Topaz ($Al_2SiO_4F_2$, $S0_5$) Structure: A2B2C4D_oP36_62_d_d_2cd_c-001

This structure previously used the label(s) `A2B2C4D_oP36_62_d_d_2cd_c`. Calls to these addresses will be redirected here.

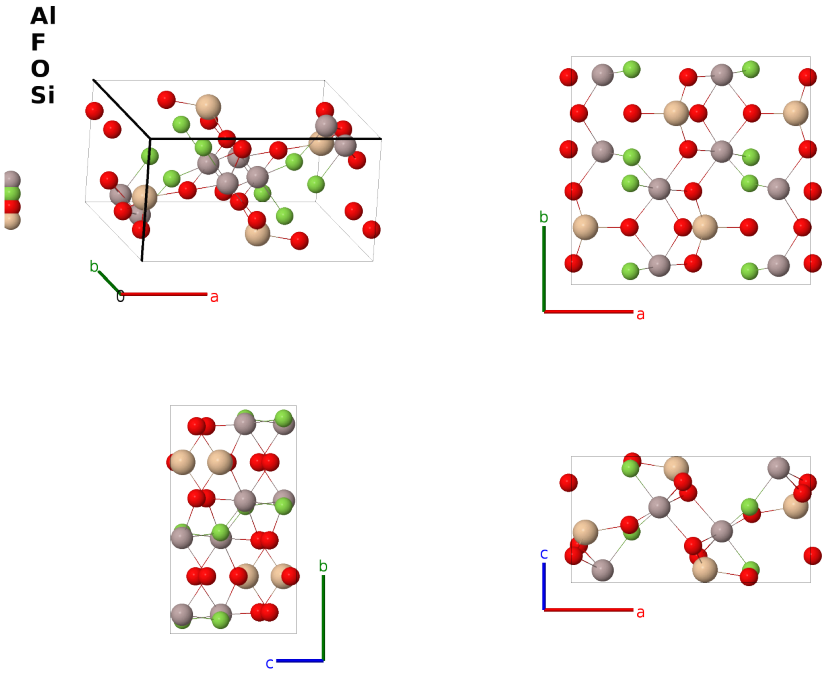
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, 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/7RBD

https://aflow.org/prototype-encyclopedia/A2B2C4D_oP36_62_d_d_2cd_c-001



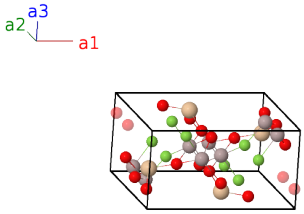
Prototype	$Al_2F_2O_4Si$
AFLOW prototype label	A2B2C4D_oP36_62_d_d_2cd_c-001
***Strukturbericht* designation**	$S0_5$
Mineral name	topaz
ICSD	55860
CCDC	1620155
Pearson symbol	oP36
Space group number	62
Space group symbol	*Pnma*
AFLOW prototype command	`aflow --proto=A2B2C4D_oP36_62_d_d_2cd_c-001 --params=`$a, b/a, c/a, x_1, z_1, x_2, z_2, x_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

Other compounds with this structure
$Al_2SiO_4(F, OH)_2$

- The fluorine (8d) site in topaz can have a composition $F_{1-x}(OH)_x$, where $x < 0.3$.
- We use the data at $T = 298$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

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{10}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{14}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Al I
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8d)	Al I
$\mathbf{B_{16}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Al I

$$\mathbf{B_{17}} = -x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3 = -ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{Al I}$$

$$\mathbf{B_{18}} = \left(x_4 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = a\left(x_4 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{Al I}$$

$$\mathbf{B_{19}} = x_4\,\mathbf{a}_1 - \left(y_4 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3 = ax_4\,\hat{\mathbf{x}} - b\left(y_4 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{Al I}$$

$$\mathbf{B_{20}} = -\left(x_4 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(x_4 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_4 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{Al I}$$

$$\mathbf{B_{21}} = x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{F I}$$

$$\mathbf{B_{22}} = -\left(x_5 - \tfrac{1}{2}\right)\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(x_5 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{F I}$$

$$\mathbf{B_{23}} = -x_5\,\mathbf{a}_1 + \left(y_5 + \tfrac{1}{2}\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}} + b\left(y_5 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{F I}$$

$$\mathbf{B_{24}} = \left(x_5 + \tfrac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5 - \tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_5 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = a\left(x_5 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_5 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_5 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{F I}$$

$$\mathbf{B_{25}} = -x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{F I}$$

$$\mathbf{B_{26}} = \left(x_5 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - \left(z_5 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = a\left(x_5 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{F I}$$

$$\mathbf{B_{27}} = x_5\,\mathbf{a}_1 - \left(y_5 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}} - b\left(y_5 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{F I}$$

$$\mathbf{B_{28}} = -\left(x_5 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_5 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(x_5 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_5 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{F I}$$

$$\mathbf{B_{29}} = x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{O III}$$

$$\mathbf{B_{30}} = -\left(x_6 - \tfrac{1}{2}\right)\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(x_6 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{O III}$$

$$\mathbf{B_{31}} = -x_6\,\mathbf{a}_1 + \left(y_6 + \tfrac{1}{2}\right)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}} + b\left(y_6 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{O III}$$

$$\mathbf{B_{32}} = \left(x_6 + \tfrac{1}{2}\right)\,\mathbf{a}_1 - \left(y_6 - \tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_6 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = a\left(x_6 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_6 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{O III}$$

$$\mathbf{B_{33}} = -x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{O III}$$

$$\mathbf{B_{34}} = \left(x_6 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - \left(z_6 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = a\left(x_6 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{O III}$$

$$\mathbf{B_{35}} = x_6\,\mathbf{a}_1 - \left(y_6 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}} - b\left(y_6 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{O III}$$

$$\mathbf{B_{36}} = -\left(x_6 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_6 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(x_6 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_6 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{O III}$$

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).

First cited in

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.