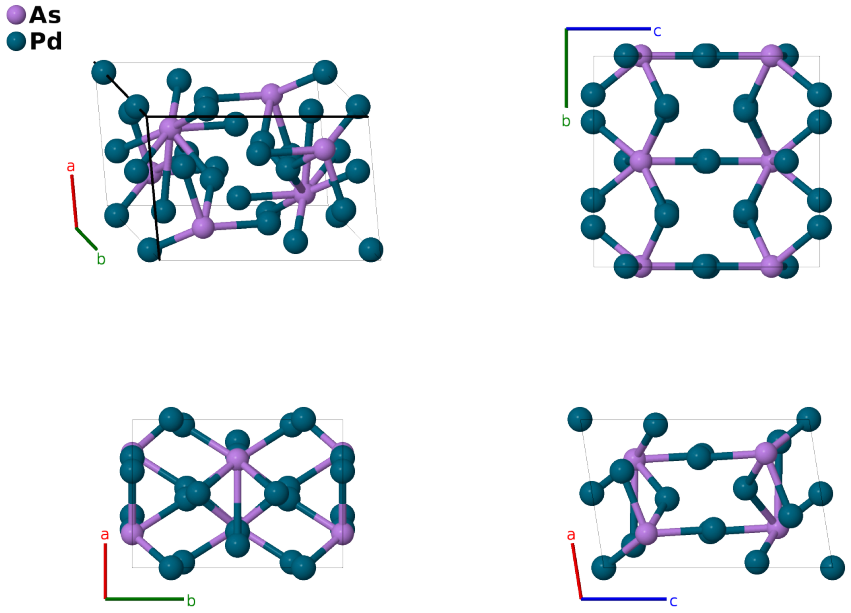
Pd_5As Structure: AB5_mC24_12_i_g2ij-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/XSQ7

https://aflow.org/p/AB5_mC24_12_i_g2ij-001

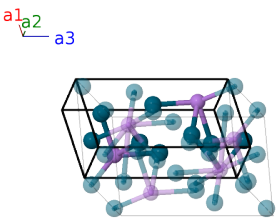


Prototype	$AsPd_5$
AFLOW prototype label	AB5_mC24_12_i_g2ij-001
ICSD	239291
Pearson symbol	mC24
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=AB5_mC24_12_i_g2ij-001 --params=`$a, b/a, c/a, \beta, y_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, y_5, z_5$

- We have shifted the origin of the z-axis by $c/2$ from that used by (Kohlman, 2016). This changes the position of the palladium atoms from the (4h) Wyckoff position to (4g).

Base-centered Monoclinic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2$	=	$by_1\,\hat{\mathbf{y}}$	(4g)	Pd I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2$	=	$-by_1\,\hat{\mathbf{y}}$	(4g)	Pd I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	As I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	As I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pd II
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pd II
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pd III
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pd III
$\mathbf{B_9}$	=	$(x_5 - y_5)\,\mathbf{a}_1 + (x_5 + y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(8j)	Pd IV
$\mathbf{B_{10}}$	=	$-(x_5 + y_5)\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(8j)	Pd IV
$\mathbf{B_{11}}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - (x_5 + y_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(8j)	Pd IV
$\mathbf{B_{12}}$	=	$(x_5 + y_5)\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(8j)	Pd IV

References

[1] H. Kohlmann, M. Vasseur, A. Sayede, G. Lefevre, J. M. Sander, and S. Doylee, *Crystal structure and hydrogenation properties of Pd_5As*, J. Alloys Compd. **664**, 256–265 (2016), doi:10.1016/j.jallcom.2015.12.039.