

β -Alumina ($D5_6$, Al_2O_3) Structure: A2B3_hP60_194_3fk_cdef2k-001

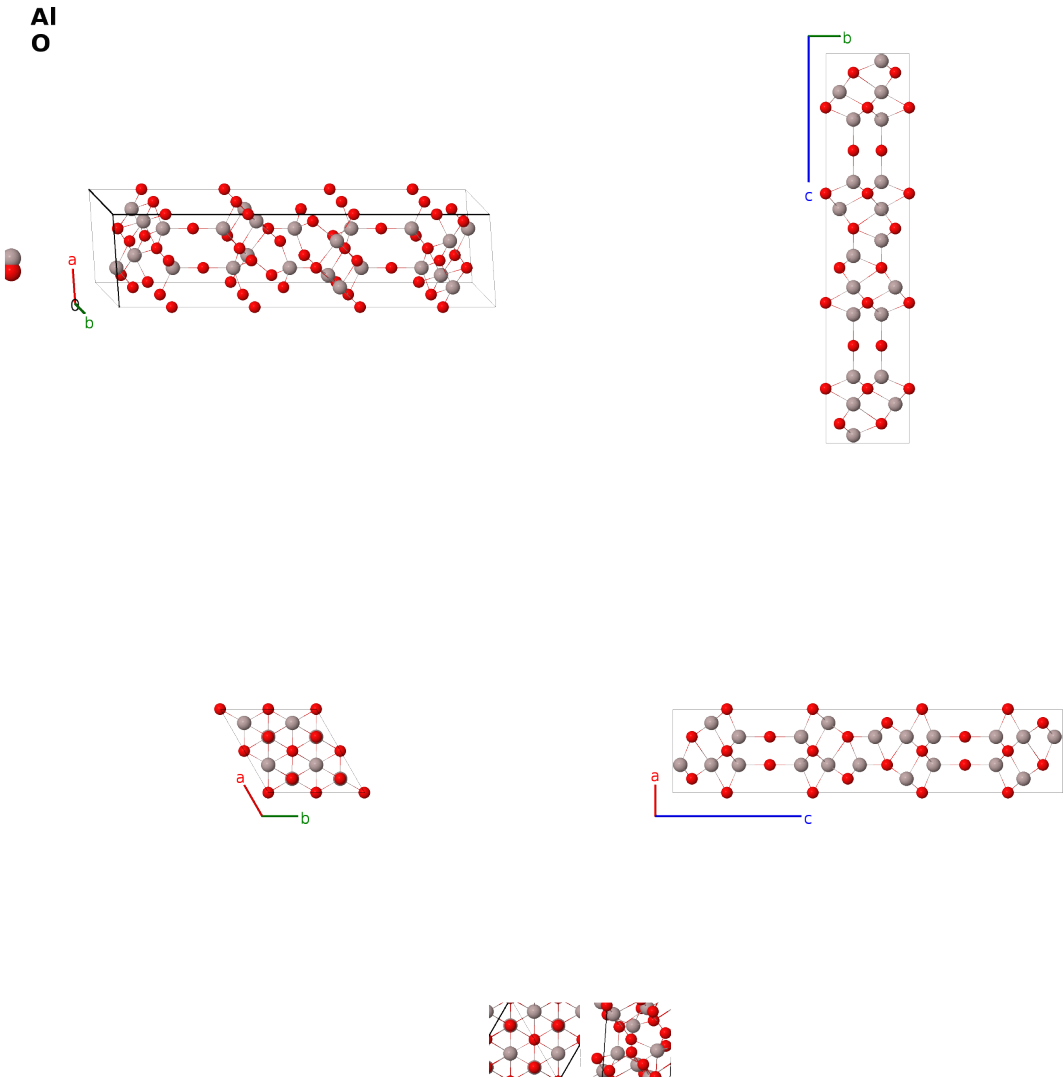
This structure previously used the label(s) **A2B3_hP60_194_3fk_cdef2k**. Calls to these addresses will be redirected here.

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/T15Z>

https://aflow.org/prototype-encyclopedia/A2B3_hP60_194_3fk_cdef2k-001



Prototype	Al_2O_3
AFLOW prototype label	A2B3_hP60_194_3fk_cdef2k-001
<i>Strukturbericht</i> designation	$D5_6$
Mineral name	β -alumina

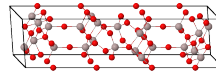
ICSD	24226
CCDC	1600272
Pearson symbol	hP60
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>aflow --proto=A2B3_hP60_194_3fk_cdef2k-001</code> <code>--params=a, c/a, z3, z4, z5, z6, z7, x8, z8, x9, z9, x10, z10</code>

- 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 ($D5_6$) (this structure)
 - 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 .
- (Hermann, 1937) assigned this the *Strukturbericht* designation $D5_6$, calling it β -corundum, and subtitles the section “with small Na_2O impurities.”
- As noted by (Gottfried, 1937) and (Le Cars, 1975), the Na impurities replace Al atoms on the (4f) Wyckoff positions, along with some unspecified O sites. More detail can be found in the ICSD CIF.
- Charge neutrality requires that some of the displaced atoms remain in the lattice, and they are moved to (2a) Wyckoff positions at (0 0 0) and (0 0 1/2), but are not shown here.
- Here we only list the “ideal” structure.

Hexagonal primitive vectors

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

$\mathbf{a}_1$
 $\mathbf{a}_2$
 $\mathbf{a}_3$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B}_2$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B}_3$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(2d)	O II
$\mathbf{B}_4$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(2d)	O II
$\mathbf{B}_5$	$= z_3\mathbf{a}_3$	$=$	$cz_3\hat{\mathbf{z}}$	(4e)	O III

$$\begin{aligned}
\mathbf{B}_{47} &= x_9 \mathbf{a}_1 + 2x_9 \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3 &= \frac{3}{2}ax_9 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9 \hat{\mathbf{y}} - c\left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) &\quad \text{O V} \\
\mathbf{B}_{48} &= x_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3 &= -\sqrt{3}ax_9 \hat{\mathbf{y}} - c\left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) &\quad \text{O V} \\
\mathbf{B}_{49} &= x_{10} \mathbf{a}_1 + 2x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= \frac{3}{2}ax_{10} \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} &(12k) &\quad \text{O VI} \\
\mathbf{B}_{50} &= -2x_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= -\frac{3}{2}ax_{10} \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} &(12k) &\quad \text{O VI} \\
\mathbf{B}_{51} &= x_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= -\sqrt{3}ax_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} &(12k) &\quad \text{O VI} \\
\mathbf{B}_{52} &= -x_{10} \mathbf{a}_1 - 2x_{10} \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 &= -\frac{3}{2}ax_{10} \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) &\quad \text{O VI} \\
\mathbf{B}_{53} &= 2x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 &= \frac{3}{2}ax_{10} \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) &\quad \text{O VI} \\
\mathbf{B}_{54} &= -x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 &= \sqrt{3}ax_{10} \hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) &\quad \text{O VI} \\
\mathbf{B}_{55} &= 2x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= \frac{3}{2}ax_{10} \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} &(12k) &\quad \text{O VI} \\
\mathbf{B}_{56} &= -x_{10} \mathbf{a}_1 - 2x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= -\frac{3}{2}ax_{10} \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} &(12k) &\quad \text{O VI} \\
\mathbf{B}_{57} &= -x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= \sqrt{3}ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} &(12k) &\quad \text{O VI} \\
\mathbf{B}_{58} &= -2x_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_3 &= -\frac{3}{2}ax_{10} \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} - c\left(z_{10} - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) &\quad \text{O VI} \\
\mathbf{B}_{59} &= x_{10} \mathbf{a}_1 + 2x_{10} \mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_3 &= \frac{3}{2}ax_{10} \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} - c\left(z_{10} - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) &\quad \text{O VI} \\
\mathbf{B}_{60} &= x_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_3 &= -\sqrt{3}ax_{10} \hat{\mathbf{y}} - c\left(z_{10} - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) &\quad \text{O VI}
\end{aligned}$$

References

- [1] W. L. Bragg, C. Gottfried, and J. West, *The Structure of β Alumina*, Z. Kristallogr. **77**, 255–274 (1931), doi:10.1524/zkri.1931.77.1.255.
- [2] Y. L. Cars, D. Gratias, R. Portier, and J. Th  ry, *Planar defects in β -alumina*, J. Solid State Chem. **15**, 218–222 (1975), doi:10.1016/0022-4596(75)90205-4.

Found in

- [1] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

First cited in

D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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.