

TaTi (BCC SQS-16) Structure: AB_aP16_2_4i_4i-001

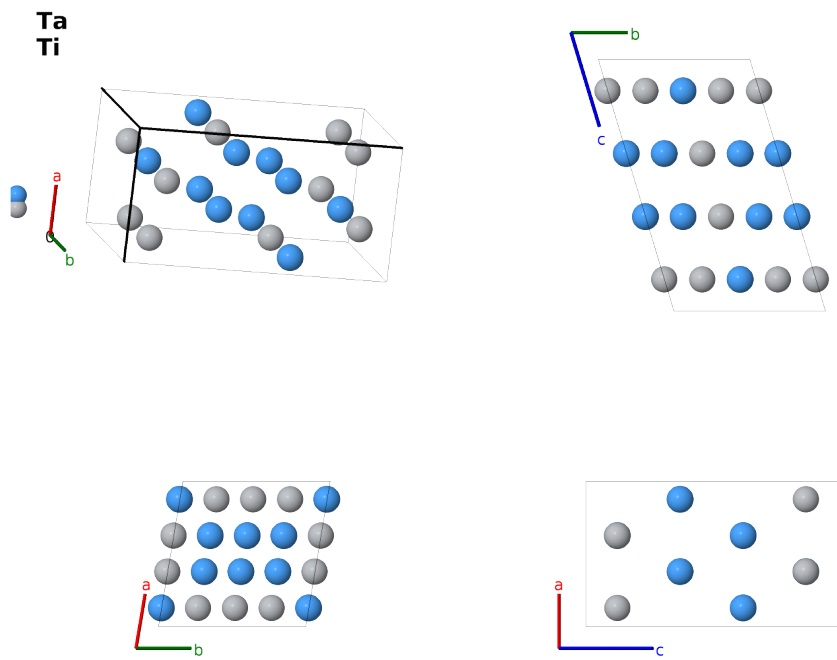
This structure previously used the label(s) **AB_aP16_2_4i_4i**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/BQ6Y>

https://aflow.org/prototype-encyclopedia/AB_aP16_2_4i_4i-001



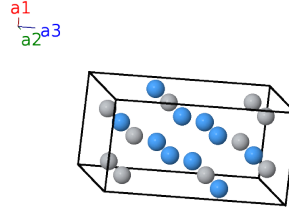
Prototype	TaTi
AFLOW prototype label	AB_aP16_2_4i_4i-001
Pearson symbol	aP16
Space group number	2
Space group symbol	$P\bar{1}$
AFLOW prototype command	<pre>aflow --proto=AB_aP16_2_4i_4i-001 --params=a,b/a,c/a,α,β,γ,x_1,y_1,z_1,x_2,y_2,z_2,x_3,y_3,z_3,x_4,y_4,z_4,x_5,y_5,z_5,x_6,y_6,z_6,x_7,y_7,z_7,x_8,y_8,z_8</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),
 - Ta₅Ti₁₁ (A5B11_mP16_6_2abc_2a3b3c),
 - Ta₃Ti₈ (A3B5_oC32_38_abce_abcdef),
 - TaTi (AB_aP16_2_4i_4i) (this structure).

Triclinic primitive vectors

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \cos \gamma \hat{\mathbf{x}} + b \sin \gamma \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c_x \hat{\mathbf{x}} + c_y \hat{\mathbf{y}} + c_z \hat{\mathbf{z}} \\
 c_x &= c \cos \beta \\
 c_y &= c(\cos \alpha - \cos \beta \cos \gamma) / \sin \gamma \\
 c_z &= \sqrt{c^2 - c_x^2 - c_y^2}
 \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$(ax_1 + by_1 \cos \gamma + c_x z_1) \hat{\mathbf{x}} + (by_1 \sin \gamma + c_y z_1) \hat{\mathbf{y}} + c_z z_1 \hat{\mathbf{z}}$	(2i)	Ta I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-(ax_1 + by_1 \cos \gamma + c_x z_1) \hat{\mathbf{x}} - (by_1 \sin \gamma + c_y z_1) \hat{\mathbf{y}} - c_z z_1 \hat{\mathbf{z}}$	(2i)	Ta I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + by_2 \cos \gamma + c_x z_2) \hat{\mathbf{x}} + (by_2 \sin \gamma + c_y z_2) \hat{\mathbf{y}} + c_z z_2 \hat{\mathbf{z}}$	(2i)	Ta II
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + by_2 \cos \gamma + c_x z_2) \hat{\mathbf{x}} - (by_2 \sin \gamma + c_y z_2) \hat{\mathbf{y}} - c_z z_2 \hat{\mathbf{z}}$	(2i)	Ta II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + by_3 \cos \gamma + c_x z_3) \hat{\mathbf{x}} + (by_3 \sin \gamma + c_y z_3) \hat{\mathbf{y}} + c_z z_3 \hat{\mathbf{z}}$	(2i)	Ta III
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + by_3 \cos \gamma + c_x z_3) \hat{\mathbf{x}} - (by_3 \sin \gamma + c_y z_3) \hat{\mathbf{y}} - c_z z_3 \hat{\mathbf{z}}$	(2i)	Ta III
$\mathbf{B}_7$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + by_4 \cos \gamma + c_x z_4) \hat{\mathbf{x}} + (by_4 \sin \gamma + c_y z_4) \hat{\mathbf{y}} + c_z z_4 \hat{\mathbf{z}}$	(2i)	Ta IV
$\mathbf{B}_8$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + by_4 \cos \gamma + c_x z_4) \hat{\mathbf{x}} - (by_4 \sin \gamma + c_y z_4) \hat{\mathbf{y}} - c_z z_4 \hat{\mathbf{z}}$	(2i)	Ta IV
$\mathbf{B}_9$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + by_5 \cos \gamma + c_x z_5) \hat{\mathbf{x}} + (by_5 \sin \gamma + c_y z_5) \hat{\mathbf{y}} + c_z z_5 \hat{\mathbf{z}}$	(2i)	Ti I
$\mathbf{B}_{10}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + by_5 \cos \gamma + c_x z_5) \hat{\mathbf{x}} - (by_5 \sin \gamma + c_y z_5) \hat{\mathbf{y}} - c_z z_5 \hat{\mathbf{z}}$	(2i)	Ti I
$\mathbf{B}_{11}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + by_6 \cos \gamma + c_x z_6) \hat{\mathbf{x}} + (by_6 \sin \gamma + c_y z_6) \hat{\mathbf{y}} + c_z z_6 \hat{\mathbf{z}}$	(2i)	Ti II
$\mathbf{B}_{12}$	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + by_6 \cos \gamma + c_x z_6) \hat{\mathbf{x}} - (by_6 \sin \gamma + c_y z_6) \hat{\mathbf{y}} - c_z z_6 \hat{\mathbf{z}}$	(2i)	Ti II

$$\begin{aligned}
\mathbf{B}_{13} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= (ax_7 + by_7 \cos \gamma + c_x z_7) \hat{\mathbf{x}} + (by_7 \sin \gamma + c_y z_7) \hat{\mathbf{y}} + c_z z_7 \hat{\mathbf{z}} &(2i) &\text{Ti III} \\
\mathbf{B}_{14} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -(ax_7 + by_7 \cos \gamma + c_x z_7) \hat{\mathbf{x}} - (by_7 \sin \gamma + c_y z_7) \hat{\mathbf{y}} - c_z z_7 \hat{\mathbf{z}} &(2i) &\text{Ti III} \\
\mathbf{B}_{15} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= (ax_8 + by_8 \cos \gamma + c_x z_8) \hat{\mathbf{x}} + (by_8 \sin \gamma + c_y z_8) \hat{\mathbf{y}} + c_z z_8 \hat{\mathbf{z}} &(2i) &\text{Ti IV} \\
\mathbf{B}_{16} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 &= -(ax_8 + by_8 \cos \gamma + c_x z_8) \hat{\mathbf{x}} - (by_8 \sin \gamma + c_y z_8) \hat{\mathbf{y}} - c_z z_8 \hat{\mathbf{z}} &(2i) &\text{Ti IV}
\end{aligned}$$

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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