

κ alumina (Al_2O_3) Structure: A2B3_oP40_33_4a_6a-001

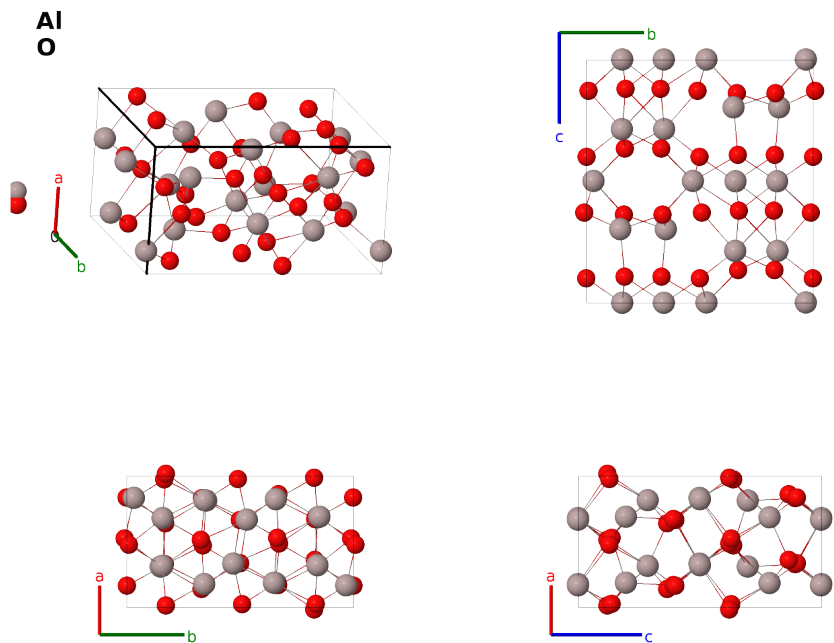
This structure previously used the label(s) **A2B3_oP40_33_4a_6a**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/SGA3>

https://aflow.org/prototype-encyclopedia/A2B3_oP40_33_4a_6a-001



Prototype	Al_2O_3
AFLOW prototype label	A2B3_oP40_33_4a_6a-001
Mineral name	κ alumina
ICSD	84375
CCDC	1644379
Pearson symbol	oP40
Space group number	33
Space group symbol	$Pna2_1$
AFLOW prototype command	<pre>aflow --proto=A2B3_oP40_33_4a_6a-001 --params=a,b/a,c/a,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,y5,z5,x6,y6,z6,x7, y7,z7,x8,y8,z8,x9,y9,z9,x10,y10,z10</pre>

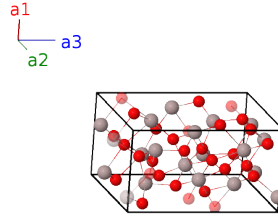
Other compounds with this structure

$(\text{Fe}_2\text{O}_3)_{1-x} \cdot (\text{Al}_2\text{O}_3)_x$, $(\text{Fe}_2\text{O}_3)_{1-x} \cdot (\text{Ga}_2\text{O}_3)_x$

- Alumina comes in a variety of forms. In the Encyclopedia we have:
 - Corundum, or α -alumina ($D5_1$) is the mineral usual found in nature.
 - β -alumina ($D5_6$)
 - We describe γ -alumina ($D5_7$) using Fe_2O_3 as the prototype.
 - δ -alumina is a tetragonal distortion of the spinel structure. It is found in nature as deltalumite.
 - κ - Al_2O_3 (this structure)
- (Hermann, 1937) assigned this the *Strukturbericht* designation $D5_6$, calling it β -corundum, and subtitles the section “with small Na_2O impurities.” (Yoshioka, 2007) use this is an approximation to the true crystal structure of ϵ - Ga_2O_3 .

Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates		Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4a)	Al I
$\mathbf{B}_2$	$=$	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Al I
$\mathbf{B}_3$	$=$	$(x_1 + \frac{1}{2}) \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4a)	Al I
$\mathbf{B}_4$	$=$	$-(x_1 - \frac{1}{2}) \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Al I
$\mathbf{B}_5$	$=$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4a)	Al II
$\mathbf{B}_6$	$=$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Al II
$\mathbf{B}_7$	$=$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4a)	Al II
$\mathbf{B}_8$	$=$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Al II
$\mathbf{B}_9$	$=$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4a)	Al III
$\mathbf{B}_{10}$	$=$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Al III
$\mathbf{B}_{11}$	$=$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4a)	Al III
$\mathbf{B}_{12}$	$=$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Al III
$\mathbf{B}_{13}$	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4a)	Al IV
$\mathbf{B}_{14}$	$=$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Al IV

$$\begin{aligned}
\mathbf{B}_{15} &= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3 = a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (4a) & \text{Al IV} \\
\mathbf{B}_{16} &= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3 = -a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{Al IV} \\
\mathbf{B}_{17} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (4a) & \text{O I} \\
\mathbf{B}_{18} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3 = -ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O I} \\
\mathbf{B}_{19} &= (x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3 = a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (4a) & \text{O I} \\
\mathbf{B}_{20} &= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3 = -a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O I} \\
\mathbf{B}_{21} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (4a) & \text{O II} \\
\mathbf{B}_{22} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 = -ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O II} \\
\mathbf{B}_{23} &= (x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3 = a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (4a) & \text{O II} \\
\mathbf{B}_{24} &= -(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 = -a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O II} \\
\mathbf{B}_{25} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (4a) & \text{O III} \\
\mathbf{B}_{26} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3 = -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O III} \\
\mathbf{B}_{27} &= (x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + z_7 \mathbf{a}_3 = a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (4a) & \text{O III} \\
\mathbf{B}_{28} &= -(x_7 - \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3 = -a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O III} \\
\mathbf{B}_{29} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 = ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (4a) & \text{O IV} \\
\mathbf{B}_{30} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 = -ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O IV} \\
\mathbf{B}_{31} &= (x_8 + \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + z_8 \mathbf{a}_3 = a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (4a) & \text{O IV} \\
\mathbf{B}_{32} &= -(x_8 - \frac{1}{2}) \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 = -a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O IV} \\
\mathbf{B}_{33} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (4a) & \text{O V} \\
\mathbf{B}_{34} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3 = -ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O V} \\
\mathbf{B}_{35} &= (x_9 + \frac{1}{2}) \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 + z_9 \mathbf{a}_3 = a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (4a) & \text{O V} \\
\mathbf{B}_{36} &= -(x_9 - \frac{1}{2}) \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3 = -a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O V} \\
\mathbf{B}_{37} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B}_{38} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3 = -ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B}_{39} &= (x_{10} + \frac{1}{2}) \mathbf{a}_1 - (y_{10} - \frac{1}{2}) \mathbf{a}_2 + z_{10} \mathbf{a}_3 = a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{10} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B}_{40} &= -(x_{10} - \frac{1}{2}) \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3 = -a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O VI}
\end{aligned}$$

References

- [1] B. Ollivier, R. Retoux, P. Lacorre, D. Massiot, and G. Férey, *Crystal structure of κ -alumina: an X-ray powder diffraction, TEM and NMR study*, J. Mater. Chem. **7**, 1049–1056 (1997), doi:10.1039/A700054E.

Found in

- [1] K. Matsuzaki, H. Yanagi, T. K. Hiramatsu, K. Nomura, and M. H. Hosono, *Field-induced current modulation in epitaxial film of deep-ultraviolet transparent oxide semiconductor Ga_2O_3* , Appl. Phys. Lett. **88**, 092106 (2006), doi:10.1063/1.2179373.
- [2] S. Yoshioka, H. Hayashi, A. Kuwabara, F. Oba, K. Matsunaga, and I. Tanaka, *Structures and energetics of Ga_2O_3 polymorphs*, J. Phys.: Condens. Matter **19**, 346211 (2007), doi:10.1088/0953-8984/19/34/346211.

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043