

β -BaB₂O₄ (High Temperature) Structure: A2BC4_hR42_167_f_ac_2f-001

This structure previously used the label(s) **A2BC4_hR42_167_f_ac_2f**. Calls to these addresses will be redirected here.

Cite this page as:

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/RYPV>

https://aflow.org/prototype-encyclopedia/A2BC4_hR42_167_f_ac_2f-001

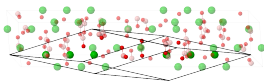
Prototype	B ₂ BaO ₄
AFLOW prototype label	A2BC4_hR42_167_f_ac_2f-001
ICSD	14376
CCDC	1595761
Pearson symbol	hR42
Space group number	167
Space group symbol	$R\bar{3}c$
AFLOW prototype command	<code>aflow --proto=A2BC4_hR42_167_f_ac_2f-001</code> <code>--params=a, c/a, x₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅</code>

- This is the high-temperature structure of BaB₂O₄. Cooling to temperatures between 100-400°C it transforms into α -BaB₂O₄. 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 BaB₂O₄ to room temperature.

Rhombohedral primitive vectors

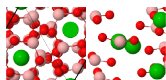
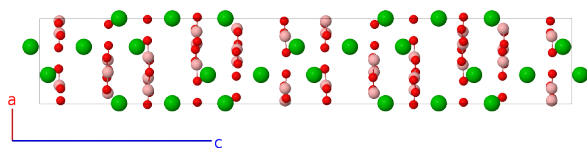
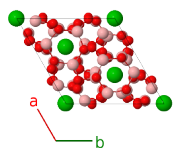
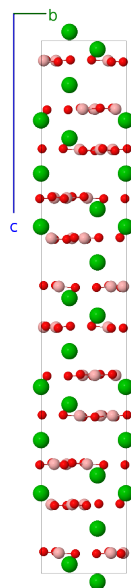
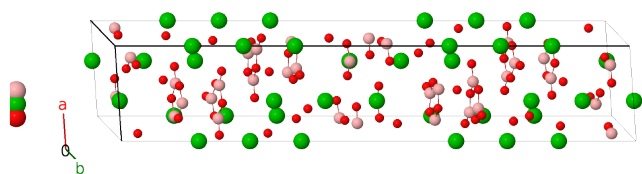
$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \end{aligned}$$

~83



Basis vectors

B
Ba
O



	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
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$c x_2 \hat{\mathbf{z}}$	(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
$\mathbf{B}_5$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-c x_2 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{22}$	$= -\left(z_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a (x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a (x_4 - 2y_4 + z_4) \hat{\mathbf{y}} - \frac{1}{6} c (2x_4 + 2y_4 + 2z_4 - 3) \hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B}_{23}$	$= -\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2} a (y_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a (2x_4 - y_4 - z_4) \hat{\mathbf{y}} - \frac{1}{6} c (2x_4 + 2y_4 + 2z_4 - 3) \hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B}_{24}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_2 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2} a (x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a (x_4 + y_4 - 2z_4) \hat{\mathbf{y}} - \frac{1}{6} c (2x_4 + 2y_4 + 2z_4 - 3) \hat{\mathbf{z}}$	(12f)	O I

$$\begin{aligned}
\mathbf{B}_{25} &= -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) &\quad \text{O I} \\
\mathbf{B}_{26} &= -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) &\quad \text{O I} \\
\mathbf{B}_{27} &= -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) &\quad \text{O I} \\
\mathbf{B}_{28} &= (z_4 + \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 + \frac{1}{2}) \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}{6}c(2x_4 + 2y_4 + 2z_4 + 3) \hat{\mathbf{z}} &(12f) &\quad \text{O I} \\
\mathbf{B}_{29} &= (y_4 + \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \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}{6}c(2x_4 + 2y_4 + 2z_4 + 3) \hat{\mathbf{z}} &(12f) &\quad \text{O I} \\
\mathbf{B}_{30} &= (x_4 + \frac{1}{2}) \mathbf{a}_1 + (z_4 + \frac{1}{2}) \mathbf{a}_2 + (y_4 + \frac{1}{2}) \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}{6}c(2x_4 + 2y_4 + 2z_4 + 3) \hat{\mathbf{z}} &(12f) &\quad \text{O I} \\
\mathbf{B}_{31} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= \frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 - 2y_5 + z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}} &(12f) &\quad \text{O II} \\
\mathbf{B}_{32} &= z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + y_5 \mathbf{a}_3 &= -\frac{1}{2}a(y_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_5 - y_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}} &(12f) &\quad \text{O II} \\
\mathbf{B}_{33} &= y_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3 &= -\frac{1}{2}a(x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 + y_5 - 2z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}} &(12f) &\quad \text{O II} \\
\mathbf{B}_{34} &= -(z_5 - \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 - (x_5 - \frac{1}{2}) \mathbf{a}_3 &= \frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - 2y_5 + z_5) \hat{\mathbf{y}} - \frac{1}{6}c(2x_5 + 2y_5 + 2z_5 - 3) \hat{\mathbf{z}} &(12f) &\quad \text{O II} \\
\mathbf{B}_{35} &= -(y_5 - \frac{1}{2}) \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3 &= -\frac{1}{2}a(y_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_5 - y_5 - z_5) \hat{\mathbf{y}} - \frac{1}{6}c(2x_5 + 2y_5 + 2z_5 - 3) \hat{\mathbf{z}} &(12f) &\quad \text{O II} \\
\mathbf{B}_{36} &= -(x_5 - \frac{1}{2}) \mathbf{a}_1 - (z_5 - \frac{1}{2}) \mathbf{a}_2 - (y_5 - \frac{1}{2}) \mathbf{a}_3 &= -\frac{1}{2}a(x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 + y_5 - 2z_5) \hat{\mathbf{y}} - \frac{1}{6}c(2x_5 + 2y_5 + 2z_5 - 3) \hat{\mathbf{z}} &(12f) &\quad \text{O II} \\
\mathbf{B}_{37} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 &= -\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - 2y_5 + z_5) \hat{\mathbf{y}} - \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}} &(12f) &\quad \text{O II} \\
\mathbf{B}_{38} &= -z_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - y_5 \mathbf{a}_3 &= \frac{1}{2}a(y_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_5 - y_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}} &(12f) &\quad \text{O II} \\
\mathbf{B}_{39} &= -y_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3 &= \frac{1}{2}a(x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 + y_5 - 2z_5) \hat{\mathbf{y}} - \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}} &(12f) &\quad \text{O II} \\
\mathbf{B}_{40} &= (z_5 + \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + (x_5 + \frac{1}{2}) \mathbf{a}_3 &= -\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 - 2y_5 + z_5) \hat{\mathbf{y}} + \frac{1}{6}c(2x_5 + 2y_5 + 2z_5 + 3) \hat{\mathbf{z}} &(12f) &\quad \text{O II} \\
\mathbf{B}_{41} &= (y_5 + \frac{1}{2}) \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3 &= \frac{1}{2}a(y_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_5 - y_5 - z_5) \hat{\mathbf{y}} + \frac{1}{6}c(2x_5 + 2y_5 + 2z_5 + 3) \hat{\mathbf{z}} &(12f) &\quad \text{O II} \\
\mathbf{B}_{42} &= (x_5 + \frac{1}{2}) \mathbf{a}_1 + (z_5 + \frac{1}{2}) \mathbf{a}_2 + (y_5 + \frac{1}{2}) \mathbf{a}_3 &= \frac{1}{2}a(x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 + y_5 - 2z_5) \hat{\mathbf{y}} + \frac{1}{6}c(2x_5 + 2y_5 + 2z_5 + 3) \hat{\mathbf{z}} &(12f) &\quad \text{O II}
\end{aligned}$$

References

- [1] A. D. Mighell, A. Perloff, and S. Block, *The crystal structure of the high temperature form of barium borate, BaO·B₂O₃*, Acta Cryst. **20**, 819–823 (1966), doi:10.1107/S0365110X66001920.

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- [1] R. Fröhlich, *Crystal Structure of the low-temperature form of BaB₂O₄*, Z. Kristallogr. **168**, 109–112 (1984), doi:10.1524/zkri.1984.168.14.109.

First cited in

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