PdTeI Structure: ABC_tP12_131_k_j_l-001

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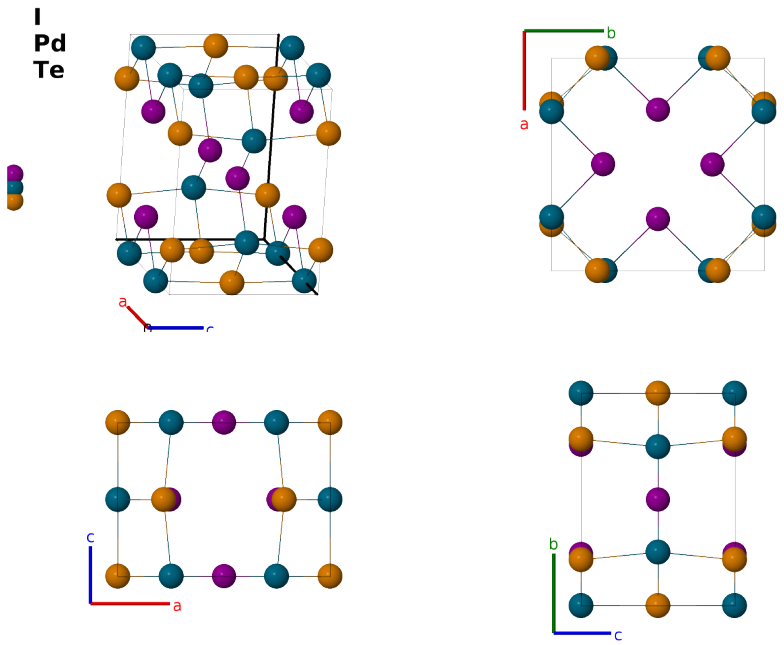
https://aflow.org/prototype-encyclopedia/ALQL

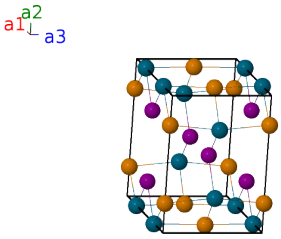
https://aflow.org/prototype-encyclopedia/ABC_tP12_131_k_j_l-001



Prototype	IPdTe
AFLOW prototype label	ABC_tP12_131_k_j_l-001
ICSD	50987
CCDC	1615886
Pearson symbol	tP12
Space group number	131
Space group symbol	$P4_2/mmc$
AFLOW prototype command	`aflow --proto=ABC_tP12_131_k_j_l-001 --params=`$a, c/a, x_1, x_2, x_3$

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1$	=	$ax_1\,\hat{\mathbf{x}}$	(4j)	Pd I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1$	=	$-ax_1\,\hat{\mathbf{x}}$	(4j)	Pd I
$\mathbf{B_3}$	=	$x_1\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4j)	Pd I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4j)	Pd I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4k)	I I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4k)	I I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$	(4k)	I I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}}$	(4k)	I I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4l)	Te I
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4l)	Te I
$\mathbf{B_{11}}$	=	$x_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{y}}$	(4l)	Te I
$\mathbf{B_{12}}$	=	$-x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{y}}$	(4l)	Te I

References

[1] D.-K. Seo, M.-H. Whangbo, K. Neininger, and G. Thiele, *Single-Crystal X-Ray Diffraction and Electronic Band Structure Studies of PdTeI*, J. Solid State Chem. **137**, 206–210 (1998), doi:10.1006/jssc.1997.7669.

Found in

[1] S. Güler-Kılıç and Ç. Kılıç, *Crystal and electronic structure of BiTeI, AuTeI, and PdTeI compounds: A dispersion-corrected density-functional study*, Phys. Rev. B **91**, 24524 (2015), doi:10.1103/PhysRevB.91.245204.

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