

α -La ($A3'$) Structure: A_hP4_194_ac-001

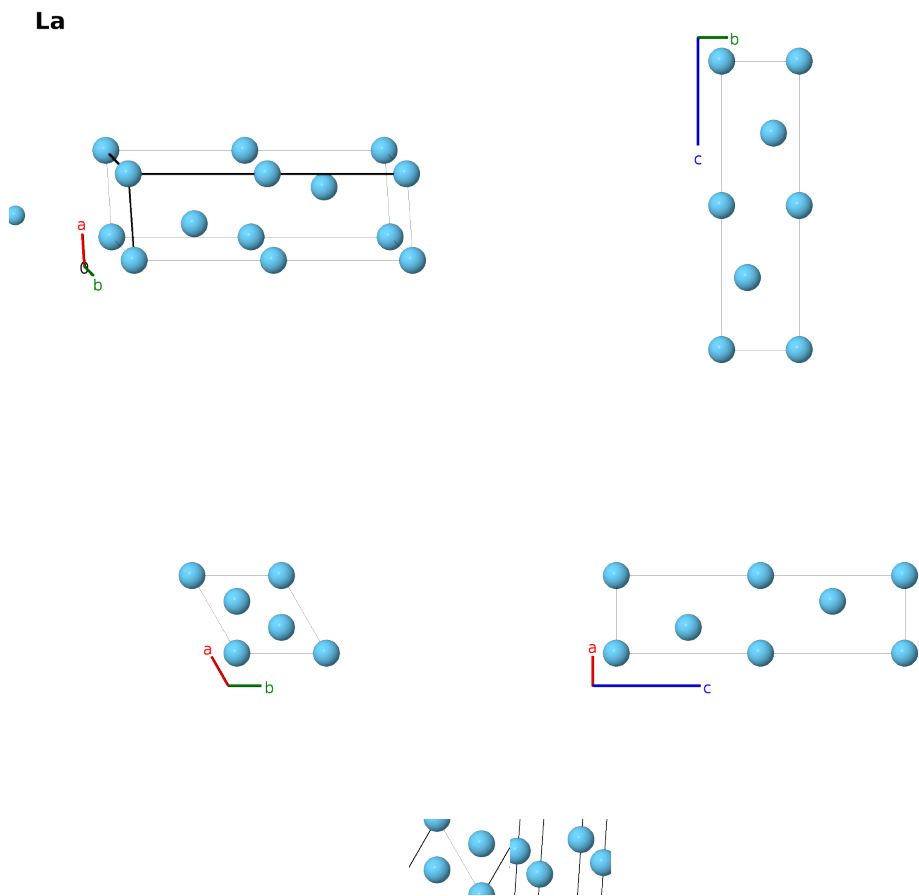
This structure previously used the label(s) **A_hP4_194_ac**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/9631>

https://aflow.org/prototype-encyclopedia/A_hP4_194_ac-001



Prototype	La
AFLOW prototype label	A_hP4_194_ac-001
<i>Strukturbericht</i> designation	$A3'$
ICSD	43573
CCDC	1613057
Pearson symbol	hP4
Space group number	194

Space group symbol $P6_3/mmc$

AFLOW prototype command `aflow --proto=A_hP4_194_ac-001`
`--params=a,c/a`

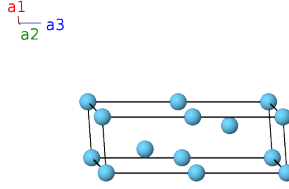
Other compounds with this structure

Am, Bk, Ce, Cf, Cm, Nd, Pm, Pr

- This crystal is close-packed, with stacking ABACABAC..., as opposed to ABAB... for the hcp (*A3*) structure and ABCABC... for the fcc (*A1*) lattice. The (2a) crystallographic sites (the A layer) form a simple hexagonal lattice. The (2c) sites (the B and C layers) form an hcp structure.

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_3 &= c\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(2a)	La I
$\mathbf{B}_2$	$\frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}c\hat{\mathbf{z}}$	(2a)	La I
$\mathbf{B}_3$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(2c)	La II
$\mathbf{B}_4$	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(2c)	La II

References

- [1] F. H. Spedding, J. J. Hanak, and A. H. Daane, *High temperature allotropy and thermal expansion of the rare-earth metals*, J. Less-Common Met. **3**, 110–124 (1961), doi:10.1016/0022-5088(61)90003-0.

Found in

- [1] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, New York, 1974).

First cited in

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