

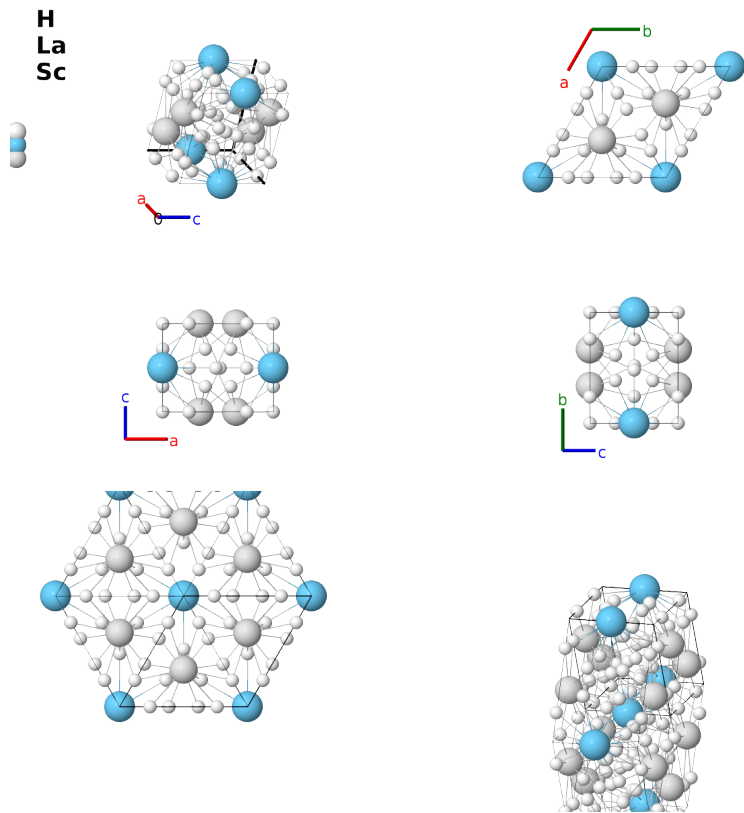
Predicted $\text{LaSc}_2\text{H}_{24}$ Superconducting Structure: A24BC2_hP27_191_jmn_b_c-001

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

https://aflow.org/prototype-encyclopedia/A24BC2_hP27_191_jmn_b_c-001

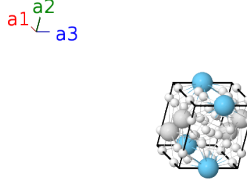


Prototype	$\text{H}_{24}\text{LaSc}_2$
AFLOW prototype label	A24BC2_hP27_191_jmn_b_c-001
Pearson symbol	hP27
Space group number	191
Space group symbol	$P6/mmm$
AFLOW prototype command	<code>aflow --proto=A24BC2_hP27_191_jmn_b_c-001 --params=a, c/a, x_3, x_4, x_5, z_5</code>

- (He, 2024) predicted this structure to be a stable form of $\text{LaSc}_2\text{H}_{24}$ at pressures in the range 167-300 GPa with T_c above 300K.

- Later (Song, 2025) found $\text{LaSc}_2\text{H}_{24}$ to be superconducting at 298K and above 195 GPa. If confirmed this is the first observed room-temperature superconductor.
- We use the prediction of the structure from (He, 2024) at 300 GPa.

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
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(1b)	La I
$\mathbf{B}_2$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}}$	(2c)	Sc I
$\mathbf{B}_3$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}}$	(2c)	Sc I
$\mathbf{B}_4$	$= x_3 \mathbf{a}_1$	$=$	$\frac{1}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}}$	(6j)	H I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_2$	$=$	$\frac{1}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}}$	(6j)	H I
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}}$	(6j)	H I
$\mathbf{B}_7$	$= -x_3 \mathbf{a}_1$	$=$	$-\frac{1}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}}$	(6j)	H I
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_2$	$=$	$-\frac{1}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}}$	(6j)	H I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}}$	(6j)	H I
$\mathbf{B}_{10}$	$= x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6m)	H II
$\mathbf{B}_{11}$	$= -2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6m)	H II
$\mathbf{B}_{12}$	$= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6m)	H II
$\mathbf{B}_{13}$	$= -x_4 \mathbf{a}_1 - 2x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6m)	H II
$\mathbf{B}_{14}$	$= 2x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6m)	H II
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\sqrt{3}ax_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6m)	H II
$\mathbf{B}_{16}$	$= x_5 \mathbf{a}_1 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(12n)	H III
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(12n)	H III
$\mathbf{B}_{18}$	$= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + cz_5 \hat{\mathbf{z}}$	(12n)	H III
$\mathbf{B}_{19}$	$= -x_5 \mathbf{a}_1 + z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(12n)	H III
$\mathbf{B}_{20}$	$= -x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(12n)	H III
$\mathbf{B}_{21}$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + cz_5 \hat{\mathbf{z}}$	(12n)	H III
$\mathbf{B}_{22}$	$= x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(12n)	H III
$\mathbf{B}_{23}$	$= x_5 \mathbf{a}_1 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(12n)	H III
$\mathbf{B}_{24}$	$= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - cz_5 \hat{\mathbf{z}}$	(12n)	H III
$\mathbf{B}_{25}$	$= -x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(12n)	H III
$\mathbf{B}_{26}$	$= -x_5 \mathbf{a}_1 - z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(12n)	H III

$$\mathbf{B}_{27} = x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 = ax_5 \hat{\mathbf{x}} - cz_5 \hat{\mathbf{z}} \quad (12n) \quad \text{H III}$$

References

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