

TaTi₇ (BCC SQS-16) Structure: AB7_hR16_166_c_c2h-001

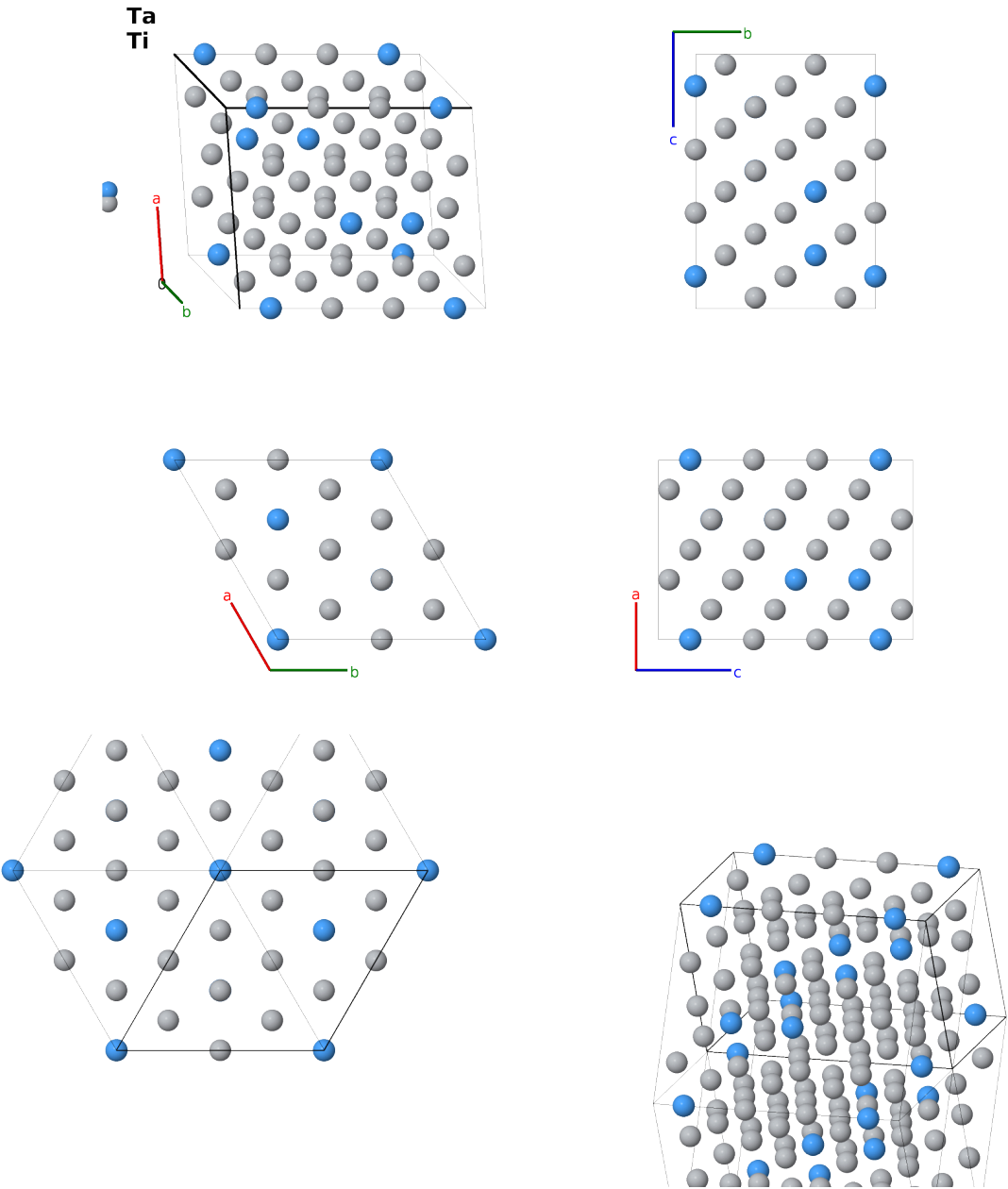
This structure previously used the label(s) **AB7_hR16_166_c_c2h**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/56NK>

https://aflow.org/prototype-encyclopedia/AB7_hR16_166_c_c2h-001

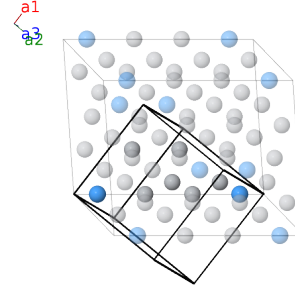


Prototype	TaTi ₇
AFLOW prototype label	AB7_hR16_166_c_c2h-001
Pearson symbol	hR16
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	aflow --proto=AB7_hR16_166_c_c2h-001 --params=a, c/a, x ₁ , x ₂ , x ₃ , z ₃ , x ₄ , z ₄

- 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) (this structure),
 - 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).

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$cx_1 \hat{\mathbf{z}}$	(2c)	Ta I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$-cx_1 \hat{\mathbf{z}}$	(2c)	Ta I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(2c)	Ti I
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-cx_2 \hat{\mathbf{z}}$	(2c)	Ti I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}}$	(6h)	Ti II
$\mathbf{B}_6$	$= z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}}$	(6h)	Ti II
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}}$	(6h)	Ti II

$$\begin{aligned}
\mathbf{B}_8 &= -z_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3 &= \frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - z_3) \hat{\mathbf{y}} - \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}} &(6h) &\text{Ti II} \\
\mathbf{B}_9 &= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= -\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - z_3) \hat{\mathbf{y}} - \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}} &(6h) &\text{Ti II} \\
\mathbf{B}_{10} &= -x_3 \mathbf{a}_1 - z_3 \mathbf{a}_2 - x_3 \mathbf{a}_3 &= \frac{1}{\sqrt{3}}a(x_3 - z_3) \hat{\mathbf{y}} - \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}} &(6h) &\text{Ti II} \\
\mathbf{B}_{11} &= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= \frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}} &(6h) &\text{Ti III} \\
\mathbf{B}_{12} &= z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3 &= -\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}} &(6h) &\text{Ti III} \\
\mathbf{B}_{13} &= x_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3 &= -\frac{1}{\sqrt{3}}a(x_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}} &(6h) &\text{Ti III} \\
\mathbf{B}_{14} &= -z_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3 &= \frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}} &(6h) &\text{Ti III} \\
\mathbf{B}_{15} &= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}} &(6h) &\text{Ti III} \\
\mathbf{B}_{16} &= -x_4 \mathbf{a}_1 - z_4 \mathbf{a}_2 - x_4 \mathbf{a}_3 &= \frac{1}{\sqrt{3}}a(x_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}} &(6h) &\text{Ti III}
\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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