$PdBr_2$ Structure: A2B_mC12_15_f_a-002

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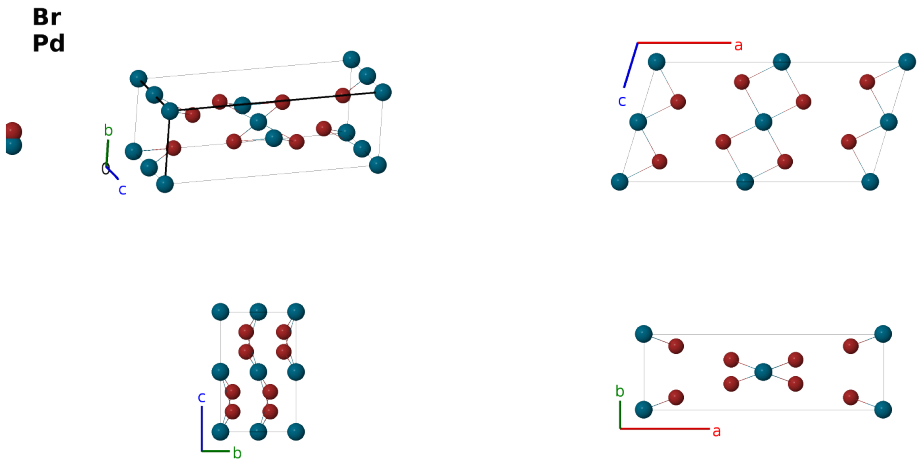
https://aflow.org/prototype-encyclopedia/M9Q8

https://aflow.org/prototype-encyclopedia/A2B_mC12_15_f_a-002

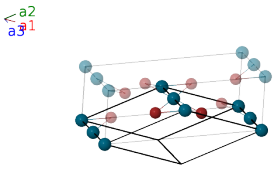


Prototype	Br_2Pd
AFLOW prototype label	A2B_mC12_15_f_a-002
ICSD	27443
CCDC	1602720
Pearson symbol	mC12
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	`aflow --proto=A2B_mC12_15_f_a-002 --params=`$a, b/a, c/a, \beta, x_2, y_2, z_2$

- (Brodersen, 1966) places this structure in space group $P2_1/c$#14 and Pearson Symbol mP24, however atomic coordinates are consistent with space group $C2/c$#15 with a primitive cell containing only six atoms. The ICSD entry uses the original structure, however (Villars, 2016) also uses the $C2/c$ structure.
- PdP_2 and $PdBr_2$ have the same AFLOW prototype label, A2B_mC12_15_f_a. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

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
$\mathbf{B_1}$	=	0	=	0	(4a)	Pd I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(4a)	Pd I
$\mathbf{B_3}$	=	$(x_2 - y_2)\,\mathbf{a}_1 + (x_2 + y_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(8f)	Br I
$\mathbf{B_4}$	=	$-(x_2 + y_2)\,\mathbf{a}_1 - (x_2 - y_2)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_2 + c\left(z_2 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Br I
$\mathbf{B_5}$	=	$-(x_2 - y_2)\,\mathbf{a}_1 - (x_2 + y_2)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(8f)	Br I
$\mathbf{B_6}$	=	$(x_2 + y_2)\,\mathbf{a}_1 + (x_2 - y_2)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_2 + c\left(z_2 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Br I

References

[1] K. Brodersen, G. Thiele, and H. Gaedcke, *Die Konstitution des Palladium(II)-bromids*, Z. Anorganische und Allgemeine Chemie **348**, 162–167 (1966), doi:10.1002/zaac.19663480307.

[2] P. V. C. Editor), *PdBr2 Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.

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