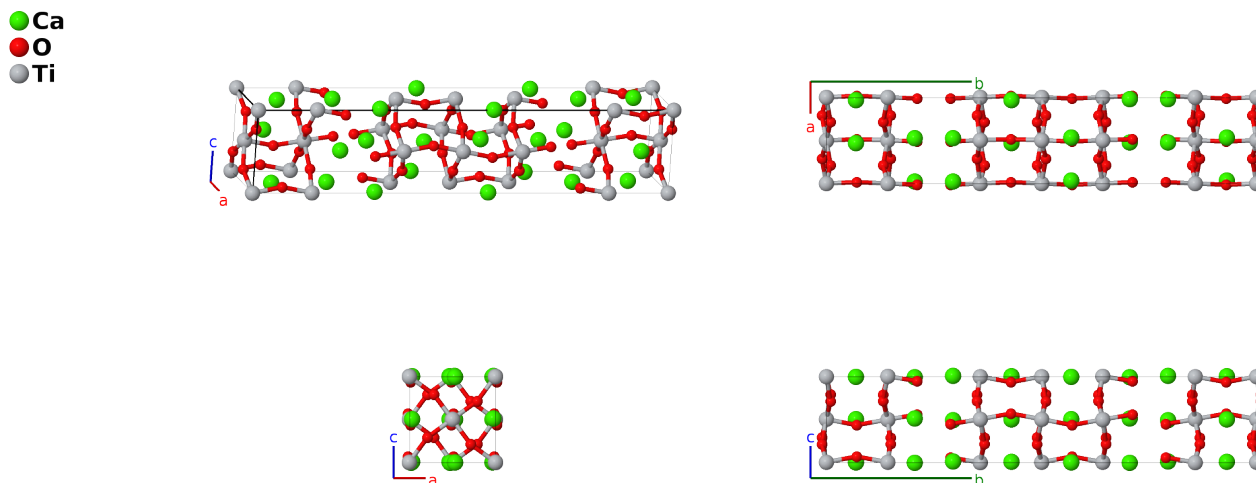


Ca₄Ti₃O₁₀ Structure: A4B10C3_oP68_61_2c_5c_ac-001

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<https://aflow.org/p/R6BH>

https://aflow.org/p/A4B10C3_oP68_61_2c_5c_ac-001



Prototype	Ca ₄ O ₁₀ Ti ₃
AFLOW prototype label	A4B10C3_oP68_61_2c_5c_ac-001
ICSD	86242
Pearson symbol	oP68
Space group number	61
Space group symbol	<i>Pbca</i>
AFLOW prototype command	<pre>aflow --proto=A4B10C3_oP68_61_2c_5c_ac-001 --params=a, b/a, c/a, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9</pre>

Other compounds with this structure

(Ca_{3.6}Sr_{0.4})Ti₃O₁₀

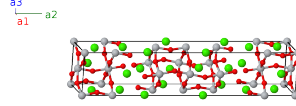
- (Hawkins, 1991) give the structure the *Pcab* setting of space group #61. We use FINDSYM to place it in the standard *Pbca* setting. This requires a 90° rotation about the *y*-axis. In addition, the origin was shifted to place a titanium atom at the origin.
- Pararammelsbergite (NiAs₂), β-TeO₂ and brookite (*C*21, TiO₂ have the same AFLOW prototype label, A2B_oP24_61_2c.c. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

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	$=$	0	$=$	0	(4a) Ti I
\mathbf{B}_2	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4a) Ti I
\mathbf{B}_3	$=$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4a) Ti I
\mathbf{B}_4	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}}$	(4a) Ti I
\mathbf{B}_5	$=$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8c) Ca I
\mathbf{B}_6	$=$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c) Ca I
\mathbf{B}_7	$=$	$-x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c) Ca I
\mathbf{B}_8	$=$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8c) Ca I
\mathbf{B}_9	$=$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8c) Ca I
\mathbf{B}_{10}	$=$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 + y_2 \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c) Ca I
\mathbf{B}_{11}	$=$	$x_2 \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c) Ca I
\mathbf{B}_{12}	$=$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8c) Ca I
\mathbf{B}_{13}	$=$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8c) Ca II
\mathbf{B}_{14}	$=$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c) Ca II
\mathbf{B}_{15}	$=$	$-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c) Ca II
\mathbf{B}_{16}	$=$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8c) Ca II
\mathbf{B}_{17}	$=$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8c) Ca II
\mathbf{B}_{18}	$=$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c) Ca II
\mathbf{B}_{19}	$=$	$x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c) Ca II
\mathbf{B}_{20}	$=$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8c) Ca II
\mathbf{B}_{21}	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8c) O I
\mathbf{B}_{22}	$=$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c) O I
\mathbf{B}_{23}	$=$	$-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c) O I
\mathbf{B}_{24}	$=$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8c) O I
\mathbf{B}_{25}	$=$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8c) O I
\mathbf{B}_{26}	$=$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c) O I
\mathbf{B}_{27}	$=$	$x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c) O I

$$\begin{aligned}
\mathbf{B}_{60} &= -\left(x_8 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 + z_8 \mathbf{a}_3 &= & -a \left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_8 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8c) & \text{O V} \\
\mathbf{B}_{61} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 &= & ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (8c) & \text{Ti II} \\
\mathbf{B}_{62} &= -\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 - y_9 \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 &= & -a \left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c \left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{Ti II} \\
\mathbf{B}_{63} &= -x_9 \mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3 &= & -ax_9 \hat{\mathbf{x}} + b \left(y_9 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{Ti II} \\
\mathbf{B}_{64} &= \left(x_9 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 - z_9 \mathbf{a}_3 &= & a \left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_9 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (8c) & \text{Ti II} \\
\mathbf{B}_{65} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 &= & -ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (8c) & \text{Ti II} \\
\mathbf{B}_{66} &= \left(x_9 + \frac{1}{2}\right) \mathbf{a}_1 + y_9 \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3 &= & a \left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - c \left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{Ti II} \\
\mathbf{B}_{67} &= x_9 \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 &= & ax_9 \hat{\mathbf{x}} - b \left(y_9 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{Ti II} \\
\mathbf{B}_{68} &= -\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_2 + z_9 \mathbf{a}_3 &= & -a \left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_9 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (8c) & \text{Ti II}
\end{aligned}$$

References

- [1] K. Hawkins and T. J. White, *Defect structure and chemistry of $(Ca_xSr_{1-x})_{n+1}Ti_nO_{3n+1}$ layer perovskites*, Philos. Trans. Royal Soc. A **336**, 541–569 (1991), doi:10.1098/rsta.1991.0099.