

Ta₃Ti₅ (BCC SQS-16) Structure: A3B5_oC32_38_abcd_abcef-001

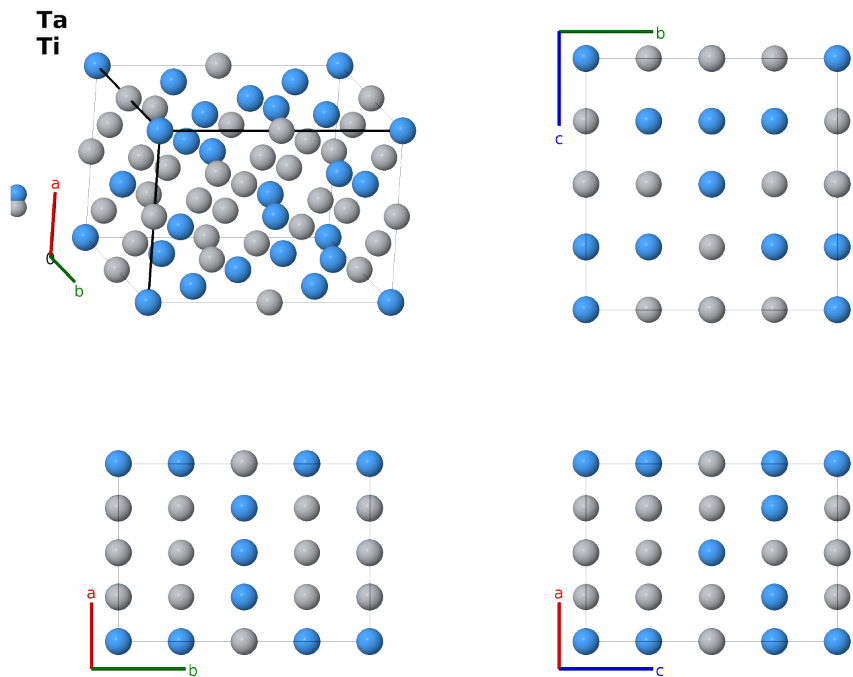
This structure previously used the label(s) **A3B5_oC32_38_abce_abcdf**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/0NF7>

https://aflow.org/prototype-encyclopedia/A3B5_oC32_38_abcd_abcef-001



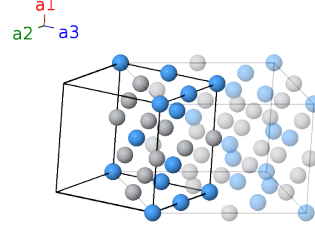
Prototype	Ta ₃ Ti ₅
AFLOW prototype label	A3B5_oC32_38_abcd_abcef-001
Pearson symbol	oC32
Space group number	38
Space group symbol	<i>Amm</i> 2
AFLOW prototype command	<code>aflow --proto=A3B5_oC32_38_abcd_abcef-001</code> <code>--params=a, b/a, c/a, z₁, z₂, z₃, z₄, x₅, z₅, x₆, z₆, y₇, z₇, y₈, z₈, x₉, y₉, z₉</code>

- 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_abcdf) (this structure),
- TaTi (AB_aP16_2_4i_4i).

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -z_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(2a)	Ta I
$\mathbf{B}_2$	$= -z_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$cz_2 \hat{\mathbf{z}}$	(2a)	Ti I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 - z_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + cz_3 \hat{\mathbf{z}}$	(2b)	Ta II
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 - z_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + cz_4 \hat{\mathbf{z}}$	(2b)	Ti II
$\mathbf{B}_5$	$= x_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + cz_5 \hat{\mathbf{z}}$	(4c)	Ta III
$\mathbf{B}_6$	$= -x_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + cz_5 \hat{\mathbf{z}}$	(4c)	Ta III
$\mathbf{B}_7$	$= x_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + cz_6 \hat{\mathbf{z}}$	(4c)	Ti III
$\mathbf{B}_8$	$= -x_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + cz_6 \hat{\mathbf{z}}$	(4c)	Ti III
$\mathbf{B}_9$	$= (y_7 - z_7) \mathbf{a}_2 + (y_7 + z_7) \mathbf{a}_3$	$=$	$by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4d)	Ta IV
$\mathbf{B}_{10}$	$= -(y_7 + z_7) \mathbf{a}_2 - (y_7 - z_7) \mathbf{a}_3$	$=$	$-by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4d)	Ta IV
$\mathbf{B}_{11}$	$= \frac{1}{2} \mathbf{a}_1 + (y_8 - z_8) \mathbf{a}_2 + (y_8 + z_8) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(4e)	Ti IV
$\mathbf{B}_{12}$	$= \frac{1}{2} \mathbf{a}_1 - (y_8 + z_8) \mathbf{a}_2 - (y_8 - z_8) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(4e)	Ti IV
$\mathbf{B}_{13}$	$= x_9 \mathbf{a}_1 + (y_9 - z_9) \mathbf{a}_2 + (y_9 + z_9) \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8f)	Ti V
$\mathbf{B}_{14}$	$= -x_9 \mathbf{a}_1 - (y_9 + z_9) \mathbf{a}_2 - (y_9 - z_9) \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8f)	Ti V
$\mathbf{B}_{15}$	$= x_9 \mathbf{a}_1 - (y_9 + z_9) \mathbf{a}_2 - (y_9 - z_9) \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8f)	Ti V
$\mathbf{B}_{16}$	$= -x_9 \mathbf{a}_1 + (y_9 - z_9) \mathbf{a}_2 + (y_9 + z_9) \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8f)	Ti V

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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