

LaH₁₀ High-T_c Superconductor Structure: A10B_cF44_225_cf_a-001

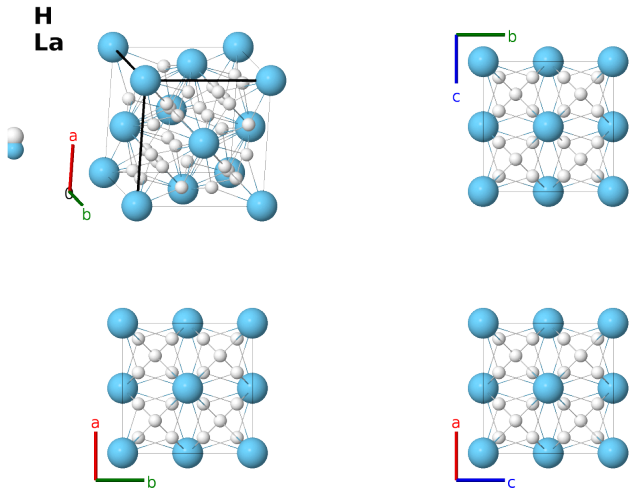
This structure previously used the label(s) **A10B_cF44_225_cf.b**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://afLOW.org/prototype-encyclopedia/8F2Q>

https://afLOW.org/prototype-encyclopedia/A10B_cF44_225_cf_a-001



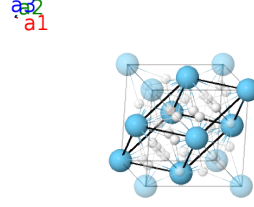
Prototype	H ₁₀ La
AFLOW prototype label	A10B_cF44_225_cf_a-001
Pearson symbol	cF44
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A10B_cF44_225_cf_a-001 --params=a, x₃</code>

- This structure was predicted by (Liu, 2017) as a possible near-room-temperature superconductor at pressures above 200 GPa. Its existence was confirmed by (Geballe, 2018).
- The lattice constant $a = 4.78\text{\AA}$ is taken from the (Liu, 2017) prediction at 300 GPa. (Geballe, 2018) found $a = 5.09\text{\AA}$ at 172 GPa, however that measurement does not appear in the ICSD, only in Table S2 of their supplementary information.
- (Liu, 2017)
- ICSD entries 259264 through 259303 are associated with (Geballe, 2018), but none of them include hydrogen positions and all have much smaller lattice constants than those given for LaH₁₀, leading us to believe that they represent calibration runs using elemental materials.

- The AFLOW prototype label convention moves the origin by (a/2 a/2 a/2) from the published version, moving the lanthanum site from (4b) to (4a).

Face-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(4a) La I
$\mathbf{B}_2$	=	$\frac{1}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	=	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(8c) H I
$\mathbf{B}_3$	=	$\frac{3}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	=	$\frac{3}{4}a\hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{y}} + \frac{3}{4}a\hat{\mathbf{z}}$	(8c) H I
$\mathbf{B}_4$	=	$x_3\mathbf{a}_1 + x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	=	$ax_3\hat{\mathbf{x}} + ax_3\hat{\mathbf{y}} + ax_3\hat{\mathbf{z}}$	(32f) H II
$\mathbf{B}_5$	=	$x_3\mathbf{a}_1 + x_3\mathbf{a}_2 - 3x_3\mathbf{a}_3$	=	$-ax_3\hat{\mathbf{x}} - ax_3\hat{\mathbf{y}} + ax_3\hat{\mathbf{z}}$	(32f) H II
$\mathbf{B}_6$	=	$x_3\mathbf{a}_1 - 3x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	=	$-ax_3\hat{\mathbf{x}} + ax_3\hat{\mathbf{y}} - ax_3\hat{\mathbf{z}}$	(32f) H II
$\mathbf{B}_7$	=	$-3x_3\mathbf{a}_1 + x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	=	$ax_3\hat{\mathbf{x}} - ax_3\hat{\mathbf{y}} - ax_3\hat{\mathbf{z}}$	(32f) H II
$\mathbf{B}_8$	=	$-x_3\mathbf{a}_1 - x_3\mathbf{a}_2 + 3x_3\mathbf{a}_3$	=	$ax_3\hat{\mathbf{x}} + ax_3\hat{\mathbf{y}} - ax_3\hat{\mathbf{z}}$	(32f) H II
$\mathbf{B}_9$	=	$-x_3\mathbf{a}_1 - x_3\mathbf{a}_2 - x_3\mathbf{a}_3$	=	$-ax_3\hat{\mathbf{x}} - ax_3\hat{\mathbf{y}} - ax_3\hat{\mathbf{z}}$	(32f) H II
$\mathbf{B}_{10}$	=	$-x_3\mathbf{a}_1 + 3x_3\mathbf{a}_2 - x_3\mathbf{a}_3$	=	$ax_3\hat{\mathbf{x}} - ax_3\hat{\mathbf{y}} + ax_3\hat{\mathbf{z}}$	(32f) H II
$\mathbf{B}_{11}$	=	$3x_3\mathbf{a}_1 - x_3\mathbf{a}_2 - x_3\mathbf{a}_3$	=	$-ax_3\hat{\mathbf{x}} + ax_3\hat{\mathbf{y}} + ax_3\hat{\mathbf{z}}$	(32f) H II

References

- [1] H. Liu, I. I. Naumov, R. Hoffmann, N. W. Ashcroft, and R. J. Hemley, *Potential high- T_c superconducting lanthanum and yttrium hydrides at high pressure*, Proc. Natl. Acad. Sci. **114**, 6990–6995 (2017), doi:10.1073/pnas.1704505114.
- [2] Z. M. Geballe, H. Liu, A. K. Mishra, M. Ahart, M. Somayazulu, Y. Meng, M. Baldini, and R. J. Hemley, *Synthesis and Stability of Lanthanum Superhydrides*, Angew. Chem. Int. Ed. **57**, 688–692 (2018), doi:10.1002/anie.201709970.

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