$CePt_2In_7$ Structure: AB7C2_tI20_139_a_bdg_e-001

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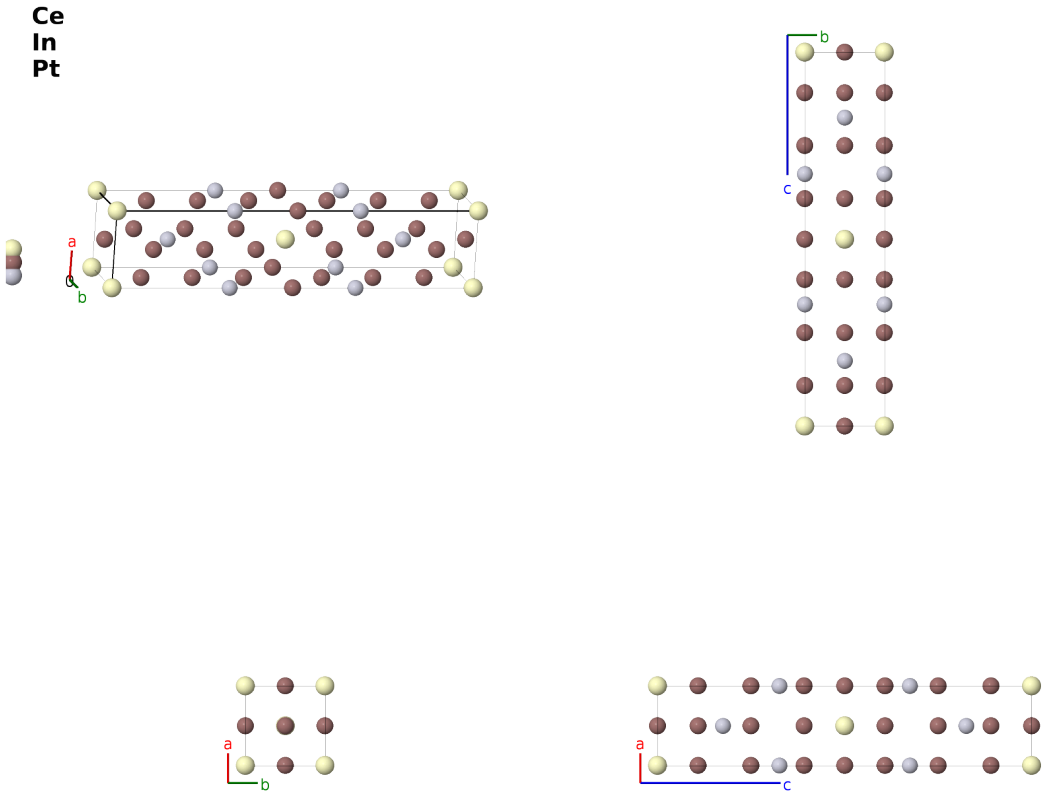
https://aflow.org/prototype-encyclopedia/P6JF

https://aflow.org/prototype-encyclopedia/AB7C2_tI20_139_a_bdg_e-001

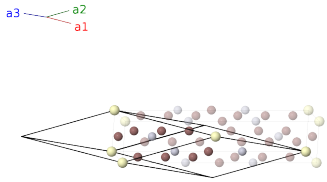


Prototype	$CeIn_7Pt_2$
AFLOW prototype label	AB7C2_tI20_139_a_bdg_e-001
ICSD	161312
CCDC	1677684
Pearson symbol	tI20
Space group number	139
Space group symbol	$I4/mmm$

AFLOW prototype command `aflow --proto=AB7C2_tI20_139_a_bdg_e-001 --params=`$a, c/a, z_4, z_5$

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ce I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	In I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	In II
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	In II
$\mathbf{B_5}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$	=	$cz_4\,\hat{\mathbf{z}}$	(4e)	Pt I
$\mathbf{B_6}$	=	$-z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2$	=	$-cz_4\,\hat{\mathbf{z}}$	(4e)	Pt I
$\mathbf{B_7}$	=	$\left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8g)	In III
$\mathbf{B_8}$	=	$z_5\,\mathbf{a}_1 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(8g)	In III
$\mathbf{B_9}$	=	$-\left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8g)	In III
$\mathbf{B_{10}}$	=	$-z_5\,\mathbf{a}_1 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_5\,\hat{\mathbf{z}}$	(8g)	In III

References

[1] Z. M. Kurenbaeva, E. V. Murashova, Y. D. Seropegin, H. Noël, and A. I. Tursina, *The crystal structure of the new indide $CePt_2In_7$ from powder data*, Intermetallics **16**, 979–981 (2008), doi:10.1016/j.intermet.2008.04.018.

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[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.

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