

α -BaB₂O₄ (Low Temperature) Structure: A2BC4_hR42_161_2b_b_4b-001

This structure previously used the label(s) **A2BC4_hR42_161_2b_b_4b**. Calls to these addresses will be redirected here.

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

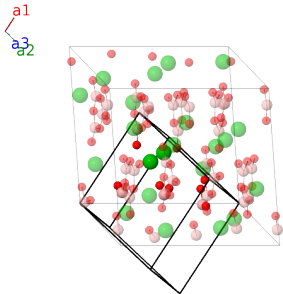
https://aflow.org/prototype-encyclopedia/A2BC4_hR42_161_2b_b_4b-001

Prototype	B ₂ BaO ₄
AFLOW prototype label	A2BC4_hR42_161_2b_b_4b-001
ICSD	30885
CCDC	1605091
Pearson symbol	hR42
Space group number	161
Space group symbol	<i>R</i> 3 <i>c</i>
AFLOW prototype command	<code>aflow --proto=A2BC4_hR42_161_2b_b_4b-001</code> <code>--params=a, c/a, x₁, y₁, z₁, x₂, y₂, z₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆, x₇, y₇, z₇</code>

- This is the low-temperature structure. Heating to temperatures between 100-400°C it transforms into β -BaB₂O₄. The principle difference between the two forms is the lack of inversion symmetry in the low-temperature structure.

Rhombohedral primitive vectors

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



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
$\mathbf{B}_4$	$=$	$(z_1 + \frac{1}{2}) \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 + (x_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_1 - z_1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_1 - 2y_1 + z_1) \hat{\mathbf{y}} + \frac{1}{6}c(2x_1 + 2y_1 + 2z_1 + 3) \hat{\mathbf{z}}$	(6b)	B I
$\mathbf{B}_5$	$=$	$(y_1 + \frac{1}{2}) \mathbf{a}_1 + (x_1 + \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_1 - z_1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_1 - y_1 - z_1) \hat{\mathbf{y}} + \frac{1}{6}c(2x_1 + 2y_1 + 2z_1 + 3) \hat{\mathbf{z}}$	(6b)	B I
$\mathbf{B}_6$	$=$	$(x_1 + \frac{1}{2}) \mathbf{a}_1 + (z_1 + \frac{1}{2}) \mathbf{a}_2 + (y_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_1 - y_1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_1 + y_1 - 2z_1) \hat{\mathbf{y}} + \frac{1}{6}c(2x_1 + 2y_1 + 2z_1 + 3) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{10}$	$=$	$(z_2 + \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_2 - z_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_2 - 2y_2 + z_2) \hat{\mathbf{y}} + \frac{1}{6}c(2x_2 + 2y_2 + 2z_2 + 3) \hat{\mathbf{z}}$	(6b)	B II
$\mathbf{B}_{11}$	$=$	$(y_2 + \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_2 - z_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_2 - y_2 - z_2) \hat{\mathbf{y}} + \frac{1}{6}c(2x_2 + 2y_2 + 2z_2 + 3) \hat{\mathbf{z}}$	(6b)	B II
$\mathbf{B}_{12}$	$=$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 + (z_2 + \frac{1}{2}) \mathbf{a}_2 + (y_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_2 + y_2 - 2z_2) \hat{\mathbf{y}} + \frac{1}{6}c(2x_2 + 2y_2 + 2z_2 + 3) \hat{\mathbf{z}}$	(6b)	B II
$\mathbf{B}_{13}$	$=$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6b)	Ba I
$\mathbf{B}_{14}$	$=$	$z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6b)	Ba I
$\mathbf{B}_{15}$	$=$	$y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6b)	Ba I
$\mathbf{B}_{16}$	$=$	$(z_3 + \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + (x_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} + \frac{1}{6}c(2x_3 + 2y_3 + 2z_3 + 3) \hat{\mathbf{z}}$	(6b)	Ba I
$\mathbf{B}_{17}$	$=$	$(y_3 + \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} + \frac{1}{6}c(2x_3 + 2y_3 + 2z_3 + 3) \hat{\mathbf{z}}$	(6b)	Ba I
$\mathbf{B}_{18}$	$=$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 + (z_3 + \frac{1}{2}) \mathbf{a}_2 + (y_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} + \frac{1}{6}c(2x_3 + 2y_3 + 2z_3 + 3) \hat{\mathbf{z}}$	(6b)	Ba I
$\mathbf{B}_{19}$	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 - 2y_4 + z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6b)	O I
$\mathbf{B}_{20}$	$=$	$z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_4 - y_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6b)	O I
$\mathbf{B}_{21}$	$=$	$y_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 + y_4 - 2z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6b)	O I
$\mathbf{B}_{22}$	$=$	$(z$				

$$\begin{aligned}
\mathbf{B}_{25} &= 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}} &(6b) & \text{O II} \\
\mathbf{B}_{26} &= 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}} &(6b) & \text{O II} \\
\mathbf{B}_{27} &= 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}} &(6b) & \text{O II} \\
\mathbf{B}_{28} &= (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}} &(6b) & \text{O II} \\
\mathbf{B}_{29} &= (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}} &(6b) & \text{O II} \\
\mathbf{B}_{30} &= (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}} &(6b) & \text{O II} \\
\mathbf{B}_{31} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= \frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 - 2y_6 + z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6b) & \text{O III} \\
\mathbf{B}_{32} &= z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + y_6 \mathbf{a}_3 &= -\frac{1}{2}a(y_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_6 - y_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6b) & \text{O III} \\
\mathbf{B}_{33} &= y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3 &= -\frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6b) & \text{O III} \\
\mathbf{B}_{34} &= (z_6 + \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + (x_6 + \frac{1}{2}) \mathbf{a}_3 &= -\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 - 2y_6 + z_6) \hat{\mathbf{y}} + \frac{1}{6}c(2x_6 + 2y_6 + 2z_6 + 3) \hat{\mathbf{z}} &(6b) & \text{O III} \\
\mathbf{B}_{35} &= (y_6 + \frac{1}{2}) \mathbf{a}_1 + (x_6 + \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 &= \frac{1}{2}a(y_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_6 - y_6 - z_6) \hat{\mathbf{y}} + \frac{1}{6}c(2x_6 + 2y_6 + 2z_6 + 3) \hat{\mathbf{z}} &(6b) & \text{O III} \\
\mathbf{B}_{36} &= (x_6 + \frac{1}{2}) \mathbf{a}_1 + (z_6 + \frac{1}{2}) \mathbf{a}_2 + (y_6 + \frac{1}{2}) \mathbf{a}_3 &= \frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} + \frac{1}{6}c(2x_6 + 2y_6 + 2z_6 + 3) \hat{\mathbf{z}} &(6b) & \text{O III} \\
\mathbf{B}_{37} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= \frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 - 2y_7 + z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}} &(6b) & \text{O IV} \\
\mathbf{B}_{38} &= z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + y_7 \mathbf{a}_3 &= -\frac{1}{2}a(y_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_7 - y_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}} &(6b) & \text{O IV} \\
\mathbf{B}_{39} &= y_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3 &= -\frac{1}{2}a(x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 + y_7 - 2z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}} &(6b) & \text{O IV} \\
\mathbf{B}_{40} &= (z_7 + \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 + (x_7 + \frac{1}{2}) \mathbf{a}_3 &= -\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 - 2y_7 + z_7) \hat{\mathbf{y}} + \frac{1}{6}c(2x_7 + 2y_7 + 2z_7 + 3) \hat{\mathbf{z}} &(6b) & \text{O IV} \\
\mathbf{B}_{41} &= (y_7 + \frac{1}{2}) \mathbf{a}_1 + (x_7 + \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3 &= \frac{1}{2}a(y_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_7 - y_7 - z_7) \hat{\mathbf{y}} + \frac{1}{6}c(2x_7 + 2y_7 + 2z_7 + 3) \hat{\mathbf{z}} &(6b) & \text{O IV} \\
\mathbf{B}_{42} &= (x_7 + \frac{1}{2}) \mathbf{a}_1 + (z_7 + \frac{1}{2}) \mathbf{a}_2 + (y_7 + \frac{1}{2}) \mathbf{a}_3 &= \frac{1}{2}a(x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 + y_7 - 2z_7) \hat{\mathbf{y}} + \frac{1}{6}c(2x_7 + 2y_7 + 2z_7 + 3) \hat{\mathbf{z}} &(6b) & \text{O IV}
\end{aligned}$$

References

- [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.

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