Ta_2PdSe_6 Structure: AB6C2_mC18_12_a_3i_i-004

This structure originally had the label `AB6C2_mC18_12_a_3i_i`. Calls to that address will be redirected here.

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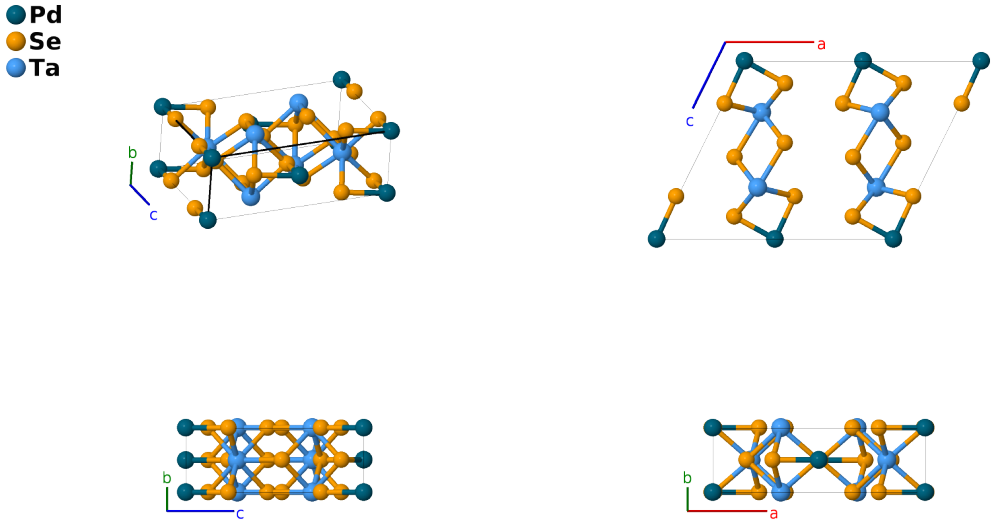
https://aflow.org/p/H8PR

https://aflow.org/p/AB6C2_mC18_12_a_3i_i-004



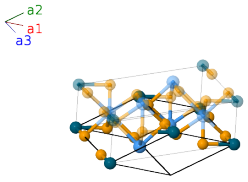
Prototype	$PdSe_6Ta_2$
AFLOW prototype label	AB6C2_mC18_12_a_3i_i-004
ICSD	61005
Pearson symbol	mC18
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=AB6C2_mC18_12_a_3i_i-004 --params=`$a, b/a, c/a, \beta, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5$

Other compounds with this structure
Nb_2PdS_6, Nb_2PdSe_6, Ta_2PdS_6

- (Keszler, 1985) gave the structure in the $I2/m$ setting of space group #12. We used FINDSYM to change this to the standard $C2/m$ setting. Because of this change our primitive vectors are linear combinations of the original ones, and the lattice has been rotated.

Base-centered Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Pd I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	Se 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)	Se I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Se II
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Se II
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Se III
$\mathbf{B_7}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Se III
$\mathbf{B_8}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ta I
$\mathbf{B_9}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ta I

References

[1] D. A. Keszler, P. J. Squattrito, N. E. Brese, J. A. Ibers, M. Shang, and J. Lu, *New layered ternary chalcogenides: tantalum palladium sulfide (Ta_2PdS_6), tantalum palladium selenide (Ta_2PdSe_6), niobium palladium sulfide (Nb_2PdS_6), niobium palladium selenide (Nb_2PdSe_6)*, Inorg. Chem. pp. 3063–3067 (1985), doi:10.1021/ic00213a038.