Theoretical Cubic LiH_{12} Structure: A12B_cP13_200_j_b-001

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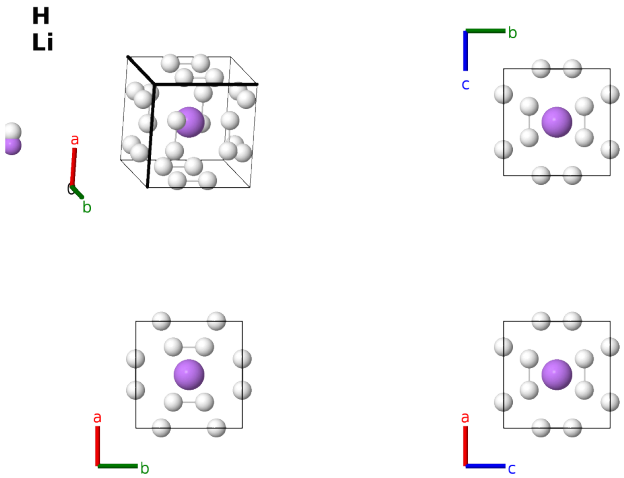
https://aflow.org/prototype-encyclopedia/7KWV

https://aflow.org/prototype-encyclopedia/A12B_cP13_200_j_b-001



Prototype	$H_{12}Li$
AFLOW prototype label	A12B_cP13_200_j_b-001
Pearson symbol	cP13
Space group number	200
Space group symbol	$Pm\overline{3}$
AFLOW prototype command	`aflow --proto=A12B_cP13_200_j_b-001 --params=`a, y_2, z_2

- (Verma, 2026) published a large number of predictions of possible superconducting Li-H compounds at 250 using the Perdew-Burke-Ernzerhof functional with VASP. They identified this structure as the best candidate for finding high-temperature superconductivity, with a transition temperature T_c above 300K.

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(1b)	Li I
$\mathbf{B_2}$	=	$y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{y}} + az_2\,\hat{\mathbf{z}}$	(12j)	H I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{y}} + az_2\,\hat{\mathbf{z}}$	(12j)	H I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{y}} - az_2\,\hat{\mathbf{z}}$	(12j)	H I
$\mathbf{B_5}$	=	$-y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{y}} - az_2\,\hat{\mathbf{z}}$	(12j)	H I
$\mathbf{B_6}$	=	$z_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_3$	=	$az_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{z}}$	(12j)	H I
$\mathbf{B_7}$	=	$z_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_3$	=	$az_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{z}}$	(12j)	H I
$\mathbf{B_8}$	=	$-z_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_3$	=	$-az_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{z}}$	(12j)	H I
$\mathbf{B_9}$	=	$-z_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_3$	=	$-az_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{z}}$	(12j)	H I
$\mathbf{B_{10}}$	=	$y_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2$	=	$ay_2\,\hat{\mathbf{x}} + az_2\,\hat{\mathbf{y}}$	(12j)	H I
$\mathbf{B_{11}}$	=	$-y_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2$	=	$-ay_2\,\hat{\mathbf{x}} + az_2\,\hat{\mathbf{y}}$	(12j)	H I
$\mathbf{B_{12}}$	=	$y_2\,\mathbf{a}_1 - z_2\,\mathbf{a}_2$	=	$ay_2\,\hat{\mathbf{x}} - az_2\,\hat{\mathbf{y}}$	(12j)	H I
$\mathbf{B_{13}}$	=	$-y_2\,\mathbf{a}_1 - z_2\,\mathbf{a}_2$	=	$-ay_2\,\hat{\mathbf{x}} - az_2\,\hat{\mathbf{y}}$	(12j)	H I

References

[1] A. K. Verma and P. Modak, *High-temperature superconductivity in compressed molecular hydrogen via controlled electron-doping*, Physica B **728**, 418355 (2026), doi:10.1016/j.physb.2026.418355.

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