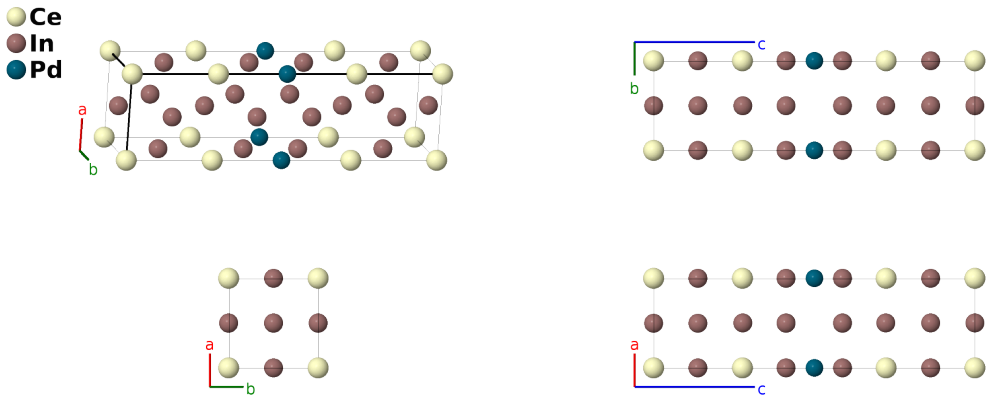
Ce_3PdIn_{11} Structure: A3B11C_tP15_123_ag_ch2i_b-001

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/7DQQ

https://aflow.org/p/A3B11C_tP15_123_ag_ch2i_b-001

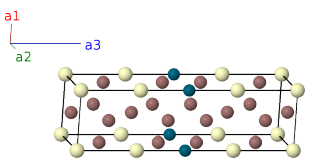


Prototype	$Ce_3In_{11}Pd$
AFLOW prototype label	A3B11C_tP15_123_ag_ch2i_b-001
ICSD	192619
Pearson symbol	tP15
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	`aflow --proto=A3B11C_tP15_123_ag_ch2i_b-001 --params=`$a, c/a, z_4, z_5, z_6, z_7$

Other compounds with this structure
Ce_3PtIn_{11}

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
$\mathbf{B_1}$	=	0	=	0	(1a)	Ce I

$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Pd I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(1c)	In I
$\mathbf{B_4}$	=	$z_4\,\mathbf{a}_3$	=	$cz_4\,\hat{\mathbf{z}}$	(2g)	Ce II
$\mathbf{B_5}$	=	$-z_4\,\mathbf{a}_3$	=	$-cz_4\,\hat{\mathbf{z}}$	(2g)	Ce II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(2h)	In II
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(2h)	In II
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4i)	In III
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_6\,\hat{\mathbf{z}}$	(4i)	In III
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(4i)	In III
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_6\,\hat{\mathbf{z}}$	(4i)	In III
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4i)	In IV
$\mathbf{B_{13}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_7\,\hat{\mathbf{z}}$	(4i)	In IV
$\mathbf{B_{14}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(4i)	In IV
$\mathbf{B_{15}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_7\,\hat{\mathbf{z}}$	(4i)	In IV

References

[1] M. Kratochvilova, M. Dusek, K. Uhlirova, A. Rudajevova, J. Prokleska, B. Vondrackova, J. Custers, and V. Sechovsky, *Single crystal study of the layered heavy fermion compounds Ce_2PdIn_8, Ce_3PdIn_{11}, Ce_2PtIn_8 and Ce_3PtIn_{11}*, J. Cryst. Growth **397**, 47–52 (2014), doi:10.1016/j.jcrysgro.2014.04.008.