Here we set $z_5 = 0$ for the Pd-III atom.
- Hexagonal settings for rhombohedral structures can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

| | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|-------------------|--|---|---|------------------|-----------|
| \mathbf{B}_1 | $x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$ | = | $cx_1 \hat{\mathbf{z}}$ | (1a) | Pd I |
| \mathbf{B}_2 | $x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$ | = | $cx_2 \hat{\mathbf{z}}$ | (1a) | Pd II |
| \mathbf{B}_3 | $x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$ | = | $\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$ | (3b) | P I |
| \mathbf{B}_4 | $z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$ | = | $-\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$ | (3b) | P I |
| \mathbf{B}_5 | $y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$ | = | $-\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$ | (3b) | P I |
| \mathbf{B}_6 | $x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$ | = | $\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 - 2y_4 + z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$ | (3b) | P II |
| \mathbf{B}_7 | $z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$ | = | $-\frac{1}{2}a(y_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_4 - y_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$ | (3b) | P II |
| \mathbf{B}_8 | $y_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$ | = | $-\frac{1}{2}a(x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 + y_4 - 2z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$ | (3b) | P II |
| \mathbf{B}_9 | $x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$ | = | $\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 - 2y_5 + z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$ | (3b) | Pd III |
| \mathbf{B}_{10} | $z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$ | = | $-\frac{1}{2}a(y_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_5 - y_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$ | (3b) | Pd III |
| \mathbf{B}_{11} | $y_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$ | = | $-\frac{1}{2}a(x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 + y_5 - 2z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$ | (3b) | Pd III |
| \mathbf{B}_{12} | $x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$ | = | $\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 - 2y_6 + z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$ | (3b) | Pd IV |
| \mathbf{B}_{13} | $z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$ | = | $-\frac{1}{2}a(y_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_6 - y_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$ | (3b) | Pd IV |
| \mathbf{B}_{14} | $y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$ | = | $-\frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$ | (3b) | Pd IV |
| \mathbf{B}_{15} | $x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$ | = | $\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 - 2y_7 + z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$ | (3b) | Pd V |
| \mathbf{B}_{16} | $z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + y_7 \mathbf{a}_3$ | = | $-\frac{1}{2}a(y_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_7 - y_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$ | (3b) | Pd V |

$$\begin{aligned}
\mathbf{B}_{17} &= y_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3 &= -\frac{1}{2}a(x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 + y_7 - 2z_7) \hat{\mathbf{y}} + & (3b) & \text{Pd V} \\
&&& \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}} \\
\mathbf{B}_{18} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= \frac{1}{2}a(x_8 - z_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_8 - 2y_8 + z_8) \hat{\mathbf{y}} + & (3b) & \text{Pd VI} \\
&&& \frac{1}{3}c(x_8 + y_8 + z_8) \hat{\mathbf{z}} \\
\mathbf{B}_{19} &= z_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + y_8 \mathbf{a}_3 &= -\frac{1}{2}a(y_8 - z_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_8 - y_8 - z_8) \hat{\mathbf{y}} + & (3b) & \text{Pd VI} \\
&&& \frac{1}{3}c(x_8 + y_8 + z_8) \hat{\mathbf{z}} \\
\mathbf{B}_{20} &= y_8 \mathbf{a}_1 + z_8 \mathbf{a}_2 + x_8 \mathbf{a}_3 &= -\frac{1}{2}a(x_8 - y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_8 + y_8 - 2z_8) \hat{\mathbf{y}} + & (3b) & \text{Pd VI} \\
&&& \frac{1}{3}c(x_8 + y_8 + z_8) \hat{\mathbf{z}}
\end{aligned}$$

References

- [1] T. Matković and K. Schubert, *Kristallstruktur von Pd₇P₃*, J. Less-Common Met. **55**, 177–184 (1977), doi:10.1016/0022-5088(77)90190-4.