Predicted Li_2MgH_{16} High-T_c Superconductor (250 GPa) Structure: A16B2C_cF152_227_eg_c_b-001

This structure originally had the label `A16B2C_cF152_227_eg_d_a`. Calls to that address will be redirected here.

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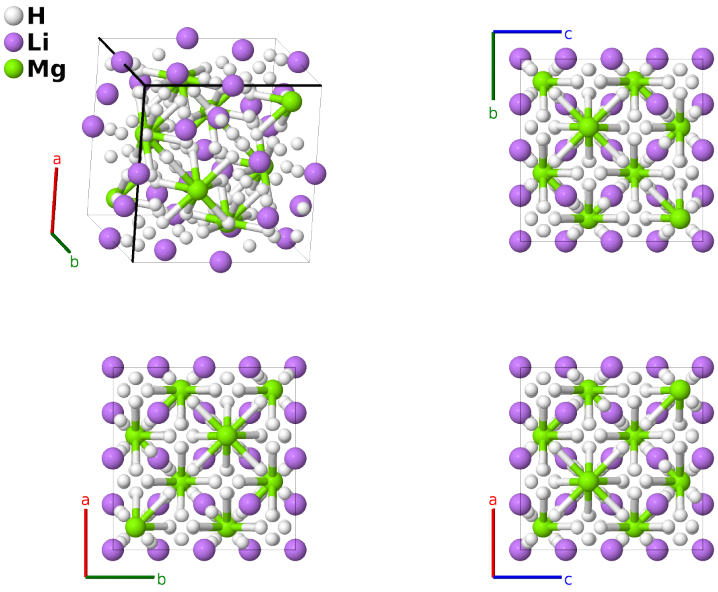
https://aflow.org/p/WZBC

https://aflow.org/p/A16B2C_cF152_227_eg_c_b-001

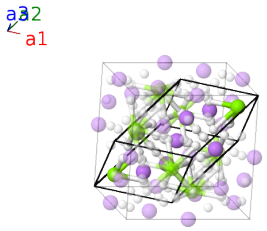


Prototype	$H_{16}Li_2Mg$
AFLOW prototype label	A16B2C_cF152_227_eg_c_b-001
ICSD	none
Pearson symbol	cF152
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	`aflow --proto=A16B2C_cF152_227_eg_c_b-001 --params=`a, x_3, x_4, z_4

- This structure was predicted by (Sun, 2019) as a metastable state of Li_2MgH_{16} at 250 GPa and $T = 0$K. If it is possible to construct this compound, or if it becomes stable due to thermodynamic considerations, it is predicted to have a superconducting transition T_c between 430 and 473K.
- The predicted $T = 0$K ground state at 300 GPa is a $P\bar{3}m1$ #164 structure with molecular hydrogen.
- (Sun, 2019) give the Wyckoff positions in setting 1 of space group $Fd\bar{3}m$ #227. (They list the Wyckoff positions of the magnesium and lithium atoms as (8b) and (16c), respectively. They are actually at (8a) and (16d), as in their 300 GPa data.) We used FINDSYM to shift this to our standard setting 2.

Face-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 + \frac{3}{8}\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(8b)	Mg I
$\mathbf{B_2}$	=	$\frac{5}{8}\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \frac{5}{8}\,\mathbf{a}_3$	=	$\frac{5}{8}a\,\hat{\mathbf{x}} + \frac{5}{8}a\,\hat{\mathbf{y}} + \frac{5}{8}a\,\hat{\mathbf{z}}$	(8b)	Mg I
$\mathbf{B_3}$	=	0	=	0	(16c)	Li I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(16c)	Li I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	Li I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	Li I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(32e)	H I
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - \left(3x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(32e)	H I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 - \left(3x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	H I
$\mathbf{B_{10}}$	=	$-\left(3x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	H I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(3x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(32e)	H I
$\mathbf{B_{12}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(32e)	H I
$\mathbf{B_{13}}$	=	$-x_3\,\mathbf{a}_1 + \left(3x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	H I
$\mathbf{B_{14}}$	=	$\left(3x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	H I
$\mathbf{B_{15}}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + (2x_4 - z_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{16}}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 - \left(2x_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{17}}$	=	$(2x_4 - z_4)\,\mathbf{a}_1 - \left(2x_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - a\left(z_4 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{18}}$	=	$-\left(2x_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + (2x_4 - z_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(z_4 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{19}}$	=	$(2x_4 - z_4)\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$az_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{20}}$	=	$-\left(2x_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$az_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{21}}$	=	$z_4\,\mathbf{a}_1 + (2x_4 - z_4)\,\mathbf{a}_2 - \left(2x_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(z_4 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{22}}$	=	$z_4\,\mathbf{a}_1 - \left(2x_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + (2x_4 - z_4)\,\mathbf{a}_3$	=	$-a\left(z_4 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{23}}$	=	$z_4\,\mathbf{a}_1 + (2x_4 - z_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + az_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{24}}$	=	$z_4\,\mathbf{a}_1 - \left(2x_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + az_4\,\hat{\mathbf{y}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	H II

$\mathbf{B_{25}}$	=	$-\left(2x_4+z_4-\frac{1}{2}\right)\,\mathbf{a}_1+z_4\,\mathbf{a}_2+(2x_4-z_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}-a\left(z_4-\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(x_4-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{26}}$	=	$(2x_4-z_4)\,\mathbf{a}_1+z_4\,\mathbf{a}_2-\left(2x_4+z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(z_4-\frac{1}{4}\right)\,\hat{\mathbf{y}}+ax_4\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{27}}$	=	$-z_4\,\mathbf{a}_1-z_4\,\mathbf{a}_2+\left(2x_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{y}}-az_4\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{28}}$	=	$-z_4\,\mathbf{a}_1-z_4\,\mathbf{a}_2-(2x_4-z_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}-az_4\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{29}}$	=	$-(2x_4-z_4)\,\mathbf{a}_1+\left(2x_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}+a\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{30}}$	=	$\left(2x_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_1-(2x_4-z_4)\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}+a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{31}}$	=	$-(2x_4-z_4)\,\mathbf{a}_1-z_4\,\mathbf{a}_2+\left(2x_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{y}}-ax_4\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{32}}$	=	$\left(2x_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_1-z_4\,\mathbf{a}_2-(2x_4-z_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}+a\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{33}}$	=	$-z_4\,\mathbf{a}_1-(2x_4-z_4)\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}-az_4\,\hat{\mathbf{y}}-ax_4\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{34}}$	=	$-z_4\,\mathbf{a}_1+\left(2x_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{x}}-az_4\,\hat{\mathbf{y}}+a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{35}}$	=	$-z_4\,\mathbf{a}_1-(2x_4-z_4)\,\mathbf{a}_2+\left(2x_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{y}}-ax_4\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{36}}$	=	$-z_4\,\mathbf{a}_1+\left(2x_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2-(2x_4-z_4)\,\mathbf{a}_3$	=	$a\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}+a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{37}}$	=	$\left(2x_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_1-z_4\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$-az_4\,\hat{\mathbf{x}}+a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	H II
$\mathbf{B_{38}}$	=	$-(2x_4-z_4)\,\mathbf{a}_1-z_4\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$-az_4\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}-ax_4\,\hat{\mathbf{z}}$	(96g)	H II

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.