

PdGa₅ Structure:

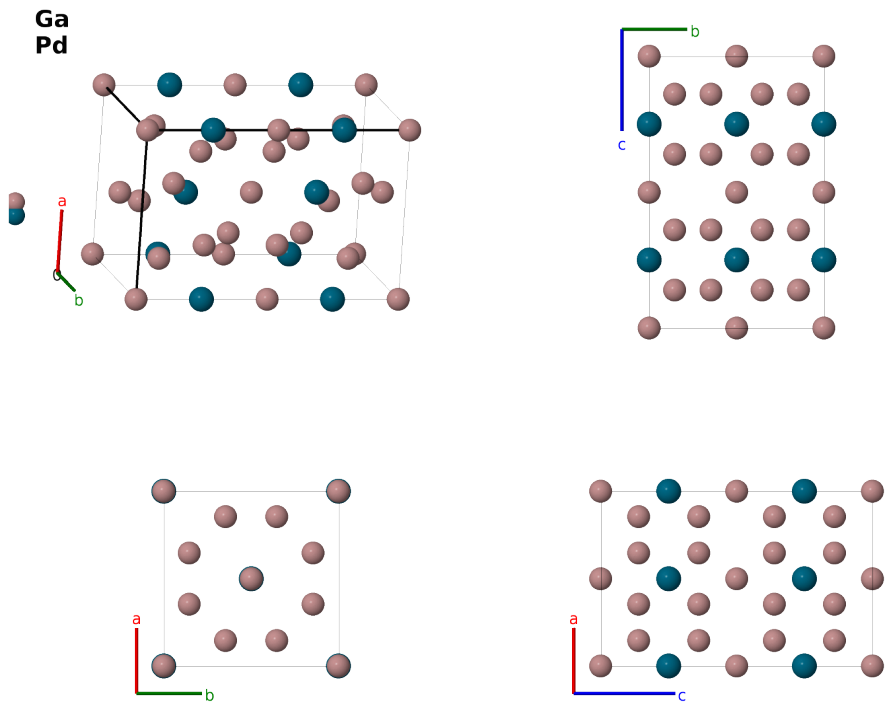
A5B_tI24_140_cl_a-001

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<https://aflow.org/prototype-encyclopedia/528Z>

https://aflow.org/prototype-encyclopedia/A5B_tI24_140_cl_a-001

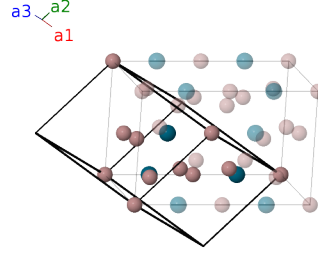


Prototype	Ga ₅ Pd
AFLOW prototype label	A5B_tI24_140_cl_a-001
ICSD	103908
CCDC	1661839
Pearson symbol	tI24
Space group number	140
Space group symbol	<i>I4/mcm</i>
AFLOW prototype command	<code>aflow --proto=A5B_tI24_140_cl_a-001</code> <code>--params=a, c/a, x₃, z₃</code>

• There is no ICSD entry for (Grin, 1997). It is a refinement of the work of (Schubert, 1959), and we list that ICSD entry.

Body-centered Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{1}{4}c \hat{\mathbf{z}}$	(4a)	Pd I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{3}{4}c \hat{\mathbf{z}}$	(4a)	Pd I
$\mathbf{B}_3$	$= 0$	$=$	0	(4c)	Ga I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(4c)	Ga I
$\mathbf{B}_5$	$= (x_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + (2x_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(16l)	Ga II
$\mathbf{B}_6$	$= (-x_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - z_3) \mathbf{a}_2 - (2x_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(16l)	Ga II
$\mathbf{B}_7$	$= (x_3 + z_3) \mathbf{a}_1 + (-x_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(16l)	Ga II
$\mathbf{B}_8$	$= -(x_3 - z_3) \mathbf{a}_1 + (x_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(16l)	Ga II
$\mathbf{B}_9$	$= (x_3 - z_3) \mathbf{a}_1 - (x_3 + z_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(16l)	Ga II
$\mathbf{B}_{10}$	$= -(x_3 + z_3) \mathbf{a}_1 + (x_3 - z_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(16l)	Ga II
$\mathbf{B}_{11}$	$= (x_3 - z_3 + \frac{1}{2}) \mathbf{a}_1 + (x_3 - z_3) \mathbf{a}_2 + (2x_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(16l)	Ga II
$\mathbf{B}_{12}$	$= -(x_3 + z_3 - \frac{1}{2}) \mathbf{a}_1 - (x_3 + z_3) \mathbf{a}_2 - (2x_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(16l)	Ga II

References

- [1] Y. Grin, K. Peters, and H. G. von Schnering, *Refinement of the crystal structure of palladium pentagallide, PdGa₅*, Z. Kristallogr. **212**, 6 (1997), doi:10.1524/zkri.1997.212.s1.6.
- [2] K. Schubert, H. Lukas, H. Mei, and S. Bhan, *Zum Aufbau der Systeme Kobalt-Gallium, Palladium-Gallium, Palladium-Zinn und verwandter Legierungen*, Z. Metallkd. **50**, 534–540 (1959).

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