

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

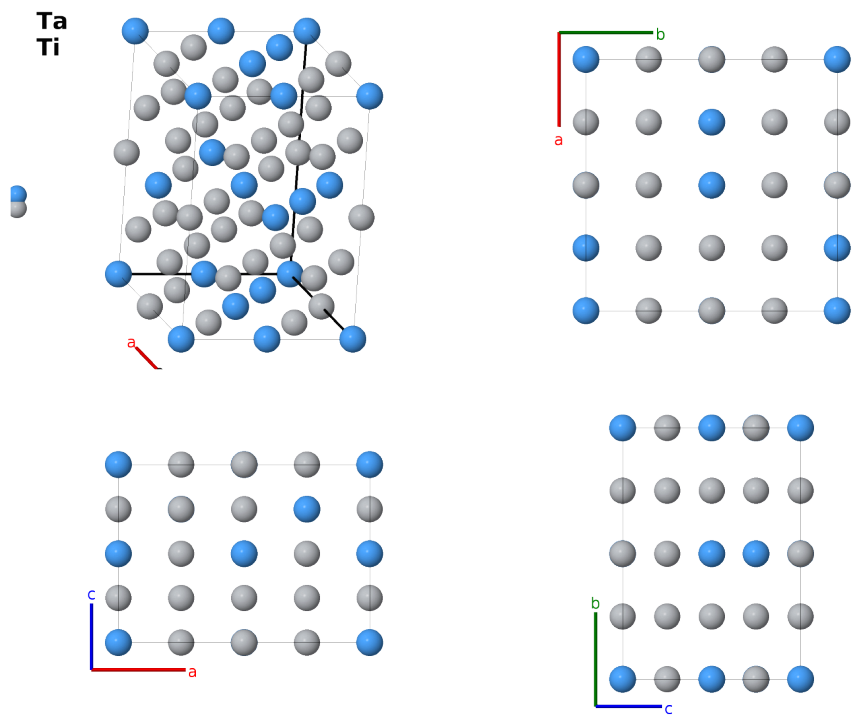
This structure previously used the label(s) **AB3_mC32_8_4a_4a4b**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/P5PQ>

https://aflow.org/prototype-encyclopedia/AB3_mC32_8_4a_4a4b-001



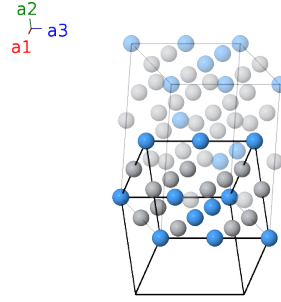
Prototype	TaTi ₃
AFLOW prototype label	AB3_mC32_8_4a_4a4b-001
Pearson symbol	mC32
Space group number	8
Space group symbol	<i>Cm</i>
AFLOW prototype command	<pre>aflow --proto=AB3_mC32_8_4a_4a4b-001 --params=a,b/a,c/a,β,x₁,z₁,x₂,z₂,x₃,z₃,x₄,z₄,x₅,z₅,x₆,z₆,x₇,z₇,x₈,z₈,x₉,y₉,z₉, x₁₀,y₁₀,z₁₀,x₁₁,y₁₁,z₁₁,x₁₂,y₁₂,z₁₂</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

$$\mathbf{B}_{16} = \begin{pmatrix} (x_{12} + y_{12}) \mathbf{a}_1 + \\ (x_{12} - y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3 \end{pmatrix} = (ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}} \quad (4b) \quad \text{Ti VIII}$$

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.

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