α-BaB_2O_4 (Low Temperature) Structure: A2BC4_hR42_161_2b_b_4b-001

This structure originally had the label `A2BC4_hR42_161_2b_b_4b`. Calls to that address will be redirected here.

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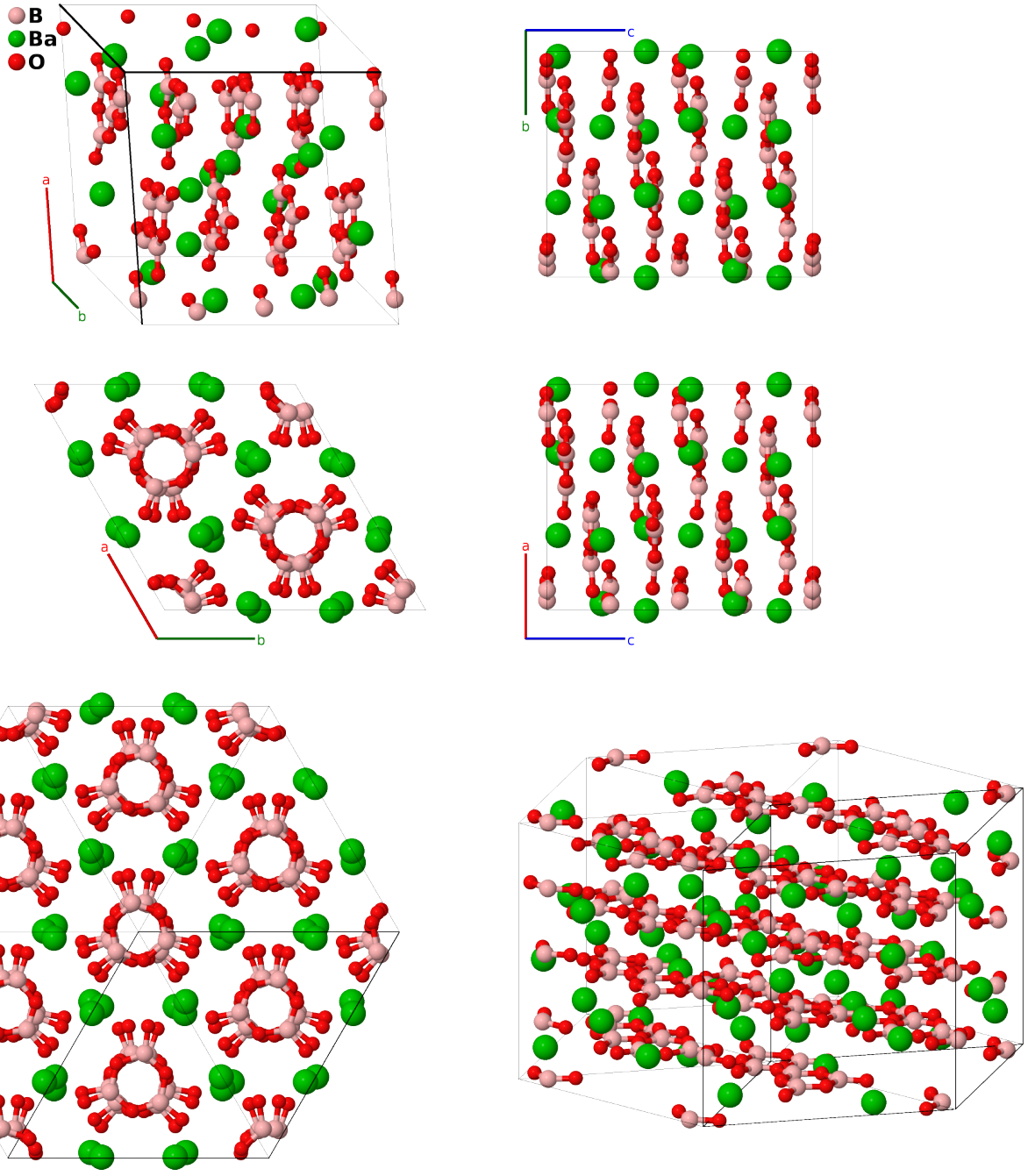
https://aflow.org/p/UFMT

https://aflow.org/p/A2BC4_hR42_161_2b_b_4b-001

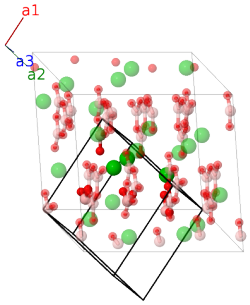


Prototype	B_2BaO_4
AFLOW prototype label	A2BC4_hR42_161_2b_b_4b-001
ICSD	30885
Pearson symbol	hR42
Space group number	161
Space group symbol	$R3c$
AFLOW prototype command	`aflow --proto=A2BC4_hR42_161_2b_b_4b-001 --params=`$a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

- This is the low-temperature structure. Heating to temperatures between 100-400°C it transforms into β-BaB_2O_4. The principle difference between the two forms is the lack of inversion symmetry in the low-temperature structure.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_1 - z_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_1 - 2y_1 + z_1)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(6b)	B I
$\mathbf{B_2}$	=	$z_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + y_1\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_1 - z_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_1 - y_1 - z_1)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(6b)	B I
$\mathbf{B_3}$	=	$y_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_1 - y_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_1 + y_1 - 2z_1)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(6b)	B I
$\mathbf{B_4}$	=	$\left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_1 - z_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_1 - 2y_1 + z_1)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_1 + 2y_1 + 2z_1 + 3)\,\hat{\mathbf{z}}$	(6b)	B I
$\mathbf{B_5}$	=	$\left(y_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_1 - z_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_1 - y_1 - z_1)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_1 + 2y_1 + 2z_1 + 3)\,\hat{\mathbf{z}}$	(6b)	B I
$\mathbf{B_6}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_1 - y_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_1 + y_1 - 2z_1)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_1 + 2y_1 + 2z_1 + 3)\,\hat{\mathbf{z}}$	(6b)	B I
$\mathbf{B_7}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_2 - 2y_2 + z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6b)	B II
$\mathbf{B_8}$	=	$z_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + y_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_2 - z_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_2 - y_2 - z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6b)	B II
$\mathbf{B_9}$	=	$y_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2 - y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_2 + y_2 - 2z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6b)	B II
$\mathbf{B_{10}}$	=	$\left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_2 - 2y_2 + z_2)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_2 + 2y_2 + 2z_2 + 3)\,\hat{\mathbf{z}}$	(6b)	B II

$$\mathbf{B_{11}} = \left(y_2+\tfrac{1}{2}\right)\mathbf{a}_1+\left(x_2+\tfrac{1}{2}\right)\mathbf{a}_2+\left(z_2+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\left(y_2-z_2\right)\hat{\mathbf{x}}+\tfrac{\sqrt{3}}{6}a\left(2x_2-y_2-z_2\right)\hat{\mathbf{y}}+\tfrac{1}{6}c\left(2x_2+2y_2+2z_2+3\right)\hat{\mathbf{z}} \quad (6b) \quad \text{B II}$$

$$\mathbf{B_{12}} = \left(x_2+\tfrac{1}{2}\right)\mathbf{a}_1+\left(z_2+\tfrac{1}{2}\right)\mathbf{a}_2+\left(y_2+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\left(x_2-y_2\right)\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\left(x_2+y_2-2z_2\right)\hat{\mathbf{y}}+\tfrac{1}{6}c\left(2x_2+2y_2+2z_2+3\right)\hat{\mathbf{z}} \quad (6b) \quad \text{B II}$$

$$\mathbf{B_{13}} = x_3\mathbf{a}_1+y_3\mathbf{a}_2+z_3\mathbf{a}_3 = \tfrac{1}{2}a\left(x_3-z_3\right)\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\left(x_3-2y_3+z_3\right)\hat{\mathbf{y}}+\tfrac{1}{3}c\left(x_3+y_3+z_3\right)\hat{\mathbf{z}} \quad (6b) \quad \text{Ba I}$$

$$\mathbf{B_{14}} = z_3\mathbf{a}_1+x_3\mathbf{a}_2+y_3\mathbf{a}_3 = -\tfrac{1}{2}a\left(y_3-z_3\right)\hat{\mathbf{x}}+\tfrac{\sqrt{3}}{6}a\left(2x_3-y_3-z_3\right)\hat{\mathbf{y}}+\tfrac{1}{3}c\left(x_3+y_3+z_3\right)\hat{\mathbf{z}} \quad (6b) \quad \text{Ba I}$$

$$\mathbf{B_{15}} = y_3\mathbf{a}_1+z_3\mathbf{a}_2+x_3\mathbf{a}_3 = -\tfrac{1}{2}a\left(x_3-y_3\right)\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\left(x_3+y_3-2z_3\right)\hat{\mathbf{y}}+\tfrac{1}{3}c\left(x_3+y_3+z_3\right)\hat{\mathbf{z}} \quad (6b) \quad \text{Ba I}$$

$$\mathbf{B_{16}} = \left(z_3+\tfrac{1}{2}\right)\mathbf{a}_1+\left(y_3+\tfrac{1}{2}\right)\mathbf{a}_2+\left(x_3+\tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\left(x_3-z_3\right)\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\left(x_3-2y_3+z_3\right)\hat{\mathbf{y}}+\tfrac{1}{6}c\left(2x_3+2y_3+2z_3+3\right)\hat{\mathbf{z}} \quad (6b) \quad \text{Ba I}$$

$$\mathbf{B_{17}} = \left(y_3+\tfrac{1}{2}\right)\mathbf{a}_1+\left(x_3+\tfrac{1}{2}\right)\mathbf{a}_2+\left(z_3+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\left(y_3-z_3\right)\hat{\mathbf{x}}+\tfrac{\sqrt{3}}{6}a\left(2x_3-y_3-z_3\right)\hat{\mathbf{y}}+\tfrac{1}{6}c\left(2x_3+2y_3+2z_3+3\right)\hat{\mathbf{z}} \quad (6b) \quad \text{Ba I}$$

$$\mathbf{B_{18}} = \left(x_3+\tfrac{1}{2}\right)\mathbf{a}_1+\left(z_3+\tfrac{1}{2}\right)\mathbf{a}_2+\left(y_3+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\left(x_3-y_3\right)\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\left(x_3+y_3-2z_3\right)\hat{\mathbf{y}}+\tfrac{1}{6}c\left(2x_3+2y_3+2z_3+3\right)\hat{\mathbf{z}} \quad (6b) \quad \text{Ba I}$$

$$\mathbf{B_{19}} = x_4\mathbf{a}_1+y_4\mathbf{a}_2+z_4\mathbf{a}_3 = \tfrac{1}{2}a\left(x_4-z_4\right)\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\left(x_4-2y_4+z_4\right)\hat{\mathbf{y}}+\tfrac{1}{3}c\left(x_4+y_4+z_4\right)\hat{\mathbf{z}} \quad (6b) \quad \text{O I}$$

$$\mathbf{B_{20}} = z_4\mathbf{a}_1+x_4\mathbf{a}_2+y_4\mathbf{a}_3 = -\tfrac{1}{2}a\left(y_4-z_4\right)\hat{\mathbf{x}}+\tfrac{\sqrt{3}}{6}a\left(2x_4-y_4-z_4\right)\hat{\mathbf{y}}+\tfrac{1}{3}c\left(x_4+y_4+z_4\right)\hat{\mathbf{z}} \quad (6b) \quad \text{O I}$$

$$\mathbf{B_{21}} = y_4\mathbf{a}_1+z_4\mathbf{a}_2+x_4\mathbf{a}_3 = -\tfrac{1}{2}a\left(x_4-y_4\right)\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\left(x_4+y_4-2z_4\right)\hat{\mathbf{y}}+\tfrac{1}{3}c\left(x_4+y_4+z_4\right)\hat{\mathbf{z}} \quad (6b) \quad \text{O I}$$

$$\mathbf{B_{22}} = \left(z_4+\tfrac{1}{2}\right)\mathbf{a}_1+\left(y_4+\tfrac{1}{2}\right)\mathbf{a}_2+\left(x_4+\tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\left(x_4-z_4\right)\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\left(x_4-2y_4+z_4\right)\hat{\mathbf{y}}+\tfrac{1}{6}c\left(2x_4+2y_4+2z_4+3\right)\hat{\mathbf{z}} \quad (6b) \quad \text{O I}$$

$$\mathbf{B_{23}} = \left(y_4+\tfrac{1}{2}\right)\mathbf{a}_1+\left(x_4+\tfrac{1}{2}\right)\mathbf{a}_2+\left(z_4+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\left(y_4-z_4\right)\hat{\mathbf{x}}+\tfrac{\sqrt{3}}{6}a\left(2x_4-y_4-z_4\right)\hat{\mathbf{y}}+\tfrac{1}{6}c\left(2x_4+2y_4+2z_4+3\right)\hat{\mathbf{z}} \quad (6b) \quad \text{O I}$$

$$\mathbf{B_{24}} = \left(x_4+\tfrac{1}{2}\right)\mathbf{a}_1+\left(z_4+\tfrac{1}{2}\right)\mathbf{a}_2+\left(y_4+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\left(x_4-y_4\right)\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\left(x_4+y_4-2z_4\right)\hat{\mathbf{y}}+\tfrac{1}{6}c\left(2x_4+2y_4+2z_4+3\right)\hat{\mathbf{z}} \quad (6b) \quad \text{O I}$$

$$\mathbf{B_{25}} = x_5\mathbf{a}_1+y_5\mathbf{a}_2+z_5\mathbf{a}_3 = \tfrac{1}{2}a\left(x_5-z_5\right)\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\left(x_5-2y_5+z_5\right)\hat{\mathbf{y}}+\tfrac{1}{3}c\left(x_5+y_5+z_5\right)\hat{\mathbf{z}} \quad (6b) \quad \text{O II}$$

$$\mathbf{B_{26}} = z_5\mathbf{a}_1+x_5\mathbf{a}_2+y_5\mathbf{a}_3 = -\tfrac{1}{2}a\left(y_5-z_5\right)\hat{\mathbf{x}}+\tfrac{\sqrt{3}}{6}a\left(2x_5-y_5-z_5\right)\hat{\mathbf{y}}+\tfrac{1}{3}c\left(x_5+y_5+z_5\right)\hat{\mathbf{z}} \quad (6b) \quad \text{O II}$$

$$\mathbf{B_{27}} = y_5\mathbf{a}_1+z_5\mathbf{a}_2+x_5\mathbf{a}_3 = -\tfrac{1}{2}a\left(x_5-y_5\right)\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\left(x_5+y_5-2z_5\right)\hat{\mathbf{y}}+\tfrac{1}{3}c\left(x_5+y_5+z_5\right)\hat{\mathbf{z}} \quad (6b) \quad \text{O II}$$

$$\mathbf{B_{28}} = \left(z_5+\tfrac{1}{2}\right)\mathbf{a}_1+\left(y_5+\tfrac{1}{2}\right)\mathbf{a}_2+\left(x_5+\tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\left(x_5-z_5\right)\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\left(x_5-2y_5+z_5\right)\hat{\mathbf{y}}+\tfrac{1}{6}c\left(2x_5+2y_5+2z_5+3\right)\hat{\mathbf{z}} \quad (6b) \quad \text{O II}$$

$$\mathbf{B_{29}} = \left(y_5+\tfrac{1}{2}\right)\mathbf{a}_1+\left(x_5+\tfrac{1}{2}\right)\mathbf{a}_2+\left(z_5+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\left(y_5-z_5\right)\hat{\mathbf{x}}+\tfrac{\sqrt{3}}{6}a\left(2x_5-y_5-z_5\right)\hat{\mathbf{y}}+\tfrac{1}{6}c\left(2x_5+2y_5+2z_5+3\right)\hat{\mathbf{z}} \quad (6b) \quad \text{O II}$$

$$\mathbf{B_{30}} = \left(x_5+\tfrac{1}{2}\right)\mathbf{a}_1+\left(z_5+\tfrac{1}{2}\right)\mathbf{a}_2+\left(y_5+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\left(x_5-y_5\right)\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\left(x_5+y_5-2z_5\right)\hat{\mathbf{y}}+\tfrac{1}{6}c\left(2x_5+2y_5+2z_5+3\right)\hat{\mathbf{z}} \quad (6b) \quad \text{O II}$$

$$\mathbf{B_{31}} = x_6\mathbf{a}_1+y_6\mathbf{a}_2+z_6\mathbf{a}_3 = \tfrac{1}{2}a\left(x_6-z_6\right)\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\left(x_6-2y_6+z_6\right)\hat{\mathbf{y}}+\tfrac{1}{3}c\left(x_6+y_6+z_6\right)\hat{\mathbf{z}} \quad (6b) \quad \text{O III}$$

$$\mathbf{B_{32}} = z_6\mathbf{a}_1+x_6\mathbf{a}_2+y_6\mathbf{a}_3 = -\tfrac{1}{2}a\left(y_6-z_6\right)\hat{\mathbf{x}}+\tfrac{\sqrt{3}}{6}a\left(2x_6-y_6-z_6\right)\hat{\mathbf{y}}+\tfrac{1}{3}c\left(x_6+y_6+z_6\right)\hat{\mathbf{z}} \quad (6b) \quad \text{O III}$$

$$\mathbf{B_{33}} = y_6\mathbf{a}_1+z_6\mathbf{a}_2+x_6\mathbf{a}_3 = -\tfrac{1}{2}a\left(x_6-y_6\right)\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\left(x_6+y_6-2z_6\right)\hat{\mathbf{y}}+\tfrac{1}{3}c\left(x_6+y_6+z_6\right)\hat{\mathbf{z}} \quad (6b) \quad \text{O III}$$

$$\mathbf{B_{34}} = \left(z_6+\tfrac{1}{2}\right)\mathbf{a}_1+\left(y_6+\tfrac{1}{2}\right)\mathbf{a}_2+\left(x_6+\tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_6-z_6)\,\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\,(x_6-2y_6+z_6)\,\hat{\mathbf{y}}+\tfrac{1}{6}c\,(2x_6+2y_6+2z_6+3)\,\hat{\mathbf{z}} \quad (6b) \quad \text{O III}$$

$$\mathbf{B_{35}} = \left(y_6+\tfrac{1}{2}\right)\mathbf{a}_1+\left(x_6+\tfrac{1}{2}\right)\mathbf{a}_2+\left(z_6+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(y_6-z_6)\,\hat{\mathbf{x}}+\tfrac{\sqrt{3}}{6}a\,(2x_6-y_6-z_6)\,\hat{\mathbf{y}}+\tfrac{1}{6}c\,(2x_6+2y_6+2z_6+3)\,\hat{\mathbf{z}} \quad (6b) \quad \text{O III}$$

$$\mathbf{B_{36}} = \left(x_6+\tfrac{1}{2}\right)\mathbf{a}_1+\left(z_6+\tfrac{1}{2}\right)\mathbf{a}_2+\left(y_6+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(x_6-y_6)\,\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\,(x_6+y_6-2z_6)\,\hat{\mathbf{y}}+\tfrac{1}{6}c\,(2x_6+2y_6+2z_6+3)\,\hat{\mathbf{z}} \quad (6b) \quad \text{O III}$$

$$\mathbf{B_{37}} = x_7\,\mathbf{a}_1+y_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_7-z_7)\,\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\,(x_7-2y_7+z_7)\,\hat{\mathbf{y}}+\tfrac{1}{3}c\,(x_7+y_7+z_7)\,\hat{\mathbf{z}} \quad (6b) \quad \text{O IV}$$

$$\mathbf{B_{38}} = z_7\,\mathbf{a}_1+x_7\,\mathbf{a}_2+y_7\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_7-z_7)\,\hat{\mathbf{x}}+\tfrac{\sqrt{3}}{6}a\,(2x_7-y_7-z_7)\,\hat{\mathbf{y}}+\tfrac{1}{3}c\,(x_7+y_7+z_7)\,\hat{\mathbf{z}} \quad (6b) \quad \text{O IV}$$

$$\mathbf{B_{39}} = y_7\,\mathbf{a}_1+z_7\,\mathbf{a}_2+x_7\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_7-y_7)\,\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\,(x_7+y_7-2z_7)\,\hat{\mathbf{y}}+\tfrac{1}{3}c\,(x_7+y_7+z_7)\,\hat{\mathbf{z}} \quad (6b) \quad \text{O IV}$$

$$\mathbf{B_{40}} = \left(z_7+\tfrac{1}{2}\right)\mathbf{a}_1+\left(y_7+\tfrac{1}{2}\right)\mathbf{a}_2+\left(x_7+\tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_7-z_7)\,\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\,(x_7-2y_7+z_7)\,\hat{\mathbf{y}}+\tfrac{1}{6}c\,(2x_7+2y_7+2z_7+3)\,\hat{\mathbf{z}} \quad (6b) \quad \text{O IV}$$

$$\mathbf{B_{41}} = \left(y_7+\tfrac{1}{2}\right)\mathbf{a}_1+\left(x_7+\tfrac{1}{2}\right)\mathbf{a}_2+\left(z_7+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(y_7-z_7)\,\hat{\mathbf{x}}+\tfrac{\sqrt{3}}{6}a\,(2x_7-y_7-z_7)\,\hat{\mathbf{y}}+\tfrac{1}{6}c\,(2x_7+2y_7+2z_7+3)\,\hat{\mathbf{z}} \quad (6b) \quad \text{O IV}$$

$$\mathbf{B_{42}} = \left(x_7+\tfrac{1}{2}\right)\mathbf{a}_1+\left(z_7+\tfrac{1}{2}\right)\mathbf{a}_2+\left(y_7+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(x_7-y_7)\,\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\,(x_7+y_7-2z_7)\,\hat{\mathbf{y}}+\tfrac{1}{6}c\,(2x_7+2y_7+2z_7+3)\,\hat{\mathbf{z}} \quad (6b) \quad \text{O IV}$$

References

[1] R. Fröhlich, *Crystal Structure of the low-temperature form of BaB_2O_4*, Z. Kristallogr. **168**, 109–112 (1984), doi:10.1524/zkri.1984.168.14.109.