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

This structure originally had the label `A_hP4_194_ac`. Calls to that address will be redirected here.

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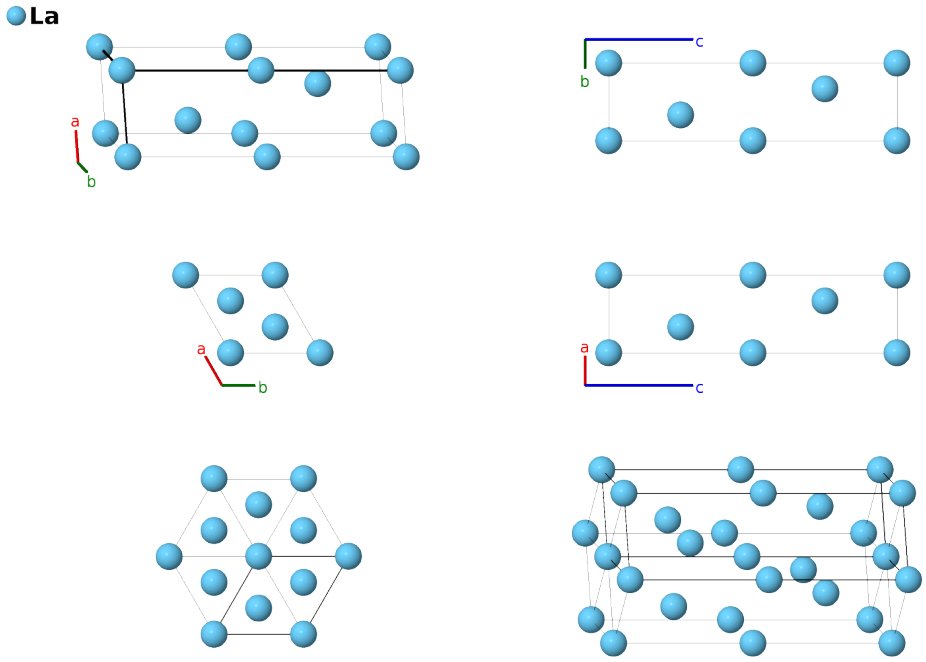
https://aflow.org/p/9631

https://aflow.org/p/A_hP4_194_ac-001



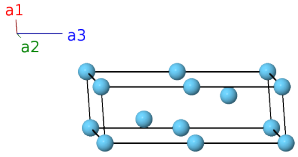
Prototype	La
AFLOW prototype label	A_hP4_194_ac-001
***Strukturbericht* designation**	$A3'$
ICSD	43573
Pearson symbol	hP4
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=A_hP4_194_ac-001 --params=`$a, c/a$

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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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).