

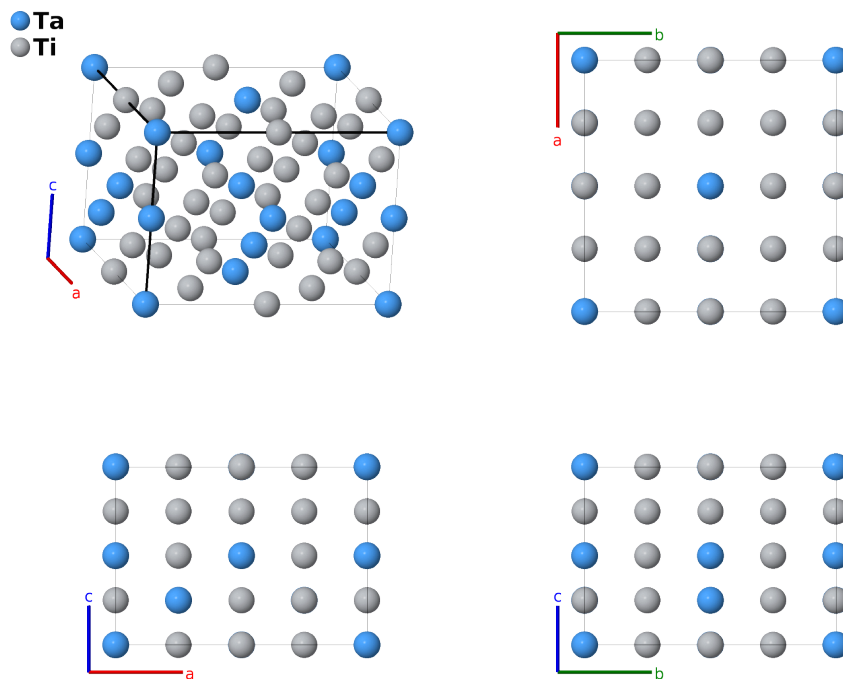
TaTi₃-II (BCC SQS-16) Structure: AB3_mC32_8_4a_4a4b-001

This structure originally had the label AB3_mC32_8_4a_4a4b. Calls to that address will be redirected here.

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<https://afLOW.org/p/P5PQ>

https://afLOW.org/p/AB3_mC32_8_4a_4a4b-001



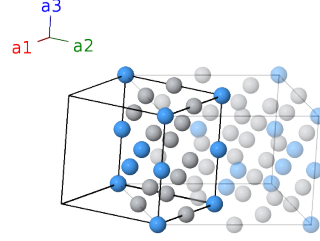
Prototype	TaTi ₃
AFLOW prototype label	AB3_mC32_8_4a_4a4b-001
ICSD	none
Pearson symbol	mC32
Space group number	8
Space group symbol	<i>Cm</i>
AFLOW prototype command	<pre>afLOW --proto=AB3_mC32_8_4a_4a4b-001 --params=a, b/a, c/a, β, x₁, z₁, x₂, z₂, x₃, z₃, x₄, z₄, x₅, z₅, x₆, z₆, x₇, z₇, x₈, z₈, x₉, y₉, z₉, x₁₀, y₁₀, z₁₀, x₁₁, y₁₁, z₁₁, x₁₂, y₁₂, z₁₂</pre>

- This is a special quasirandom structure with 16 atoms per unit cell (SQS-16) for a bcc binary substitutional alloy A_xB_{1-x} (Jiang, 2004; Chakraborty, 2016)).
- Several compositions are available:

- TaTi₇ (AB7_hR16_166_c_c2h),
- Ta₃Ti₁₃ (A3B13_oC32_38_ac_a2bcdef),
- TaTi₃-I (AB3_mC32_8_4a_12a) ,
- TaTi₃-II (AB3_mC32_8_4a_4a4b) (this structure),
- Ta₅Ti₁₁ (A5B11_mP16_6_2abc_2a3b3c) ,
- Ta₃Ti₈ (A3B5_oC32_38_abce_abcdef) ,
- TaTi (AB_aP16_2_4i_4i).

Base-centered Monoclinic primitive vectors

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\
 \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}
 \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(2a)	Ta I
\mathbf{B}_2	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(2a)	Ta II
\mathbf{B}_3	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(2a)	Ta III
\mathbf{B}_4	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(2a)	Ta IV
\mathbf{B}_5	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(2a)	Ti I
\mathbf{B}_6	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(2a)	Ti II
\mathbf{B}_7	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(2a)	Ti III
\mathbf{B}_8	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(2a)	Ti IV
\mathbf{B}_9	$(x_9 - y_9) \mathbf{a}_1 + (x_9 + y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(4b)	Ti V
\mathbf{B}_{10}	$(x_9 + y_9) \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(4b)	Ti V
\mathbf{B}_{11}	$(x_{10} - y_{10}) \mathbf{a}_1 + (x_{10} + y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3$	=	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(4b)	Ti VI
\mathbf{B}_{12}	$(x_{10} + y_{10}) \mathbf{a}_1 + (x_{10} - y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3$	=	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(4b)	Ti VI
\mathbf{B}_{13}	$(x_{11} - y_{11}) \mathbf{a}_1 + (x_{11} + y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$	=	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(4b)	Ti VII
\mathbf{B}_{14}	$(x_{11} + y_{11}) \mathbf{a}_1 + (x_{11} - y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$	=	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(4b)	Ti VII
\mathbf{B}_{15}	$(x_{12} - y_{12}) \mathbf{a}_1 + (x_{12} + y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3$	=	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(4b)	Ti VIII
\mathbf{B}_{16}	$(x_{12} + y_{12}) \mathbf{a}_1 + (x_{12} - y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3$	=	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(4b)	Ti VIII

References

- [1] C. Jiang, C. Wolverton, J. Sofo, L.-Q. Chen, and Z.-K. Liu, *First-principles study of binary bcc alloys using special quasirandom structures*, Phys. Rev. B **69**, 214202 (2004), doi:10.1103/PhysRevB.69.214202.
- [2] T. Chakraborty, J. Rogal, and R. Drautz, *Unraveling the composition dependence of the martensitic transformation temperature: A first-principles study of Ti-Ta alloys*, Phys. Rev. B **94**, 224104 (2016), doi:10.1103/PhysRevB.94.224104.