Corundum (α-alumina, Al_2O_3, $D5_1$) Structure: A2B3_hR10_167_c_e-001

This structure originally had the label `A2B3_hR10_167_c_e`. Calls to that address will be redirected here.

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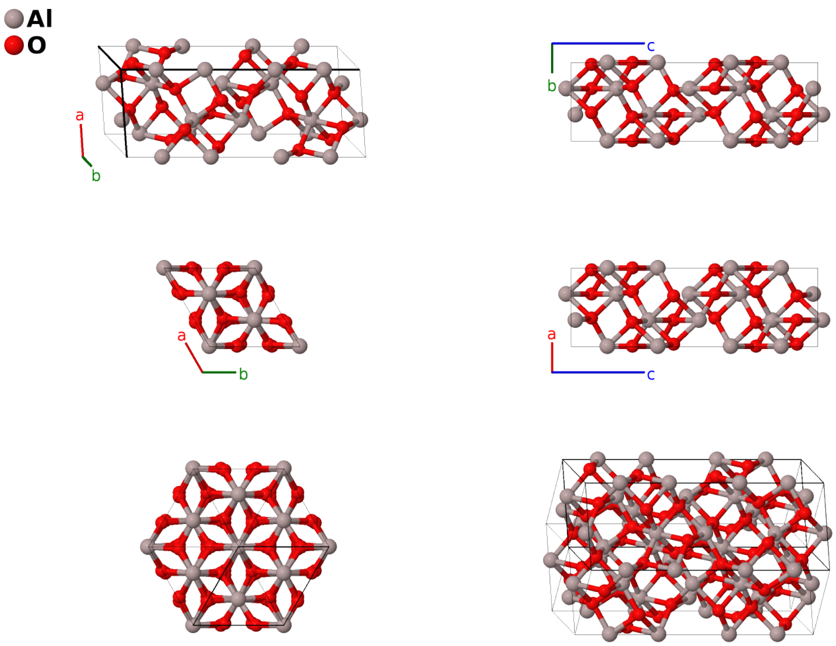
https://aflow.org/p/CBQY

https://aflow.org/p/A2B3_hR10_167_c_e-001



Prototype	Al_2O_3
AFLOW prototype label	A2B3_hR10_167_c_e-001
***Strukturbericht* designation**	$D5_1$
Mineral name	corundum
ICSD	9770
Pearson symbol	hR10
Space group number	167
Space group symbol	$R\bar{3}c$
AFLOW prototype command	`aflow --proto=A2B3_hR10_167_c_e-001 --params=`$a, c/a, x_1, x_2$

Other compounds with this structure
γ-Al_2S_3, Cr_2O_3 (Eskolaite), Fe_2O_3 (Hematite), α-Ga_2O_3, Lu_2S_3, Rh_2O_3, Ti_2O_3 (Tistarite), V_2O_3 (Karelianite), Yb_2S_3

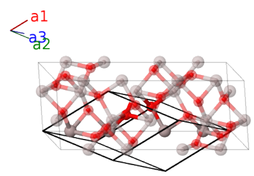
- Alumina comes in a variety of forms. In the Encyclopedia we have:

- Corundum, or α-alumina ($D5_1$) (this structure) 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.

- In corundum the aluminum atoms can be replaced by two different species of atoms stacked in alternating layers along the c-axis, forming the ilmenite structure.
- Alloying with Fe and Ti produces sapphire (a blue crystal), and alloying with Cr produces ruby (a red crystal).
- Hexagonal settings of rhombohedral structures can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-c\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-cx_1\,\hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,(4x_2 - 1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a\,(4x_2 - 1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_6}$	=	$\frac{1}{4}\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,(4x_2 - 1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{8}a\,(4x_2 - 1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_7}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_8}$	=	$-x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,(4x_2 + 3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{24}a\,(12x_2 + 1)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_9}$	=	$\frac{3}{4}\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,(4x_2 - 1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{24}a\,(12x_2 + 5)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_{10}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O I

References

[1] L. W. Finger and R. M. Hazen, *Crystal structure and compression of ruby to 46 kbar*, J. Appl. Phys. **49**, 5823–5826 (1978), doi:10.1063/1.324598.