$BaMgSiO_4$ Structure: ABC4D_hP42_173_a2b_c_4c_c-001

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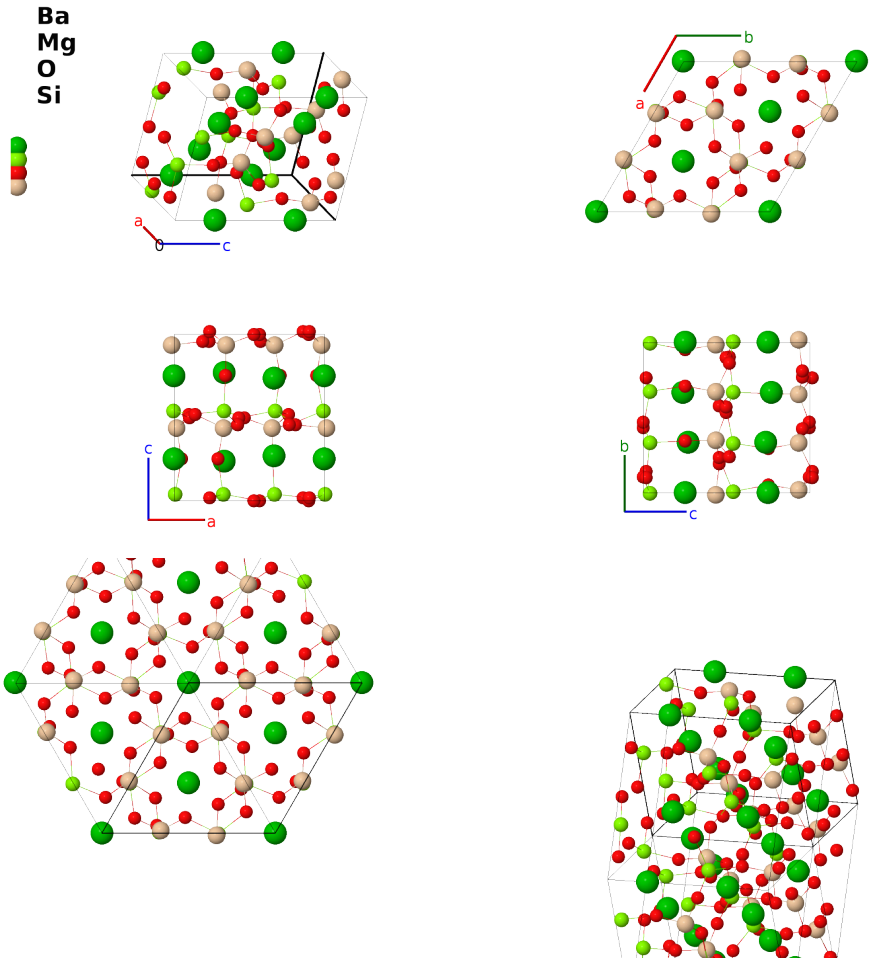
https://aflow.org/prototype-encyclopedia/0URG

https://aflow.org/prototype-encyclopedia/ABC4D_hP42_173_a2b_c_4c_c-001



Prototype	$BaMgO_4Si$
AFLOW prototype label	ABC4D_hP42_173_a2b_c_4c_c-001
ICSD	73776
CCDC	1634532
Pearson symbol	hP42
Space group number	173
Space group symbol	$P6_3$

AFLOW prototype command `aflow --proto=ABC4D_hP42_173_a2b_c_4c_c-001 --params=`$a, c/a, z_1, z_2, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9$

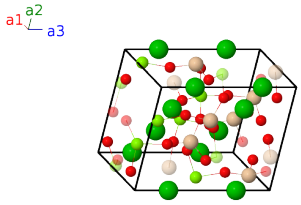
Other compounds with this structure

$BNaSiO_4$, Ba(Ge, Zn)SiO_4, $BaCoSiO_4$, $BaZnSiO_4$, $CaAl_2O_4$, $NaGaSiO_4$ (sodalite), ($Na_{0.7}K_{0.3}GaSiO_4$, $NaZnAsO_4$, $NaZnPO_4$, $SrAl_2O_4$

- Even though (Liu, 1993) give the most complete data for $BaCoSiO_4$, the ICSD selects $BaMgSiO_4$ as the prototype, and we follow that.
- We use the neutron powder data for $BaMgSiO_4$ from (Liu, 1993).
- Space group $P6_3$ #173 does not specify the origin of the z-axis. We follow (Liu, 1993) and set $z_1 = 1/4$ for the Ba I site.

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
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Ba I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Ba I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(2b)	Ba II
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Ba II
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(2b)	Ba III
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Ba III
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1+y_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4+y_4)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_4-y_4)\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(6c)	Mg I
$\mathbf{B_8}$	=	$-y_4\,\mathbf{a}_1+(x_4-y_4)\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4-2y_4)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(6c)	Mg I
$\mathbf{B_9}$	=	$-(x_4-y_4)\,\mathbf{a}_1-x_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_4-y_4)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(6c)	Mg I
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1-y_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_4+y_4)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_4-y_4)\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Mg I
$\mathbf{B_{11}}$	=	$y_4\,\mathbf{a}_1-(x_4-y_4)\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_4+2y_4)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Mg I
$\mathbf{B_{12}}$	=	$(x_4-y_4)\,\mathbf{a}_1+x_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_4-y_4)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Mg I
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1+y_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5+y_5)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_5-y_5)\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{14}}$	=	$-y_5\,\mathbf{a}_1+(x_5-y_5)\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5-2y_5)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{15}}$	=	$-(x_5-y_5)\,\mathbf{a}_1-x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_5-y_5)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{16}}$	=	$-x_5\,\mathbf{a}_1-y_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5+y_5)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_5-y_5)\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{17}}$	=	$y_5\,\mathbf{a}_1-(x_5-y_5)\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_5+2y_5)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{18}}$	=	$(x_5-y_5)\,\mathbf{a}_1+x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_5-y_5)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O I

$$\mathbf{B_{19}} = x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_6+y_6)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_6-y_6)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{O II}$$

$$\mathbf{B_{20}} = -y_6\,\mathbf{a}_1 + (x_6-y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_6-2y_6)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{O II}$$

$$\mathbf{B_{21}} = -(x_6-y_6)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_6-y_6)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{O II}$$

$$\mathbf{B_{22}} = -x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6+\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_6+y_6)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_6-y_6)\,\hat{\mathbf{y}} + c\left(z_6+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{O II}$$

$$\mathbf{B_{23}} = y_6\,\mathbf{a}_1 - (x_6-y_6)\,\mathbf{a}_2 + \left(z_6+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_6+2y_6)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + c\left(z_6+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{O II}$$

$$\mathbf{B_{24}} = (x_6-y_6)\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + \left(z_6+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_6-y_6)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + c\left(z_6+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{O II}$$

$$\mathbf{B_{25}} = x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_7+y_7)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_7-y_7)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{O III}$$

$$\mathbf{B_{26}} = -y_7\,\mathbf{a}_1 + (x_7-y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_7-2y_7)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{O III}$$

$$\mathbf{B_{27}} = -(x_7-y_7)\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_7-y_7)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{O III}$$

$$\mathbf{B_{28}} = -x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7+\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_7+y_7)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_7-y_7)\,\hat{\mathbf{y}} + c\left(z_7+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{O III}$$

$$\mathbf{B_{29}} = y_7\,\mathbf{a}_1 - (x_7-y_7)\,\mathbf{a}_2 + \left(z_7+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_7+2y_7)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + c\left(z_7+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{O III}$$

$$\mathbf{B_{30}} = (x_7-y_7)\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + \left(z_7+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_7-y_7)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + c\left(z_7+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{O III}$$

$$\mathbf{B_{31}} = x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_8+y_8)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_8-y_8)\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{O IV}$$

$$\mathbf{B_{32}} = -y_8\,\mathbf{a}_1 + (x_8-y_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_8-2y_8)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{O IV}$$

$$\mathbf{B_{33}} = -(x_8-y_8)\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_8-y_8)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{O IV}$$

$$\mathbf{B_{34}} = -x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + \left(z_8+\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_8+y_8)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_8-y_8)\,\hat{\mathbf{y}} + c\left(z_8+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{O IV}$$

$$\mathbf{B_{35}} = y_8\,\mathbf{a}_1 - (x_8-y_8)\,\mathbf{a}_2 + \left(z_8+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_8+2y_8)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + c\left(z_8+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{O IV}$$

$$\mathbf{B_{36}} = (x_8-y_8)\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + \left(z_8+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_8-y_8)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} + c\left(z_8+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{O IV}$$

$$\mathbf{B_{37}} = x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_9+y_9)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_9-y_9)\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{Si I}$$

$$\mathbf{B_{38}} = -y_9\,\mathbf{a}_1 + (x_9-y_9)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_9-2y_9)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{Si I}$$

$$\mathbf{B_{39}} = -(x_9-y_9)\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_9-y_9)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{Si I}$$

$$\mathbf{B_{40}} = -x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + \left(z_9+\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_9+y_9)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_9-y_9)\,\hat{\mathbf{y}} + c\left(z_9+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{Si I}$$

$$\mathbf{B_{41}} = y_9\,\mathbf{a}_1 - (x_9-y_9)\,\mathbf{a}_2 + \left(z_9+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_9+2y_9)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + c\left(z_9+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{Si I}$$

$$\mathbf{B_{42}} = (x_9-y_9)\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + \left(z_9+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_9-y_9)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}} + c\left(z_9+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{Si I}$$

References

[1] B. Liu and J. Barbier, *Structures of the Stuffed Tridymite Derivatives, $BaMSiO_4$ (M = Co, Zn, Mg)*, J. Solid State Chem. **102**, 115–125 (1993), doi:10.1006/jssc.1993.1013.

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