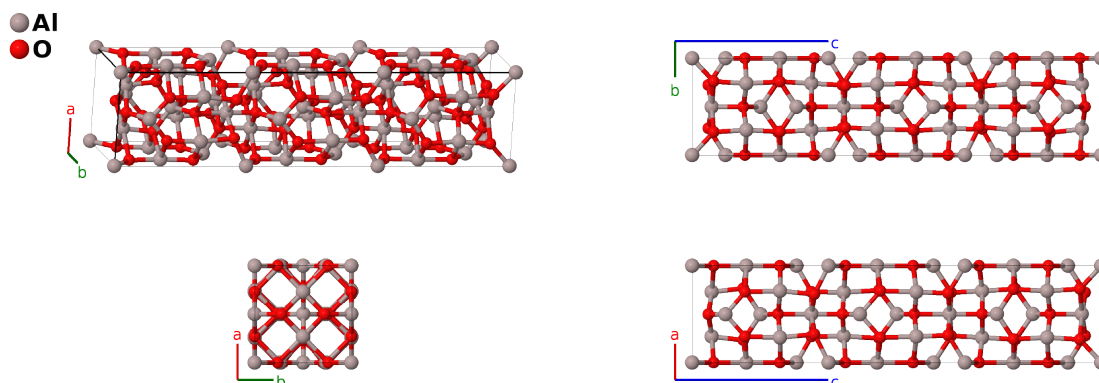


Deltalumite (δ -alumina, Al_2O_3) Structure: A3B4_tP84_115_acef3g3j3k_6j6k-001

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<https://afLOW.org/p/YL8L>

https://afLOW.org/p/A3B4_tP84_115_acef3g3j3k_6j6k-001

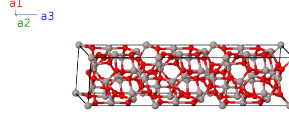


Prototype	Al_2O_3
AFLOW prototype label	A3B4_tP84_115_acef3g3j3k_6j6k-001
Mineral name	deltalumite
ICSD	40200
Pearson symbol	tP84
Space group number	115
Space group symbol	$P\bar{4}m2$
AFLOW prototype command	<pre>afLOW --proto=A3B4_tP84_115_acef3g3j3k_6j6k-001 --params=a, c/a, z3, z4, z5, z6, z7, x8, z8, x9, z9, x10, z10, x11, z11, x12, z12, x13, z13, x14, z14, x15, z15, x16, z16, x17, z17, x18, z18, x19, z19, x20, z20, x21, z21, x22, z22, x23, z23, x24, z24, x25, z25</pre>

- 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 (this structure) is a tetragonal distortion of the spinel structure. It is found in nature as deltalumite.
 - κ - Al_2O_3 .
- Only 5/6 of the aluminum (4j) and (4k) sites in deltalumite are occupied, giving the observed alumina stoichiometry, Al_2O_3 .

Simple Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	$=$	0	(1a)	Al I
\mathbf{B}_2	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(1c)	Al II
\mathbf{B}_3	$z_3 \mathbf{a}_3$	$=$	$cz_3 \hat{\mathbf{z}}$	(2e)	Al III
\mathbf{B}_4	$-z_3 \mathbf{a}_3$	$=$	$-cz_3 \hat{\mathbf{z}}$	(2e)	Al III
\mathbf{B}_5	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2f)	Al IV
\mathbf{B}_6	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(2f)	Al IV
\mathbf{B}_7	$\frac{1}{2} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(2g)	Al V
\mathbf{B}_8	$\frac{1}{2} \mathbf{a}_1 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - cz_5 \hat{\mathbf{z}}$	(2g)	Al V
\mathbf{B}_9	$\frac{1}{2} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(2g)	Al VI
\mathbf{B}_{10}	$\frac{1}{2} \mathbf{a}_1 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - cz_6 \hat{\mathbf{z}}$	(2g)	Al VI
\mathbf{B}_{11}	$\frac{1}{2} \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(2g)	Al VII
\mathbf{B}_{12}	$\frac{1}{2} \mathbf{a}_1 - z_7 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - cz_7 \hat{\mathbf{z}}$	(2g)	Al VII
\mathbf{B}_{13}	$x_8 \mathbf{a}_1 + z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + cz_8 \hat{\mathbf{z}}$	(4j)	Al VIII
\mathbf{B}_{14}	$-x_8 \mathbf{a}_1 + z_8 \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} + cz_8 \hat{\mathbf{z}}$	(4j)	Al VIII
\mathbf{B}_{15}	$-x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(4j)	Al VIII
\mathbf{B}_{16}	$x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(4j)	Al VIII
\mathbf{B}_{17}	$x_9 \mathbf{a}_1 + z_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + cz_9 \hat{\mathbf{z}}$	(4j)	Al IX
\mathbf{B}_{18}	$-x_9 \mathbf{a}_1 + z_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} + cz_9 \hat{\mathbf{z}}$	(4j)	Al IX
\mathbf{B}_{19}	$-x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(4j)	Al IX
\mathbf{B}_{20}	$x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(4j)	Al IX
\mathbf{B}_{21}	$x_{10} \mathbf{a}_1 + z_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} + cz_{10} \hat{\mathbf{z}}$	(4j)	Al X
\mathbf{B}_{22}	$-x_{10} \mathbf{a}_1 + z_{10} \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} + cz_{10} \hat{\mathbf{z}}$	(4j)	Al X
\mathbf{B}_{23}	$-x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(4j)	Al X
\mathbf{B}_{24}	$x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(4j)	Al X
\mathbf{B}_{25}	$x_{11} \mathbf{a}_1 + z_{11} \mathbf{a}_3$	$=$	$ax_{11} \hat{\mathbf{x}} + cz_{11} \hat{\mathbf{z}}$	(4j)	O I
\mathbf{B}_{26}	$-x_{11} \mathbf{a}_1 + z_{11} \mathbf{a}_3$	$=$	$-ax_{11} \hat{\mathbf{x}} + cz_{11} \hat{\mathbf{z}}$	(4j)	O I
\mathbf{B}_{27}	$-x_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-ax_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(4j)	O I
\mathbf{B}_{28}	$x_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$ax_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(4j)	O I
\mathbf{B}_{29}	$x_{12} \mathbf{a}_1 + z_{12} \mathbf{a}_3$	$=$	$ax_{12} \hat{\mathbf{x}} + cz_{12} \hat{\mathbf{z}}$	(4j)	O II
\mathbf{B}_{30}	$-x_{12} \mathbf{a}_1 + z_{12} \mathbf{a}_3$	$=$	$-ax_{12} \hat{\mathbf{x}} + cz_{12} \hat{\mathbf{z}}$	(4j)	O II
\mathbf{B}_{31}	$-x_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-ax_{12} \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}}$	(4j)	O II
\mathbf{B}_{32}	$x_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$ax_{12} \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}}$	(4j)	O II

$$\begin{aligned}
\mathbf{B}_{74} &= -x_{23} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_{23} \mathbf{a}_3 &= & -ax_{23} \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + cz_{23} \hat{\mathbf{z}} & (4k) & \text{O X} \\
\mathbf{B}_{75} &= \frac{1}{2} \mathbf{a}_1 - x_{23} \mathbf{a}_2 - z_{23} \mathbf{a}_3 &= & \frac{1}{2}a \hat{\mathbf{x}} - ax_{23} \hat{\mathbf{y}} - cz_{23} \hat{\mathbf{z}} & (4k) & \text{O X} \\
\mathbf{B}_{76} &= \frac{1}{2} \mathbf{a}_1 + x_{23} \mathbf{a}_2 - z_{23} \mathbf{a}_3 &= & \frac{1}{2}a \hat{\mathbf{x}} + ax_{23} \hat{\mathbf{y}} - cz_{23} \hat{\mathbf{z}} & (4k) & \text{O X} \\
\mathbf{B}_{77} &= x_{24} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_{24} \mathbf{a}_3 &= & ax_{24} \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + cz_{24} \hat{\mathbf{z}} & (4k) & \text{O XI} \\
\mathbf{B}_{78} &= -x_{24} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_{24} \mathbf{a}_3 &= & -ax_{24} \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + cz_{24} \hat{\mathbf{z}} & (4k) & \text{O XI} \\
\mathbf{B}_{79} &= \frac{1}{2} \mathbf{a}_1 - x_{24} \mathbf{a}_2 - z_{24} \mathbf{a}_3 &= & \frac{1}{2}a \hat{\mathbf{x}} - ax_{24} \hat{\mathbf{y}} - cz_{24} \hat{\mathbf{z}} & (4k) & \text{O XI} \\
\mathbf{B}_{80} &= \frac{1}{2} \mathbf{a}_1 + x_{24} \mathbf{a}_2 - z_{24} \mathbf{a}_3 &= & \frac{1}{2}a \hat{\mathbf{x}} + ax_{24} \hat{\mathbf{y}} - cz_{24} \hat{\mathbf{z}} & (4k) & \text{O XI} \\
\mathbf{B}_{81} &= x_{25} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_{25} \mathbf{a}_3 &= & ax_{25} \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + cz_{25} \hat{\mathbf{z}} & (4k) & \text{O XII} \\
\mathbf{B}_{82} &= -x_{25} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_{25} \mathbf{a}_3 &= & -ax_{25} \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + cz_{25} \hat{\mathbf{z}} & (4k) & \text{O XII} \\
\mathbf{B}_{83} &= \frac{1}{2} \mathbf{a}_1 - x_{25} \mathbf{a}_2 - z_{25} \mathbf{a}_3 &= & \frac{1}{2}a \hat{\mathbf{x}} - ax_{25} \hat{\mathbf{y}} - cz_{25} \hat{\mathbf{z}} & (4k) & \text{O XII} \\
\mathbf{B}_{84} &= \frac{1}{2} \mathbf{a}_1 + x_{25} \mathbf{a}_2 - z_{25} \mathbf{a}_3 &= & \frac{1}{2}a \hat{\mathbf{x}} + ax_{25} \hat{\mathbf{y}} - cz_{25} \hat{\mathbf{z}} & (4k) & \text{O XII}
\end{aligned}$$

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