Ga_2Mg_5 ($D8_g$) Structure: A2B5_oI28_72_j_afj-001

This structure originally had the label `A2B5_oI28_72_j_bfj`. Calls to that address will be redirected here.

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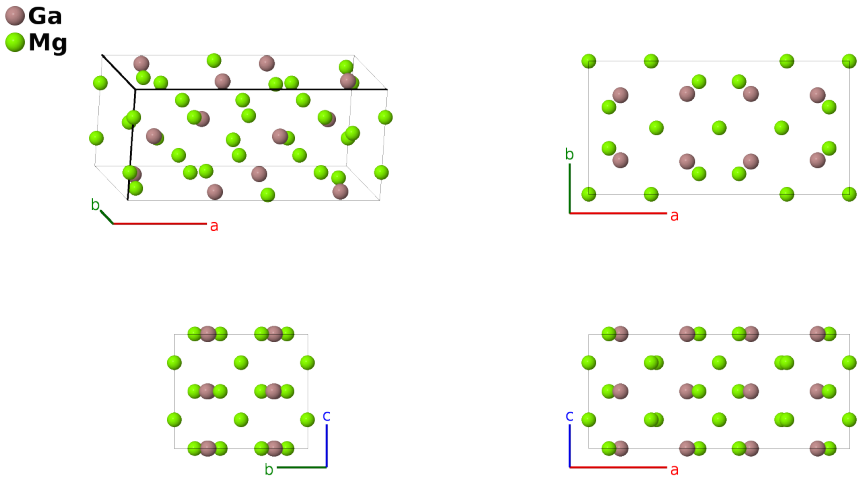
https://aflow.org/p/AB10

https://aflow.org/p/A2B5_oI28_72_j_afj-001



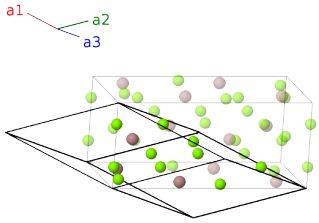
Prototype	Ga_2Mg_5
AFLOW prototype label	A2B5_oI28_72_j_afj-001
***Strukturbericht* designation**	$D8_g$
ICSD	103794
Pearson symbol	oI28
Space group number	72
Space group symbol	*Ibam*
AFLOW prototype command	`aflow --proto=A2B5_oI28_72_j_afj-001 --params=`$a, b/a, c/a, x_2, x_3, y_3, x_4, y_4$

Other compounds with this structure
As_2Cu_5, In_2Mg_5, Tl_2Mg_5, Mn_2Ge_5

- We corrected an error in the Mg III (8j) coordinates and shifted the Mg I atoms from the (2b) to the (2a) site.

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\tfrac{1}{4}\,\mathbf{a}_1 + \tfrac{1}{4}\,\mathbf{a}_2$	=	$\tfrac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	Mg I
$\mathbf{B_2}$	=	$\tfrac{3}{4}\,\mathbf{a}_1 + \tfrac{3}{4}\,\mathbf{a}_2$	=	$\tfrac{3}{4}c\,\hat{\mathbf{z}}$	(4a)	Mg I
$\mathbf{B_3}$	=	$\tfrac{1}{4}\,\mathbf{a}_1 + \left(x_2 + \tfrac{1}{4}\right)\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(8f)	Mg II
$\mathbf{B_4}$	=	$\tfrac{1}{4}\,\mathbf{a}_1 - \left(x_2 - \tfrac{1}{4}\right)\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(8f)	Mg II
$\mathbf{B_5}$	=	$\tfrac{3}{4}\,\mathbf{a}_1 - \left(x_2 - \tfrac{3}{4}\right)\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(8f)	Mg II
$\mathbf{B_6}$	=	$\tfrac{3}{4}\,\mathbf{a}_1 + \left(x_2 + \tfrac{3}{4}\right)\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(8f)	Mg II
$\mathbf{B_7}$	=	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + (x_3 + y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}}$	(8j)	Ga I
$\mathbf{B_8}$	=	$-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - (x_3 + y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}}$	(8j)	Ga I
$\mathbf{B_9}$	=	$\left(y_3 + \tfrac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 - \tfrac{1}{2}\right)\,\mathbf{a}_2 - (x_3 - y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(8j)	Ga I
$\mathbf{B_{10}}$	=	$-\left(y_3 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + (x_3 - y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(8j)	Ga I
$\mathbf{B_{11}}$	=	$y_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + (x_4 + y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}}$	(8j)	Mg III
$\mathbf{B_{12}}$	=	$-y_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - (x_4 + y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}}$	(8j)	Mg III
$\mathbf{B_{13}}$	=	$\left(y_4 + \tfrac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4 - \tfrac{1}{2}\right)\,\mathbf{a}_2 - (x_4 - y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(8j)	Mg III
$\mathbf{B_{14}}$	=	$-\left(y_4 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + (x_4 - y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(8j)	Mg III

References

[1] K. Schubert, K. Frank, R. Gohle, A. Maldonado, H. G. Meissner, A. Raman, and W. Rossteutscher, *Einige Strukturdaten metallischer Phasen (8)*, Naturwissenschaften **50**, 41 (1963), doi:10.1007/BF00622812.

Found in

[1] V. Vreshch, *Crystallography online.com* (2018). Crystal Structure of Ga_2Mg_5.