

# Pt<sub>6</sub>Si<sub>5</sub> Structure:

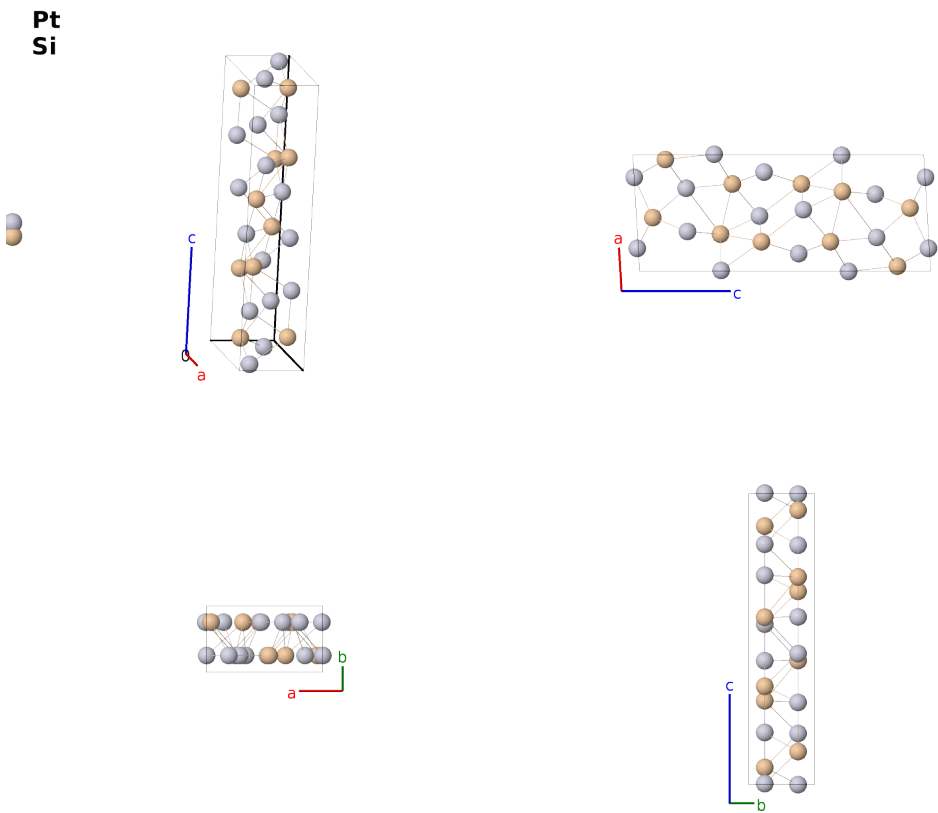
## A6B5\_mP22\_11\_6e\_5e-001

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<https://aflow.org/prototype-encyclopedia/H63U>

[https://aflow.org/prototype-encyclopedia/A6B5\\_mP22\\_11\\_6e\\_5e-001](https://aflow.org/prototype-encyclopedia/A6B5_mP22_11_6e_5e-001)

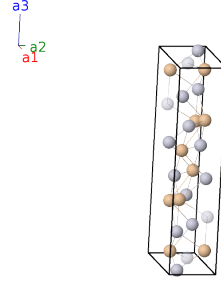


|                         |                                                                                                                                                                                                                                                   |
|-------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prototype               | Pt <sub>6</sub> Si <sub>5</sub>                                                                                                                                                                                                                   |
| AFLOW prototype label   | A6B5_mP22_11_6e_5e-001                                                                                                                                                                                                                            |
| ICSD                    | 43283                                                                                                                                                                                                                                             |
| CCDC                    | 1612800                                                                                                                                                                                                                                           |
| Pearson symbol          | mP22                                                                                                                                                                                                                                              |
| Space group number      | 11                                                                                                                                                                                                                                                |
| Space group symbol      | $P2_1/m$                                                                                                                                                                                                                                          |
| AFLOW prototype command | <code>aflow --proto=A6B5_mP22_11_6e_5e-001</code><br><code>--params=a, b/a, c/a, <math>\beta</math>, <math>x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, z_{11}</math></code> |

- Our rendition of this structure swaps the x- and z-axis used by (Gohle, 1964).

## Simple Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors

|                   | Lattice<br>coordinates                                                  |   | Cartesian<br>coordinates                                                                                                  | Wyckoff<br>position | Atom<br>type |
|-------------------|-------------------------------------------------------------------------|---|---------------------------------------------------------------------------------------------------------------------------|---------------------|--------------|
| $\mathbf{B}_1$    | $x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$        | = | $(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$           | (2e)                | Pt I         |
| $\mathbf{B}_2$    | $-x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$       | = | $-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$          | (2e)                | Pt I         |
| $\mathbf{B}_3$    | $x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$        | = | $(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$           | (2e)                | Pt II        |
| $\mathbf{B}_4$    | $-x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$       | = | $-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$          | (2e)                | Pt II        |
| $\mathbf{B}_5$    | $x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$        | = | $(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$           | (2e)                | Pt III       |
| $\mathbf{B}_6$    | $-x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$       | = | $-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$          | (2e)                | Pt III       |
| $\mathbf{B}_7$    | $x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$        | = | $(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$           | (2e)                | Pt IV        |
| $\mathbf{B}_8$    | $-x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$       | = | $-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$          | (2e)                | Pt IV        |
| $\mathbf{B}_9$    | $x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$        | = | $(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$           | (2e)                | Pt V         |
| $\mathbf{B}_{10}$ | $-x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3$       | = | $-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$          | (2e)                | Pt V         |
| $\mathbf{B}_{11}$ | $x_6 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_6 \mathbf{a}_3$        | = | $(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$           | (2e)                | Pt VI        |
| $\mathbf{B}_{12}$ | $-x_6 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_6 \mathbf{a}_3$       | = | $-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$          | (2e)                | Pt VI        |
| $\mathbf{B}_{13}$ | $x_7 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_7 \mathbf{a}_3$        | = | $(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$           | (2e)                | Si I         |
| $\mathbf{B}_{14}$ | $-x_7 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_7 \mathbf{a}_3$       | = | $-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$          | (2e)                | Si I         |
| $\mathbf{B}_{15}$ | $x_8 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_8 \mathbf{a}_3$        | = | $(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$           | (2e)                | Si II        |
| $\mathbf{B}_{16}$ | $-x_8 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_8 \mathbf{a}_3$       | = | $-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$          | (2e)                | Si II        |
| $\mathbf{B}_{17}$ | $x_9 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_9 \mathbf{a}_3$        | = | $(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$           | (2e)                | Si III       |
| $\mathbf{B}_{18}$ | $-x_9 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_9 \mathbf{a}_3$       | = | $-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}}$          | (2e)                | Si III       |
| $\mathbf{B}_{19}$ | $x_{10} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{10} \mathbf{a}_3$  | = | $(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$  | (2e)                | Si IV        |
| $\mathbf{B}_{20}$ | $-x_{10} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{10} \mathbf{a}_3$ | = | $-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_{10} \sin \beta \hat{\mathbf{z}}$ | (2e)                | Si IV        |
| $\mathbf{B}_{21}$ | $x_{11} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{11} \mathbf{a}_3$  | = | $(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$  | (2e)                | Si V         |
| $\mathbf{B}_{22}$ | $-x_{11} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{11} \mathbf{a}_3$ | = | $-(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_{11} \sin \beta \hat{\mathbf{z}}$ | (2e)                | Si V         |

## References

- [1] R. Gohle and K. Schubert, *Zum Aufbau des Systems Platin-Silizium*, Z. Metallkd. **55**, 503–511 (1964), doi:10.1515/ijmr-1964-550901.

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- [1] G. Majni, M. Costato, F. anini, and G. Celotti, *The film compounds in planar Pt-Si reaction*, J. Phys. Chem. Solids **46**, 631–641 (1985), doi:10.1016/0022-3697(85)90227-6. (Majni, 1985) erroneously identify R. Gohle as W. Gold (see Ref. 12).

### First cited in

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.