Mg_2Cu (C_b) Structure: AB2_oF48_70_e_ef-002

This structure previously used the label(s) `AB2_oF48_70_g_fg`. Calls to these addresses will be redirected here.

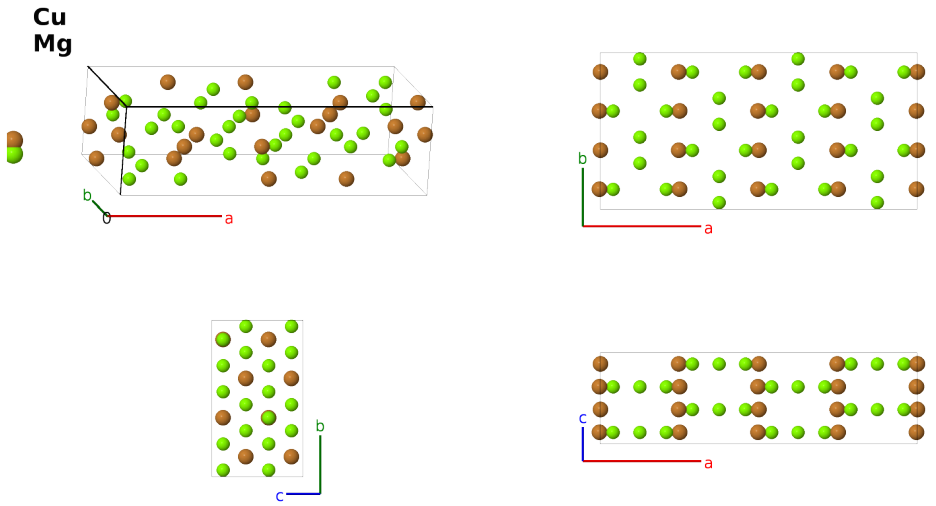
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

---

https://aflow.org/prototype-encyclopedia/S336

https://aflow.org/prototype-encyclopedia/AB2_oF48_70_e_ef-002



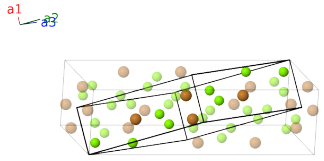
Prototype	$CuMg_2$
AFLOW prototype label	AB2_oF48_70_e_ef-002
***Strukturbericht* designation**	C_b
ICSD	695334
CCDC	2461839
Pearson symbol	oF48
Space group number	70
Space group symbol	$Fddd$
AFLOW prototype command	`aflow --proto=AB2_oF48_70_e_ef-002 --params=`$a, b/a, c/a, x_1, x_2, y_3$

Other compounds with this structure
In_2Ir, $NbSn_2$, $TiBi_2$, FeGaGe, SbSnTi

- Mn_2B ($D1_f$) and $CuMg_2$ (C_b) have the same AFLOW prototype label, AB2_oF48_70_e_ef. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Face-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-\left(x_1 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Cu I
$\mathbf{B_2}$	=	$x_1\,\mathbf{a}_1 - \left(x_1 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_1 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Cu I
$\mathbf{B_3}$	=	$\left(x_1 + \frac{3}{4}\right)\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{8}b\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Cu I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_1 + \left(x_1 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_1 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{3}{4}\right)\,\hat{\mathbf{x}} + \frac{3}{8}b\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Cu I
$\mathbf{B_5}$	=	$-\left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Mg I
$\mathbf{B_6}$	=	$x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Mg I
$\mathbf{B_7}$	=	$\left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{8}b\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Mg I
$\mathbf{B_8}$	=	$-x_2\,\mathbf{a}_1 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{3}{4}\right)\,\hat{\mathbf{x}} + \frac{3}{8}b\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Mg I
$\mathbf{B_9}$	=	$y_3\,\mathbf{a}_1 - \left(y_3 - \frac{1}{4}\right)\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	Mg II
$\mathbf{B_{10}}$	=	$-\left(y_3 - \frac{1}{4}\right)\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - \left(y_3 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	Mg II
$\mathbf{B_{11}}$	=	$-y_3\,\mathbf{a}_1 + \left(y_3 + \frac{3}{4}\right)\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16f)	Mg II
$\mathbf{B_{12}}$	=	$\left(y_3 + \frac{3}{4}\right)\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(y_3 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + b\left(y_3 + \frac{3}{4}\right)\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16f)	Mg II

References

[1] F. Gingl, P. Selvam, and K. Yvon, *Structure refinement of Mg_2Cu and a comparison of the Mg_2Cu, Mg_2Ni and Al_2Cu structure types*, Acta Crystallogr. Sect. B **49**, 201–203 (1993), doi:10.1107/S0108768192008723.

Found in

[1] V. Vreshch, *Crystal Structure of $CuMg_2$* (2018). Crystallography online.com.

First cited in

D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.