

BaAl₂O₄ (*H*2₈) Structure: A2BC6_hP18_182_f_b_gh-001

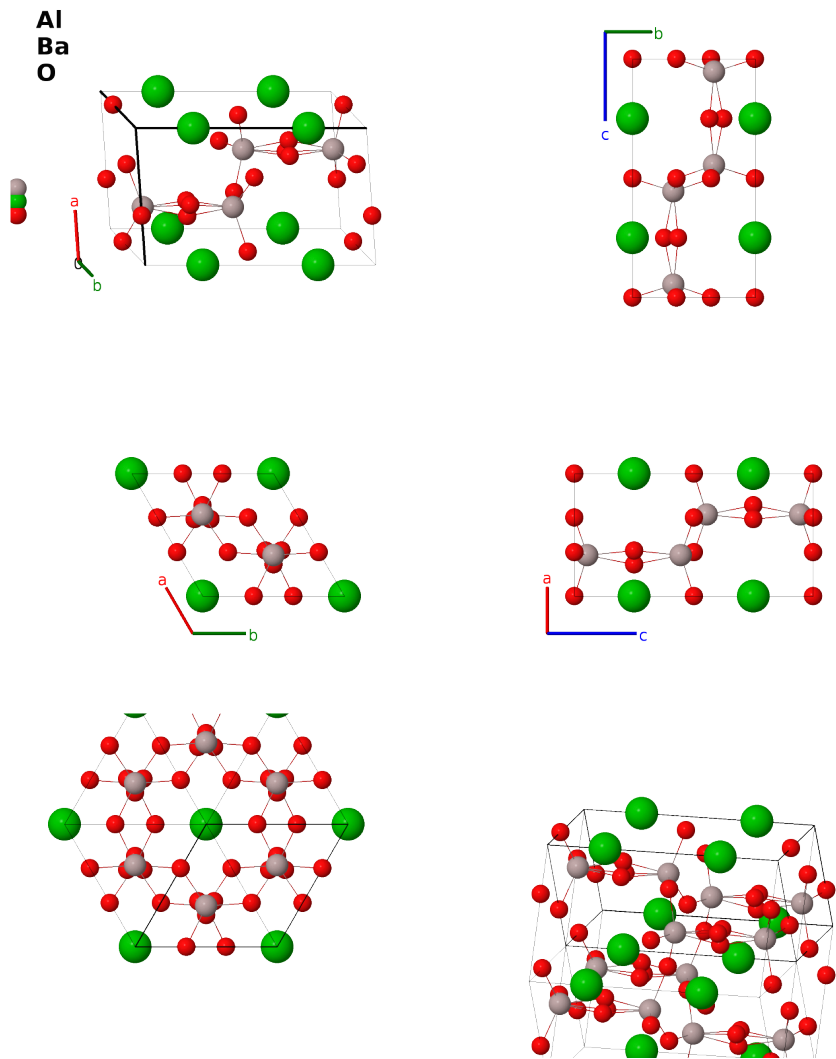
This structure previously used the label(s) **A2BC6_hP18_182_f_b_gh**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/6VW9>

https://aflow.org/prototype-encyclopedia/A2BC6_hP18_182_f_b_gh-001

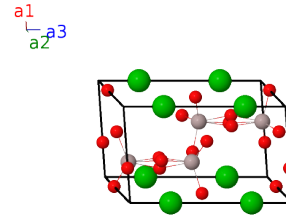


Prototype	Al ₂ BaO ₄
AFLOW prototype label	A2BC6_hP18_182_f_b_gh-001
Strukturbericht designation	<i>H</i> 2 ₈
ICSD	15728

CCDC	1596429
Pearson symbol	hP18
Space group number	182
Space group symbol	$P6_322$
AFLOW prototype command	<code>aflow --proto=A2BC6_hP18_182_f_b_gh-001</code> <code>--params=a, c/a, z₂, x₃, x₄</code>

- The structure of BaAl_2O_4 was originally determined by (Wallmark, 1937) and designated $H2_8$ by (Gottfried, 1940). This had two oxygen atoms at the (2c) Wyckoff position, $\pm(1/3, 2/3, z)$. (Perrotta, 1968) redetermined the structure and found that the best fit to external data required the (2c) oxygen atoms to be distributed among the (6h) sites. Thus each of the (6h) sites in this structure is 1/3 occupied.

Hexagonal primitive vectors

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


Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \hat{\mathbf{z}}$	(2b)	Ba I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \hat{\mathbf{z}}$	(2b)	Ba I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4f)	Al I
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Al I
$\mathbf{B}_5$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4f)	Al I
$\mathbf{B}_6$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Al I
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1$	$=$	$\frac{1}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}}$	(6g)	O I
$\mathbf{B}_8$	$= x_3 \mathbf{a}_2$	$=$	$\frac{1}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}}$	(6g)	O I
$\mathbf{B}_9$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}}$	(6g)	O I
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B}_{12}$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B}_{14}$	$= -2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B}_{15}$	$= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B}_{16}$	$= -x_4 \mathbf{a}_1 - 2x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B}_{17}$	$= 2x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	O II

$$\mathbf{B}_{18} = -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 = \sqrt{3}ax_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}} \quad (6h) \quad \text{O II}$$

References

- [1] A. J. Perrotta and J. V. Smith, *The Crystal Structure of BaAl₂O₄*, Bull. Soc. franç. de Minéral. Cristal. **91**, 85–87 (1968), doi:10.3406/bulmi.1968.6190.
- [2] S. Wallmark and A. Westgren, *X-Ray Analysis of Barium Aluminates*, Ark. Kem. Mineral. Geol. B **12** (1937).
- [3] C. Gottfried, ed., *Strukturbericht Band V 1937* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1940).

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