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

This structure previously used the label(s) `A16B2C_cF152_227_eg_d_a`. Calls to these addresses will be redirected here.

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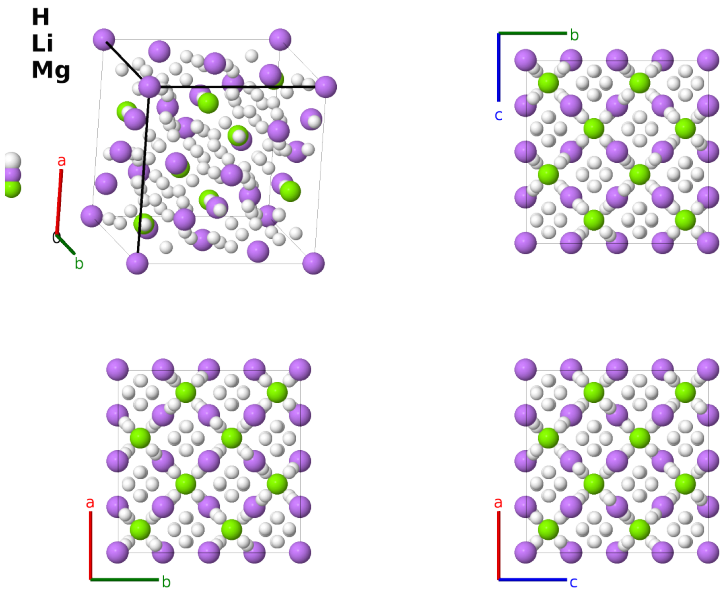
https://aflow.org/prototype-encyclopedia/WZBC

https://aflow.org/prototype-encyclopedia/A16B2C_cF152_227_eg_c_b-001

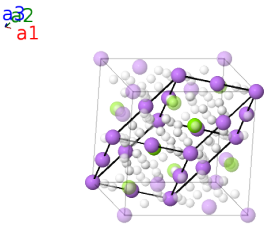


Prototype	$H_{16}Li_2Mg$
AFLOW prototype label	A16B2C_cF152_227_eg_c_b-001
Pearson symbol	cF152
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	`aflow --proto=A16B2C_cF152_227_eg_c_b-001 --params=`a, x_3, x_4, z_4

- 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. We used FINDSYM to shift this to our standard setting 2.

Face-centered Cubic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$$



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

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

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