Predicted Li_2MgH_{16} 300 GPa Structure: A16B2C_hP19_164_2d2i_d_a-001

This structure originally had the label `A16B2C_hP19_164_2d2i_d_b`. Calls to that address will be redirected here.

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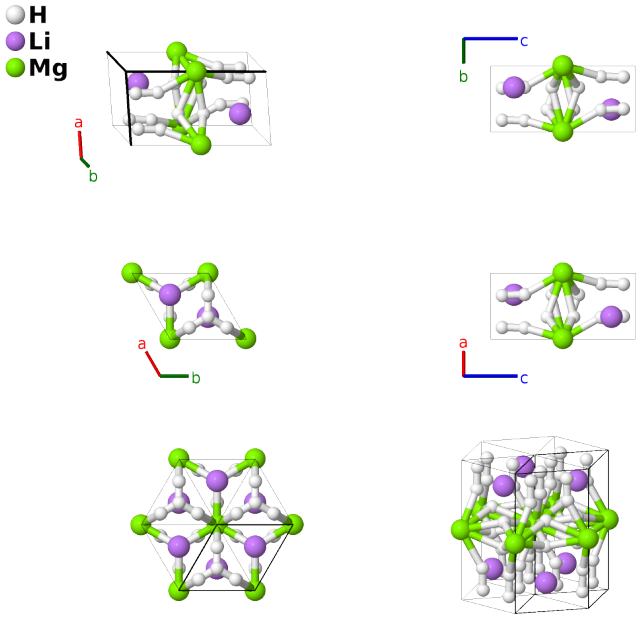
https://aflow.org/p/LLDQ

https://aflow.org/p/A16B2C_hP19_164_2d2i_d_a-001

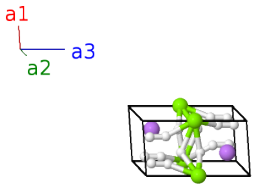


Prototype	$H_{16}Li_2Mg$
AFLOW prototype label	A16B2C_hP19_164_2d2i_d_a-001
ICSD	none
Pearson symbol	hP19
Space group number	164
Space group symbol	$P\bar{3}m1$
AFLOW prototype command	`aflow --proto=A16B2C_hP19_164_2d2i_d_a-001 --params=`$a, c/a, z_2, z_3, z_4, x_5, z_5, x_6, z_6$

- This structure is predicted to be the zero-temperature ground state of Li_2MgH_{16} at 300 GPa. It is of primarily of interest because a metastable cubic structure with the same composition is predicted to be superconducting at 250 GPa with $T_c = 430 - 473$K.

Trigonal (Hexagonal) primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Mg I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2d)	H I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2d)	H I
$\mathbf{B_4}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2d)	H II
$\mathbf{B_5}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2d)	H II
$\mathbf{B_6}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2d)	Li I
$\mathbf{B_7}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(2d)	Li I
$\mathbf{B_8}$	=	$x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-\sqrt{3}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6i)	H III
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + 2x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{3}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6i)	H III
$\mathbf{B_{10}}$	=	$-2x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6i)	H III
$\mathbf{B_{11}}$	=	$-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\sqrt{3}ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(6i)	H III
$\mathbf{B_{12}}$	=	$2x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{3}{2}ax_5\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(6i)	H III
$\mathbf{B_{13}}$	=	$-x_5\,\mathbf{a}_1 - 2x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_5\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(6i)	H III
$\mathbf{B_{14}}$	=	$x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-\sqrt{3}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6i)	H IV
$\mathbf{B_{15}}$	=	$x_6\,\mathbf{a}_1 + 2x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{3}{2}ax_6\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6i)	H IV
$\mathbf{B_{16}}$	=	$-2x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_6\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6i)	H IV
$\mathbf{B_{17}}$	=	$-x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\sqrt{3}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6i)	H IV
$\mathbf{B_{18}}$	=	$2x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{3}{2}ax_6\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6i)	H IV
$\mathbf{B_{19}}$	=	$-x_6\,\mathbf{a}_1 - 2x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_6\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6i)	H IV

References

[1] Y. Sun, J. Lv, Y. Xie, H. Liu, and Y. Ma, *Route to a Superconducting Phase above Room Temperature in Electron-Doped Hydride Compounds under High Pressure*, Phys. Rev. Lett. **123**, 097001 (2019), doi:10.1103/PhysRevLett.123.097001.