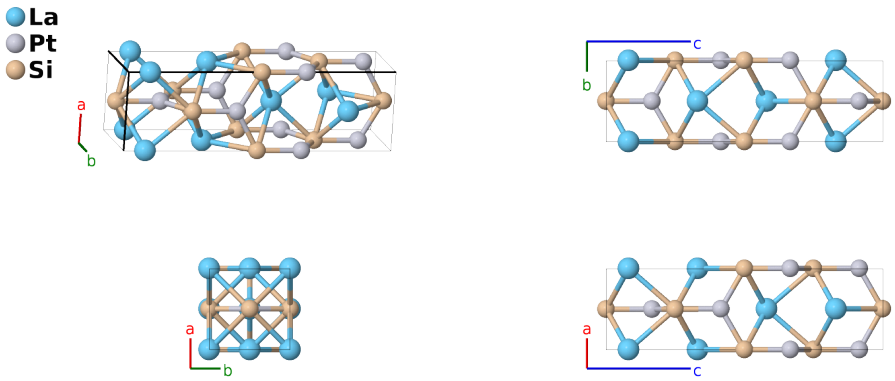
LaPtSi Structure: ABC_tI12_109_a_a_a-001

This structure originally had the label `ABC_tI12_109_a_a_a`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

https://aflow.org/p/RTEY

https://aflow.org/p/ABC_tI12_109_a_a_a-001



Prototype	LaPtSi
AFLOW prototype label	ABC_tI12_109_a_a_a-001
ICSD	27224
Pearson symbol	tI12
Space group number	109
Space group symbol	$I4_1md$
AFLOW prototype command	`aflow --proto=ABC_tI12_109_a_a_a-001 --params=`$a, c/a, z_1, z_2, z_3$

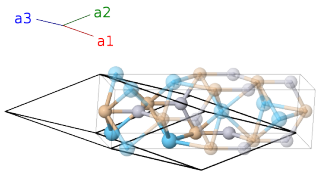
Other compounds with this structure

EuPtAs, CeAlSi, CeIrP, CeNiSi, CePtSi, GdGaSi, LaAlGe, LaAlSi, LaIrP, LaNiSi, LaPrP, LaPtGe, LaRhAs, NdAlSi, NdIrP, NdNiSi, NdPtSi, PrAlGe, PrAlSi, PrIrP, PrPtSi, PtSmSi, SmAlSi

- The sample examined by (Klepp, 1982) has 2% silicon on the platinum site and 2% platinum on the silicon site.

Body-centered Tetragonal primitive vectors

$$\mathbf{a_1} = -\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - \frac{1}{2}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2$	=	$cz_1\,\hat{\mathbf{z}}$	(4a)	La I
$\mathbf{B_2}$	=	$\left(z_1+\frac{3}{4}\right)\,\mathbf{a}_1 + \left(z_1+\frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(4a)	La I
$\mathbf{B_3}$	=	$z_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2$	=	$cz_2\,\hat{\mathbf{z}}$	(4a)	Pt I
$\mathbf{B_4}$	=	$\left(z_2+\frac{3}{4}\right)\,\mathbf{a}_1 + \left(z_2+\frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(4a)	Pt I
$\mathbf{B_5}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$	=	$cz_3\,\hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B_6}$	=	$\left(z_3+\frac{3}{4}\right)\,\mathbf{a}_1 + \left(z_3+\frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(4a)	Si I

References

[1] K. Klepp and E. Parthé, *RPtSi phases (R = La, Ce, Pr, Nd, Sm and Gd) with an ordered $ThSi_2$ derivative structure*, Acta Crystallogr. Sect. B **38**, 1105–1108 (1982), doi:10.1107/S056774088200507X.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.