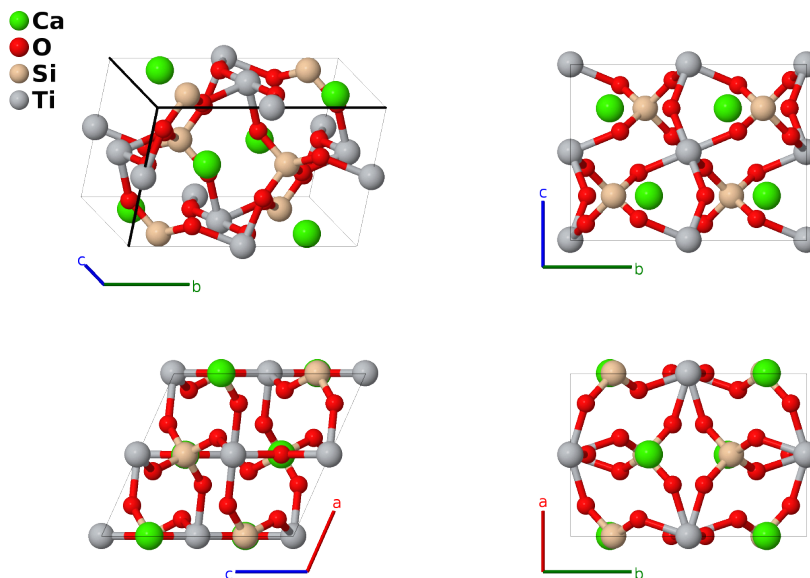# Titanite (CaTiSiO$_5$, $S0_6$) Structure: AB5CD_mC32_15_e_e2f_e_a-001

This structure originally had the label `AB5CD_mC32_15_e_e2f_e_b`. Calls to that address will be redirected here.

https://aflow.org/p/EDTK

https://aflow.org/p/AB5CD_mC32_15_e_e2f_e_a-001

Prototype	CaO$_5$SiTi
AFLOW prototype label	AB5CD_mC32_15_e_e2f_e_a-001
***Strukturbericht* designation**	$S0_6$
Mineral name	titanite
ICSD	159337
Pearson symbol	mC32
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	aflow --proto=AB5CD_mC32_15_e_e2f_e_a-001 --params=$a, b/a, c/a, \beta, y_2, y_3, y_4, x_5, y_5, z_5, x_6, y_6, z_6$

- We use the data from sample M28658 to construct our titanite cell.

- (Hermann, 1937) places the titanium atoms at the (4c) Wyckoff position rather than the (4b) position favored by (Hawthorne, 1991). The biggest difference between the two structures is the distance between the silicon and titantium atoms, which is 3.81Å in Hawthorne and a rather short 2Å in Hermann. We therefore favor the Hawthorne structure, and, since it does not otherwise substantially change the results, we continue to use $S0_6$ to describe it.

- (Hermann, 1937) also listed this as the $H5_6$ structure in the index.

Base-centered Monoclinic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$
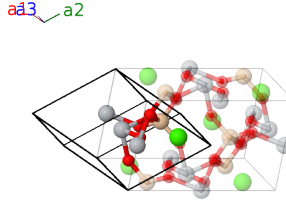
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	0	$=$	0	(4a)	Ti I
$\mathbf{B_2}$	$=$	$\tfrac{1}{2}\mathbf{a_3}$	$=$	$\tfrac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \tfrac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(4a)	Ti I
$\mathbf{B_3}$	$=$	$-y_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \tfrac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Ca I
$\mathbf{B_4}$	$=$	$y_2\,\mathbf{a_1} - y_2\,\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + \tfrac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Ca I
$\mathbf{B_5}$	$=$	$-y_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \tfrac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_6}$	$=$	$y_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \tfrac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_7}$	$=$	$-y_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \tfrac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_8}$	$=$	$y_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \tfrac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_9}$	$=$	$(x_5 - y_5)\,\mathbf{a_1} + (x_5 + y_5)\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	$=$	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{10}}$	$=$	$-(x_5 + y_5)\,\mathbf{a_1} - (x_5 - y_5)\,\mathbf{a_2} - \left(z_5 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_5 + c\left(z_5 - \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{11}}$	$=$	$-(x_5 - y_5)\,\mathbf{a_1} - (x_5 + y_5)\,\mathbf{a_2} - z_5\,\mathbf{a_3}$	$=$	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{12}}$	$=$	$(x_5 + y_5)\,\mathbf{a_1} + (x_5 - y_5)\,\mathbf{a_2} + \left(z_5 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_5 + c\left(z_5 + \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{13}}$	$=$	$(x_6 - y_6)\,\mathbf{a_1} + (x_6 + y_6)\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	$=$	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{14}}$	$=$	$-(x_6 + y_6)\,\mathbf{a_1} - (x_6 - y_6)\,\mathbf{a_2} - \left(z_6 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_6 + c\left(z_6 - \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{15}}$	$=$	$-(x_6 - y_6)\,\mathbf{a_1} - (x_6 + y_6)\,\mathbf{a_2} - z_6\,\mathbf{a_3}$	$=$	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{16}}$	$=$	$(x_6 + y_6)\,\mathbf{a_1} + (x_6 - y_6)\,\mathbf{a_2} + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_6 + c\left(z_6 + \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III

References

[1] F. C. Hawthorne, L. A. Groat, M. Raudsepp, N. A. Ball, M. Kimata, F. D. Spike, R. Gaba, N. M. Halden, G. R. Lumpkin, R. C. Ewing, R. B. Greegor, F. Lytle, T. S. Ercit, G. R. Rossman, F. J. Wicks, R. A. Ramik, B. L. Sherriff, M. E. Fleet, and C. McCammon, *Alpha-decay damage in titanite*, Am. Mineral. **76**, 370–396 (1991).

[2] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).