

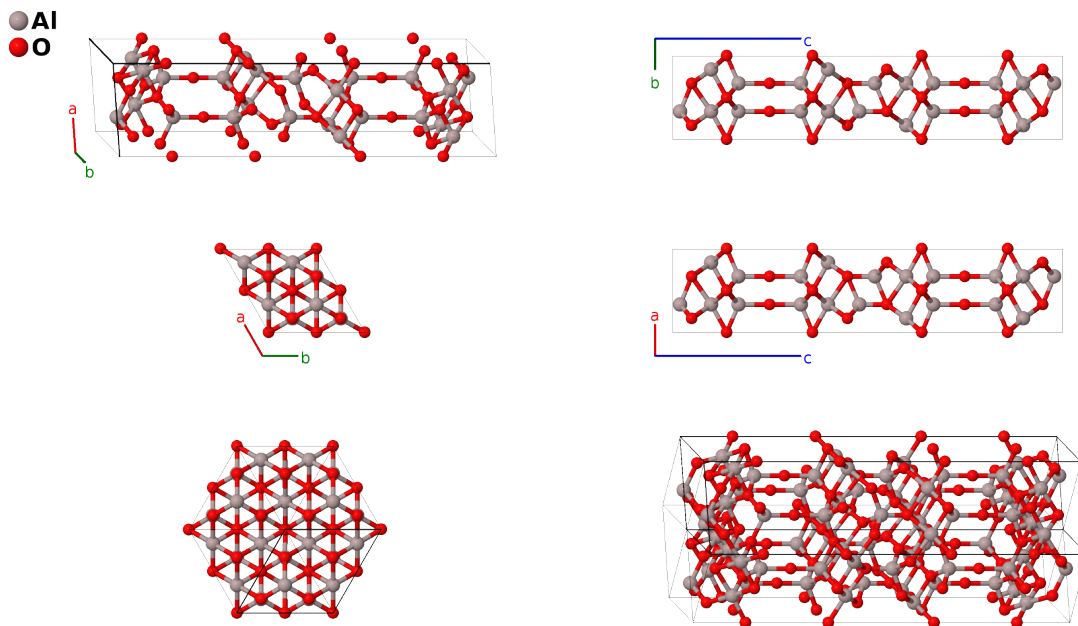
# $\beta$ -Alumina ( $D_{5_6}$ , $\text{Al}_2\text{O}_3$ ) Structure: A2B3\_hP60\_194\_3fk\_cdef2k-001

This structure originally had the label A2B3\_hP60\_194\_3fk\_cdef2k. Calls to that address will be redirected here.

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<https://aflow.org/p/T15Z>

[https://aflow.org/p/A2B3\\_hP60\\_194\\_3fk\\_cdef2k-001](https://aflow.org/p/A2B3_hP60_194_3fk_cdef2k-001)



Prototype	$\text{Al}_2\text{O}_3$
AFLOW prototype label	A2B3_hP60_194_3fk_cdef2k-001
<i>Strukturbericht</i> designation	$D_{5_6}$
Mineral name	$\beta$ -alumina
ICSD	24226
Pearson symbol	hP60
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<pre>aflow --proto=A2B3_hP60_194_3fk_cdef2k-001 --params=a, c/a, z3, z4, z5, z6, z7, x8, z8, x9, z9, x10, z10</pre>

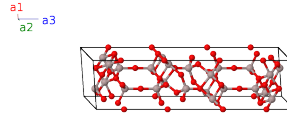
- Alumina comes in a variety of forms. In the Encyclopedia we have:
  - Corundum, or  $\alpha$ -alumina ( $D_{5_1}$ ) is the mineral usual found in nature.
  - $\beta$ -alumina ( $D_{5_6}$ ) (this structure)

- We describe  $\gamma$ -alumina ( $D5_7$ ) using  $\text{Fe}_2\text{O}_3$  as the prototype.
- $\delta$ -alumina is a tetragonal distortion of the spinel structure. It is found in nature as deltalumite.
- $\kappa$ - $\text{Al}_2\text{O}_3$ .
- (Hermann, 1937) assigned this the *Strukturbericht* designation  $D5_6$ , calling it  $\beta$ -corundum, and subtitles the section “with small  $\text{Na}_2\text{O}$  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).
- Here we only list the “ideal” structure.

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### Hexagonal primitive vectors

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




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### 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
$\mathbf{B}_6$	$= (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_7$	$= -z_3 \mathbf{a}_3$	$=$	$-cz_3 \hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_8$	$= -(z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_9$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4f)	Al I
$\mathbf{B}_{10}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Al I
$\mathbf{B}_{11}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4f)	Al I
$\mathbf{B}_{12}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Al I
$\mathbf{B}_{13}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4f)	Al II
$\mathbf{B}_{14}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Al II
$\mathbf{B}_{15}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4f)	Al II
$\mathbf{B}_{16}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Al II
$\mathbf{B}_{17}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4f)	Al III
$\mathbf{B}_{18}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Al III
$\mathbf{B}_{19}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4f)	Al III
$\mathbf{B}_{20}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Al III
$\mathbf{B}_{21}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4f)	O IV
$\mathbf{B}_{22}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	O IV



## References

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- [2] Y. L. Cars, D. Gratias, R. Portier, and J. Théry, *Planar defects in  $\beta$ -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).