$PdGa_5$ Structure: A5B_tI24_140_cl_a-001

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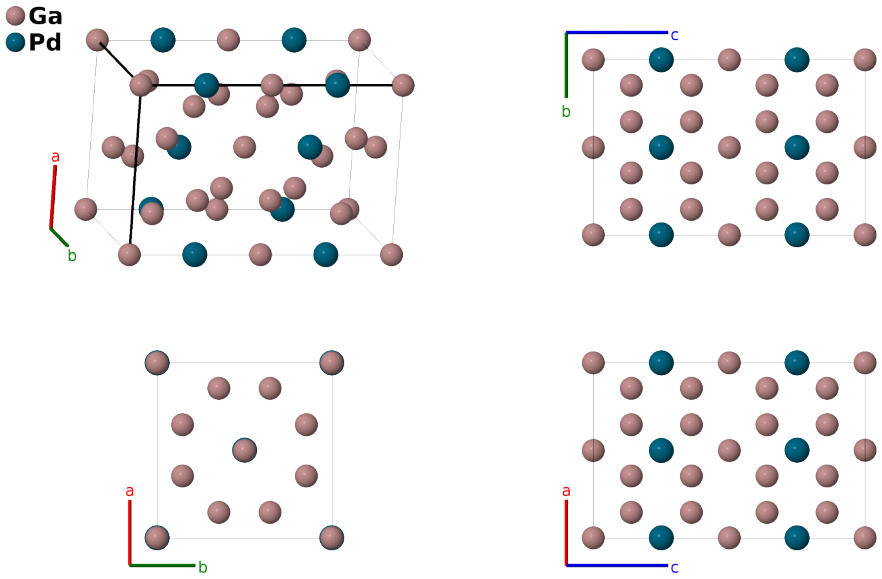
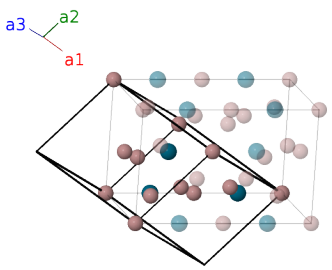


Prototype	Ga_5Pd
AFLOW prototype label	A5B_tI24_140_cl_a-001
ICSD	103908
Pearson symbol	tI24
Space group number	140
Space group symbol	$I4/mcm$
AFLOW prototype command	`aflow --proto=A5B_tI24_140_cl_a-001 --params=`$a, c/a, x_3, z_3$

- 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

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



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
$\mathbf{B_5}$	=	$\left(x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 + z_3\right)\,\mathbf{a}_2 + \left(2x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16l)	Ga II
$\mathbf{B_6}$	=	$\left(-x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 - z_3\right)\,\mathbf{a}_2 - \left(2x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16l)	Ga II
$\mathbf{B_7}$	=	$\left(x_3 + z_3\right)\,\mathbf{a}_1 + \left(-x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16l)	Ga II
$\mathbf{B_8}$	=	$-\left(x_3 - z_3\right)\,\mathbf{a}_1 + \left(x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16l)	Ga II
$\mathbf{B_9}$	=	$\left(x_3 - z_3\right)\,\mathbf{a}_1 - \left(x_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16l)	Ga II
$\mathbf{B_{10}}$	=	$-\left(x_3 + z_3\right)\,\mathbf{a}_1 + \left(x_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16l)	Ga II
$\mathbf{B_{11}}$	=	$\left(x_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 - z_3\right)\,\mathbf{a}_2 + \left(2x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16l)	Ga II
$\mathbf{B_{12}}$	=	$-\left(x_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 + z_3\right)\,\mathbf{a}_2 - \left(2x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16l)	Ga II

References

[1] Y. Grin, K. Peters, and H. G. von Schnering, *Refinement of the crystal structure of palladium pentagallide, $PdGa_5$*, 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).