

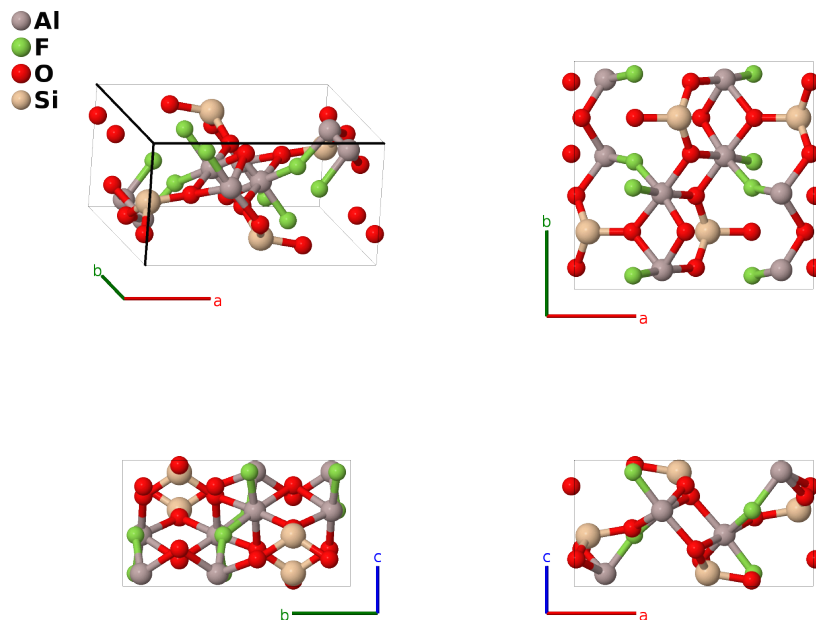
Topaz ($\text{Al}_2\text{SiO}_4\text{F}_2$, $S0_5$) Structure: A2B2C4D_oP36_62_d_d_2cd_c-001

This structure originally had the label A2B2C4D_oP36_62_d_d_2cd_c. Calls to that address will be redirected here.

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<https://aflow.org/p/7RBD>

https://aflow.org/p/A2B2C4D_oP36_62_d_d_2cd_c-001



Prototype	$\text{Al}_2\text{F}_2\text{O}_4\text{Si}$
AFLOW prototype label	A2B2C4D_oP36_62_d_d_2cd_c-001
Strukturbericht designation	$S0_5$
Mineral name	topaz
ICSD	55860
Pearson symbol	oP36
Space group number	62
Space group symbol	$Pnma$
AFLOW prototype command	<pre>aflow --proto=A2B2C4D_oP36_62_d_d_2cd_c-001 --params=a, b/a, c/a, x1, z1, x2, z2, x3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6</pre>

Other compounds with this structure

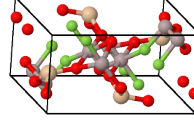
$\text{Al}_2\text{SiO}_4(\text{F}, \text{OH})_2$

- The fluorine (8d) site in topaz can have a composition $F_{1-x}(\text{OH})_x$, where $x < 0.3$.
- We use the data at $T = 298\text{K}$ from the ‘‘Pax08’’ sample in (Komatsu, 2003) with $x = 0.215$.
- The data was presented in the $Pbnm$ setting of space group #62. We used FINDSYM to transform this into the standard $Pnma$ setting.
- (Herman, 1937) gave this the $S0_5$ designation, but co-listed it as $H5_5$ in the index.

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	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_2	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_3	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_4	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_6	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_7	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_8	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	Si I
\mathbf{B}_{10}	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Si I
\mathbf{B}_{11}	$= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4c)	Si I
\mathbf{B}_{12}	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Si I
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8d)	Al I
\mathbf{B}_{14}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Al I
\mathbf{B}_{15}	$= -x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8d)	Al I
\mathbf{B}_{16}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Al I
\mathbf{B}_{17}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8d)	Al I
\mathbf{B}_{18}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Al I
\mathbf{B}_{19}	$= x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8d)	Al I

$$\begin{aligned}
\mathbf{B}_{20} &= -\begin{pmatrix} x_4 - \frac{1}{2} \\ z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_4 + \frac{1}{2} \\ z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 &= -a \begin{pmatrix} x_4 - \frac{1}{2} \\ z_4 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + b \begin{pmatrix} y_4 + \frac{1}{2} \\ z_4 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + c \begin{pmatrix} z_4 + \frac{1}{2} \\ z_4 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (8d) & \text{Al I} \\
\mathbf{B}_{21} &= 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}} & (8d) & \text{F I} \\
\mathbf{B}_{22} &= -\begin{pmatrix} x_5 - \frac{1}{2} \\ z_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - y_5 \mathbf{a}_2 + \mathbf{a}_3 &= -a \begin{pmatrix} x_5 - \frac{1}{2} \\ z_5 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c \begin{pmatrix} z_5 + \frac{1}{2} \\ z_5 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (8d) & \text{F I} \\
\mathbf{B}_{23} &= -x_5 \mathbf{a}_1 + \begin{pmatrix} y_5 + \frac{1}{2} \\ z_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - z_5 \mathbf{a}_3 &= -ax_5 \hat{\mathbf{x}} + b \begin{pmatrix} y_5 + \frac{1}{2} \\ z_5 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} & (8d) & \text{F I} \\
\mathbf{B}_{24} &= \begin{pmatrix} x_5 + \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_5 - \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \mathbf{a}_3 &= a \begin{pmatrix} x_5 + \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - b \begin{pmatrix} y_5 - \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - c \begin{pmatrix} z_5 - \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (8d) & \text{F I} \\
\mathbf{B}_{25} &= -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}} & (8d) & \text{F I} \\
\mathbf{B}_{26} &= \begin{pmatrix} x_5 + \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + y_5 \mathbf{a}_2 - \begin{pmatrix} y_5 - \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \begin{pmatrix} x_5 + \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c \begin{pmatrix} y_5 - \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (8d) & \text{F I} \\
\mathbf{B}_{27} &= x_5 \mathbf{a}_1 - \begin{pmatrix} y_5 - \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + z_5 \mathbf{a}_3 &= ax_5 \hat{\mathbf{x}} - b \begin{pmatrix} y_5 - \frac{1}{2} \\ z_5 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (8d) & \text{F I} \\
\mathbf{B}_{28} &= -\begin{pmatrix} x_5 - \frac{1}{2} \\ z_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_5 + \frac{1}{2} \\ z_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 &= -a \begin{pmatrix} x_5 - \frac{1}{2} \\ z_5 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + b \begin{pmatrix} y_5 + \frac{1}{2} \\ z_5 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + c \begin{pmatrix} z_5 + \frac{1}{2} \\ z_5 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (8d) & \text{F I} \\
\mathbf{B}_{29} &= 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}} & (8d) & \text{O III} \\
\mathbf{B}_{30} &= -\begin{pmatrix} x_6 - \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - y_6 \mathbf{a}_2 + \mathbf{a}_3 &= -a \begin{pmatrix} x_6 - \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c \begin{pmatrix} z_6 + \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (8d) & \text{O III} \\
\mathbf{B}_{31} &= -x_6 \mathbf{a}_1 + \begin{pmatrix} y_6 + \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -ax_6 \hat{\mathbf{x}} + b \begin{pmatrix} y_6 + \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (8d) & \text{O III} \\
\mathbf{B}_{32} &= \begin{pmatrix} x_6 + \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_6 - \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \mathbf{a}_3 &= a \begin{pmatrix} x_6 + \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - b \begin{pmatrix} y_6 - \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - c \begin{pmatrix} z_6 - \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (8d) & \text{O III} \\
\mathbf{B}_{33} &= -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}} & (8d) & \text{O III} \\
\mathbf{B}_{34} &= \begin{pmatrix} x_6 + \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + y_6 \mathbf{a}_2 - \begin{pmatrix} y_6 - \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \begin{pmatrix} x_6 + \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c \begin{pmatrix} y_6 - \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (8d) & \text{O III} \\
\mathbf{B}_{35} &= x_6 \mathbf{a}_1 - \begin{pmatrix} y_6 - \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + z_6 \mathbf{a}_3 &= ax_6 \hat{\mathbf{x}} - b \begin{pmatrix} y_6 - \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (8d) & \text{O III} \\
\mathbf{B}_{36} &= -\begin{pmatrix} x_6 - \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_6 + \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 &= -a \begin{pmatrix} x_6 - \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + b \begin{pmatrix} y_6 + \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + c \begin{pmatrix} z_6 + \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (8d) & \text{O III}
\end{aligned}$$

References

- [1] K. Komatsu, T. Kuribayashi, and Y. Kudoh, *Effect of temperature and pressure on the crystal structure of topaz, $Al_2SiO_4(OH, F)_2$* , J. of Mineral. Petro. Sci. **98**, 167–180 (2003), doi:10.2465/jmps.98.167.
- [2] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).