β-BaB_2O_4 (High Temperature) Structure: A2BC4_hR42_167_f_ac_2f-001

This structure originally had the label `A2BC4_hR42_167_f_ac_2f`. Calls to that address will be redirected here.

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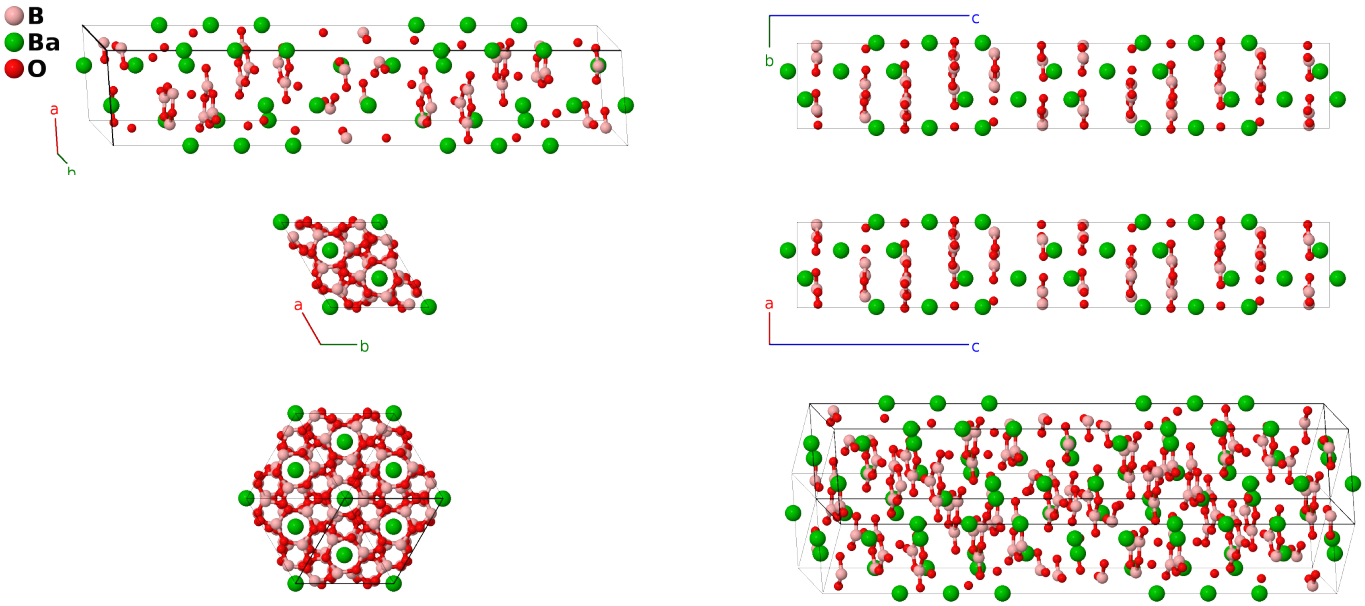
https://aflow.org/p/RYPV

https://aflow.org/p/A2BC4_hR42_167_f_ac_2f-001

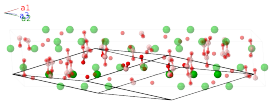


Prototype	B_2BaO_4
AFLOW prototype label	A2BC4_hR42_167_f_ac_2f-001
ICSD	14376
Pearson symbol	hR42
Space group number	167
Space group symbol	$R\bar{3}c$
AFLOW prototype command	`aflow --proto=A2BC4_hR42_167_f_ac_2f-001 --params=`$a, c/a, x_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5$

- This is the high-temperature structure of BaB_2O_4. Cooling to temperatures between 100-400°C it transforms into α-BaB_2O_4. The principle difference between the two forms is the lack of inversion symmetry in the low-temperature structure.
- This structure was determined by cooling liquid BaB_2O_4 to room temperature.

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
$\mathbf{B_1}$	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(2a)	Ba I
$\mathbf{B_2}$	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(2a)	Ba I
$\mathbf{B_3}$	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	$cx_2\,\hat{\mathbf{z}}$	(4c)	Ba II
$\mathbf{B_4}$	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	$-c\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Ba II
$\mathbf{B_5}$	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	$-cx_2\,\hat{\mathbf{z}}$	(4c)	Ba II
$\mathbf{B_6}$	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	$c\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Ba II
$\mathbf{B_7}$	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	$\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_3 - 2y_3 + z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(12f)	B I
$\mathbf{B_8}$	$z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	$-\frac{1}{2}a\,(y_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_3 - y_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(12f)	B I
$\mathbf{B_9}$	$y_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	$-\frac{1}{2}a\,(x_3 - y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_3 + y_3 - 2z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(12f)	B I
$\mathbf{B_{10}}$	$-\left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	$\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - 2y_3 + z_3)\,\hat{\mathbf{y}} - \frac{1}{6}c\,(2x_3 + 2y_3 + 2z_3 - 3)\,\hat{\mathbf{z}}$	(12f)	B I
$\mathbf{B_{11}}$	$-\left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	$-\frac{1}{2}a\,(y_3 - z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_3 - y_3 - z_3)\,\hat{\mathbf{y}} - \frac{1}{6}c\,(2x_3 + 2y_3 + 2z_3 - 3)\,\hat{\mathbf{z}}$	(12f)	B I
$\mathbf{B_{12}}$	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	$-\frac{1}{2}a\,(x_3 - y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 + y_3 - 2z_3)\,\hat{\mathbf{y}} - \frac{1}{6}c\,(2x_3 + 2y_3 + 2z_3 - 3)\,\hat{\mathbf{z}}$	(12f)	B I
$\mathbf{B_{13}}$	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	$-\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - 2y_3 + z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(12f)	B I
$\mathbf{B_{14}}$	$-z_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	$\frac{1}{2}a\,(y_3 - z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_3 - y_3 - z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(12f)	B I
$\mathbf{B_{15}}$	$-y_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	$\frac{1}{2}a\,(x_3 - y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 + y_3 - 2z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(12f)	B I
$\mathbf{B_{16}}$	$\left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	$-\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_3 - 2y_3 + z_3)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_3 + 2y_3 + 2z_3 + 3)\,\hat{\mathbf{z}}$	(12f)	B I
$\mathbf{B_{17}}$	$\left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	$\frac{1}{2}a\,(y_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_3 - y_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_3 + 2y_3 + 2z_3 + 3)\,\hat{\mathbf{z}}$	(12f)	B I
$\mathbf{B_{18}}$	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	$\frac{1}{2}a\,(x_3 - y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_3 + y_3 - 2z_3)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_3 + 2y_3 + 2z_3 + 3)\,\hat{\mathbf{z}}$	(12f)	B I
$\mathbf{B_{19}}$	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	$\frac{1}{2}a\,(x_4 - z_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_4 - 2y_4 + z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{20}}$	$z_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	$-\frac{1}{2}a\,(y_4 - z_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_4 - y_4 - z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{21}}$	$y_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	$-\frac{1}{2}a\,(x_4 - y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_4 + y_4 - 2z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(12f)	O I

$\mathbf{B_{22}}$	$= -\left(z_4-\frac{1}{2}\right)\mathbf{a}_1-\left(y_4-\frac{1}{2}\right)\mathbf{a}_2-\left(x_4-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(x_4-z_4\right)\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\left(x_4-2y_4+z_4\right)\hat{\mathbf{y}}-\frac{1}{6}c\left(2x_4+2y_4+2z_4-3\right)\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{23}}$	$= -\left(y_4-\frac{1}{2}\right)\mathbf{a}_1-\left(x_4-\frac{1}{2}\right)\mathbf{a}_2-\left(z_4-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-\frac{1}{2}a\left(y_4-z_4\right)\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\left(2x_4-y_4-z_4\right)\hat{\mathbf{y}}-\frac{1}{6}c\left(2x_4+2y_4+2z_4-3\right)\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{24}}$	$= -\left(x_4-\frac{1}{2}\right)\mathbf{a}_1-\left(z_4-\frac{1}{2}\right)\mathbf{a}_2-\left(y_4-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-\frac{1}{2}a\left(x_4-y_4\right)\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\left(x_4+y_4-2z_4\right)\hat{\mathbf{y}}-\frac{1}{6}c\left(2x_4+2y_4+2z_4-3\right)\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{25}}$	$= -x_4\,\mathbf{a}_1-y_4\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\left(x_4-z_4\right)\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\left(x_4-2y_4+z_4\right)\hat{\mathbf{y}}-\frac{1}{3}c\left(x_4+y_4+z_4\right)\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{26}}$	$= -z_4\,\mathbf{a}_1-x_4\,\mathbf{a}_2-y_4\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(y_4-z_4\right)\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\left(2x_4-y_4-z_4\right)\hat{\mathbf{y}}-\frac{1}{3}c\left(x_4+y_4+z_4\right)\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{27}}$	$= -y_4\,\mathbf{a}_1-z_4\,\mathbf{a}_2-x_4\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(x_4-y_4\right)\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\left(x_4+y_4-2z_4\right)\hat{\mathbf{y}}-\frac{1}{3}c\left(x_4+y_4+z_4\right)\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{28}}$	$= \left(z_4+\frac{1}{2}\right)\mathbf{a}_1+\left(y_4+\frac{1}{2}\right)\mathbf{a}_2+\left(x_4+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-\frac{1}{2}a\left(x_4-z_4\right)\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\left(x_4-2y_4+z_4\right)\hat{\mathbf{y}}+\frac{1}{6}c\left(2x_4+2y_4+2z_4+3\right)\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{29}}$	$= \left(y_4+\frac{1}{2}\right)\mathbf{a}_1+\left(x_4+\frac{1}{2}\right)\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(y_4-z_4\right)\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\left(2x_4-y_4-z_4\right)\hat{\mathbf{y}}+\frac{1}{6}c\left(2x_4+2y_4+2z_4+3\right)\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{30}}$	$= \left(x_4+\frac{1}{2}\right)\mathbf{a}_1+\left(z_4+\frac{1}{2}\right)\mathbf{a}_2+\left(y_4+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(x_4-y_4\right)\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\left(x_4+y_4-2z_4\right)\hat{\mathbf{y}}+\frac{1}{6}c\left(2x_4+2y_4+2z_4+3\right)\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{31}}$	$= x_5\,\mathbf{a}_1+y_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(x_5-z_5\right)\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\left(x_5-2y_5+z_5\right)\hat{\mathbf{y}}+\frac{1}{3}c\left(x_5+y_5+z_5\right)\hat{\mathbf{z}}$	(12f)	O II
$\mathbf{B_{32}}$	$= z_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2+y_5\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\left(y_5-z_5\right)\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\left(2x_5-y_5-z_5\right)\hat{\mathbf{y}}+\frac{1}{3}c\left(x_5+y_5+z_5\right)\hat{\mathbf{z}}$	(12f)	O II
$\mathbf{B_{33}}$	$= y_5\,\mathbf{a}_1+z_5\,\mathbf{a}_2+x_5\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\left(x_5-y_5\right)\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\left(x_5+y_5-2z_5\right)\hat{\mathbf{y}}+\frac{1}{3}c\left(x_5+y_5+z_5\right)\hat{\mathbf{z}}$	(12f)	O II
$\mathbf{B_{34}}$	$= -\left(z_5-\frac{1}{2}\right)\mathbf{a}_1-\left(y_5-\frac{1}{2}\right)\mathbf{a}_2-\left(x_5-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(x_5-z_5\right)\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\left(x_5-2y_5+z_5\right)\hat{\mathbf{y}}-\frac{1}{6}c\left(2x_5+2y_5+2z_5-3\right)\hat{\mathbf{z}}$	(12f)	O II
$\mathbf{B_{35}}$	$= -\left(y_5-\frac{1}{2}\right)\mathbf{a}_1-\left(x_5-\frac{1}{2}\right)\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-\frac{1}{2}a\left(y_5-z_5\right)\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\left(2x_5-y_5-z_5\right)\hat{\mathbf{y}}-\frac{1}{6}c\left(2x_5+2y_5+2z_5-3\right)\hat{\mathbf{z}}$	(12f)	O II
$\mathbf{B_{36}}$	$= -\left(x_5-\frac{1}{2}\right)\mathbf{a}_1-\left(z_5-\frac{1}{2}\right)\mathbf{a}_2-\left(y_5-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-\frac{1}{2}a\left(x_5-y_5\right)\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\left(x_5+y_5-2z_5\right)\hat{\mathbf{y}}-\frac{1}{6}c\left(2x_5+2y_5+2z_5-3\right)\hat{\mathbf{z}}$	(12f)	O II
$\mathbf{B_{37}}$	$= -x_5\,\mathbf{a}_1-y_5\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\left(x_5-z_5\right)\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\left(x_5-2y_5+z_5\right)\hat{\mathbf{y}}-\frac{1}{3}c\left(x_5+y_5+z_5\right)\hat{\mathbf{z}}$	(12f)	O II
$\mathbf{B_{38}}$	$= -z_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2-y_5\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(y_5-z_5\right)\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\left(2x_5-y_5-z_5\right)\hat{\mathbf{y}}-\frac{1}{3}c\left(x_5+y_5+z_5\right)\hat{\mathbf{z}}$	(12f)	O II
$\mathbf{B_{39}}$	$= -y_5\,\mathbf{a}_1-z_5\,\mathbf{a}_2-x_5\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(x_5-y_5\right)\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\left(x_5+y_5-2z_5\right)\hat{\mathbf{y}}-\frac{1}{3}c\left(x_5+y_5+z_5\right)\hat{\mathbf{z}}$	(12f)	O II
$\mathbf{B_{40}}$	$= \left(z_5+\frac{1}{2}\right)\mathbf{a}_1+\left(y_5+\frac{1}{2}\right)\mathbf{a}_2+\left(x_5+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-\frac{1}{2}a\left(x_5-z_5\right)\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\left(x_5-2y_5+z_5\right)\hat{\mathbf{y}}+\frac{1}{6}c\left(2x_5+2y_5+2z_5+3\right)\hat{\mathbf{z}}$	(12f)	O II
$\mathbf{B_{41}}$	$= \left(y_5+\frac{1}{2}\right)\mathbf{a}_1+\left(x_5+\frac{1}{2}\right)\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(y_5-z_5\right)\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\left(2x_5-y_5-z_5\right)\hat{\mathbf{y}}+\frac{1}{6}c\left(2x_5+2y_5+2z_5+3\right)\hat{\mathbf{z}}$	(12f)	O II
$\mathbf{B_{42}}$	$= \left(x_5+\frac{1}{2}\right)\mathbf{a}_1+\left(z_5+\frac{1}{2}\right)\mathbf{a}_2+\left(y_5+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(x_5-y_5\right)\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\left(x_5+y_5-2z_5\right)\hat{\mathbf{y}}+\frac{1}{6}c\left(2x_5+2y_5+2z_5+3\right)\hat{\mathbf{z}}$	(12f)	O II

References

[1] A. D. Mighell, A. Perloff, and S. Block, *The crystal structure of the high temperature form of barium borate, $BaO{\cdot}B_2O_3$*, Acta Cryst. **20**, 819–823 (1966), doi:10.1107/S0365110X66001920.

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