AlB_4Mg Structure: AB4C_hP6_191_a_h_b-001

This structure originally had the label `AB4C_hP6_191_a_h_b`. Calls to that address will be redirected here.

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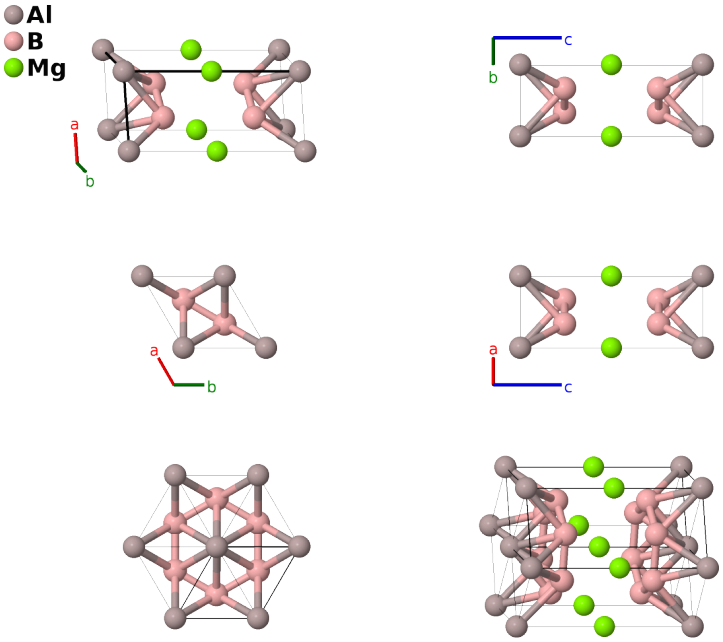
https://aflow.org/p/PDN7

https://aflow.org/p/AB4C_hP6_191_a_h_b-001

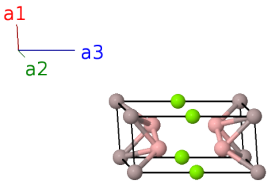


Prototype	AlB_4Mg
AFLOW prototype label	AB4C_hP6_191_a_h_b-001
ICSD	97224
Pearson symbol	hP6
Space group number	191
Space group symbol	$P6/mmm$
AFLOW prototype command	`aflow --proto=AB4C_hP6_191_a_h_b-001 --params=`$a, c/a, z_3$

- Note that Table I of (Margadonna, 2002) mislabels the (1a) and (1b) Wyckoff positions.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Mg I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4h)	B I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4h)	B I
$\mathbf{B_5}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4h)	B I
$\mathbf{B_6}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4h)	B I

References

[1] S. Margadonna, K. Prassides, I. Arvanitidis, M. Pissas, G. Papavassiliou, and A. N. Fitch, *Crystal structure of the $Mg_{1-x}Al_xB_2$ superconductors near $x \approx 0.5$*, Phys. Rev. B **66**, 014518 (2002), doi:10.1103/PhysRevB.66.014518.