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

This structure originally had the label `AB_aP16_2_4i_4i`. Calls to that address will be redirected here.

https://aflow.org/p/BQ6Y

https://aflow.org/p/AB_aP16_2_4i_4i-001
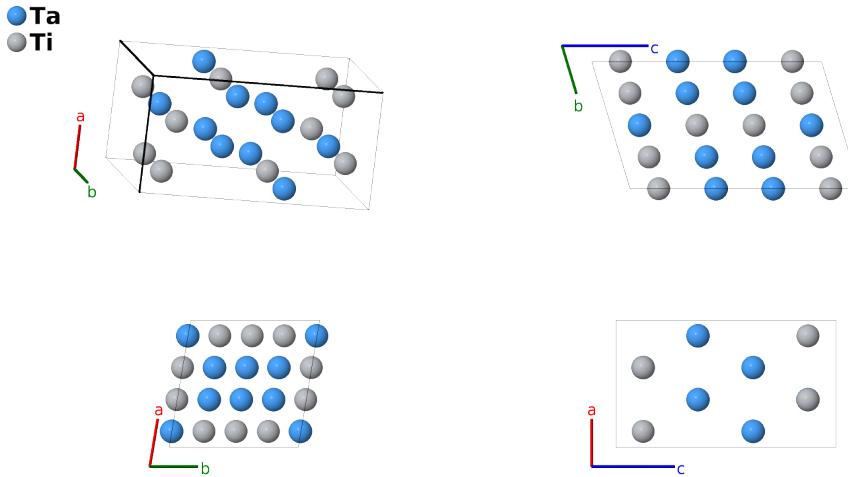
Prototype	TaTi
AFLOW prototype label	AB_aP16_2_4i_4i-001
ICSD	none
Pearson symbol	aP16
Space group number	2
Space group symbol	$P\bar{1}$
AFLOW prototype command	aflow --proto=AB_aP16_2_4i_4i-001 --params=$a, b/a, c/a, \alpha, \beta, \gamma, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$

- 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:

    - TaTi$_7$ (AB7_hR16_166_c_c2h),
    - Ta$_3$Ti$_{13}$ (A3B13_oC32_38_ac_a2bcdef),
    - TaTi$_3$-I (AB3_mC32_8_4a_12a) ,
    - TaTi$_3$-II (AB3_mC32_8_4a_4a4b),
    - Ta$_5$Ti$_{11}$ (A5B11_mP16_6_2abc_2a3b3c),

- Ta$_3$Ti$_8$ (A3B5_oC32_38_abce_abcdf),
- TaTi (AB_aP16_2_4i_4i) (this structure).

Triclinic primitive vectors

$$\mathbf{a_1} \quad = \quad a\,\hat{\mathbf{x}}$$

$$\mathbf{a_2} \quad = \quad b\cos\gamma\,\hat{\mathbf{x}} + b\sin\gamma\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} \quad = \quad c_x\,\hat{\mathbf{x}} + c_y\,\hat{\mathbf{y}} + c_z\,\hat{\mathbf{z}}$$

$$c_x \quad = \quad c\cos\beta$$

$$c_y \quad = \quad c(\cos\alpha - \cos\beta\cos\gamma)/\sin\gamma$$

$$c_z \quad = \quad \sqrt{c^2 - c_x^2 - c_y^2}$$
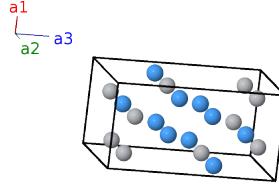
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a_1} + y_1\,\mathbf{a_2} + z_1\,\mathbf{a_3}$	=	$(ax_1 + by_1\cos\gamma + c_xz_1)\,\hat{\mathbf{x}} + (by_1\sin\gamma + c_yz_1)\,\hat{\mathbf{y}} + c_zz_1\,\hat{\mathbf{z}}$	(2i)	Ta I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a_1} - y_1\,\mathbf{a_2} - z_1\,\mathbf{a_3}$	=	$-(ax_1 + by_1\cos\gamma + c_xz_1)\,\hat{\mathbf{x}} - (by_1\sin\gamma + c_yz_1)\,\hat{\mathbf{y}} - c_zz_1\,\hat{\mathbf{z}}$	(2i)	Ta I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	=	$(ax_2 + by_2\cos\gamma + c_xz_2)\,\hat{\mathbf{x}} + (by_2\sin\gamma + c_yz_2)\,\hat{\mathbf{y}} + c_zz_2\,\hat{\mathbf{z}}$	(2i)	Ta II
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a_1} - y_2\,\mathbf{a_2} - z_2\,\mathbf{a_3}$	=	$-(ax_2 + by_2\cos\gamma + c_xz_2)\,\hat{\mathbf{x}} - (by_2\sin\gamma + c_yz_2)\,\hat{\mathbf{y}} - c_zz_2\,\hat{\mathbf{z}}$	(2i)	Ta II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	=	$(ax_3 + by_3\cos\gamma + c_xz_3)\,\hat{\mathbf{x}} + (by_3\sin\gamma + c_yz_3)\,\hat{\mathbf{y}} + c_zz_3\,\hat{\mathbf{z}}$	(2i)	Ta III
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	=	$-(ax_3 + by_3\cos\gamma + c_xz_3)\,\hat{\mathbf{x}} - (by_3\sin\gamma + c_yz_3)\,\hat{\mathbf{y}} - c_zz_3\,\hat{\mathbf{z}}$	(2i)	Ta III
$\mathbf{B_7}$	=	$x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	=	$(ax_4 + by_4\cos\gamma + c_xz_4)\,\hat{\mathbf{x}} + (by_4\sin\gamma + c_yz_4)\,\hat{\mathbf{y}} + c_zz_4\,\hat{\mathbf{z}}$	(2i)	Ta IV
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	=	$-(ax_4 + by_4\cos\gamma + c_xz_4)\,\hat{\mathbf{x}} - (by_4\sin\gamma + c_yz_4)\,\hat{\mathbf{y}} - c_zz_4\,\hat{\mathbf{z}}$	(2i)	Ta IV
$\mathbf{B_9}$	=	$x_5\,\mathbf{a_1} + y_5\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	=	$(ax_5 + by_5\cos\gamma + c_xz_5)\,\hat{\mathbf{x}} + (by_5\sin\gamma + c_yz_5)\,\hat{\mathbf{y}} + c_zz_5\,\hat{\mathbf{z}}$	(2i)	Ti I
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a_1} - y_5\,\mathbf{a_2} - z_5\,\mathbf{a_3}$	=	$-(ax_5 + by_5\cos\gamma + c_xz_5)\,\hat{\mathbf{x}} - (by_5\sin\gamma + c_yz_5)\,\hat{\mathbf{y}} - c_zz_5\,\hat{\mathbf{z}}$	(2i)	Ti I
$\mathbf{B_{11}}$	=	$x_6\,\mathbf{a_1} + y_6\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	=	$(ax_6 + by_6\cos\gamma + c_xz_6)\,\hat{\mathbf{x}} + (by_6\sin\gamma + c_yz_6)\,\hat{\mathbf{y}} + c_zz_6\,\hat{\mathbf{z}}$	(2i)	Ti II
$\mathbf{B_{12}}$	=	$-x_6\,\mathbf{a_1} - y_6\,\mathbf{a_2} - z_6\,\mathbf{a_3}$	=	$-(ax_6 + by_6\cos\gamma + c_xz_6)\,\hat{\mathbf{x}} - (by_6\sin\gamma + c_yz_6)\,\hat{\mathbf{y}} - c_zz_6\,\hat{\mathbf{z}}$	(2i)	Ti II
$\mathbf{B_{13}}$	=	$x_7\,\mathbf{a_1} + y_7\,\mathbf{a_2} + z_7\,\mathbf{a_3}$	=	$(ax_7 + by_7\cos\gamma + c_xz_7)\,\hat{\mathbf{x}} + (by_7\sin\gamma + c_yz_7)\,\hat{\mathbf{y}} + c_zz_7\,\hat{\mathbf{z}}$	(2i)	Ti III
$\mathbf{B_{14}}$	=	$-x_7\,\mathbf{a_1} - y_7\,\mathbf{a_2} - z_7\,\mathbf{a_3}$	=	$-(ax_7 + by_7\cos\gamma + c_xz_7)\,\hat{\mathbf{x}} - (by_7\sin\gamma + c_yz_7)\,\hat{\mathbf{y}} - c_zz_7\,\hat{\mathbf{z}}$	(2i)	Ti III
$\mathbf{B_{15}}$	=	$x_8\,\mathbf{a_1} + y_8\,\mathbf{a_2} + z_8\,\mathbf{a_3}$	=	$(ax_8 + by_8\cos\gamma + c_xz_8)\,\hat{\mathbf{x}} + (by_8\sin\gamma + c_yz_8)\,\hat{\mathbf{y}} + c_zz_8\,\hat{\mathbf{z}}$	(2i)	Ti IV
$\mathbf{B_{16}}$	=	$-x_8\,\mathbf{a_1} - y_8\,\mathbf{a_2} - z_8\,\mathbf{a_3}$	=	$-(ax_8 + by_8\cos\gamma + c_xz_8)\,\hat{\mathbf{x}} - (by_8\sin\gamma + c_yz_8)\,\hat{\mathbf{y}} - c_zz_8\,\hat{\mathbf{z}}$	(2i)	Ti IV

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.