$TaTi_7$ (BCC SQS-16) Structure: AB7_hR16_166_c_c2h-001

This structure originally had the label `AB7_hR16_166_c_c2h`. Calls to that address will be redirected here.

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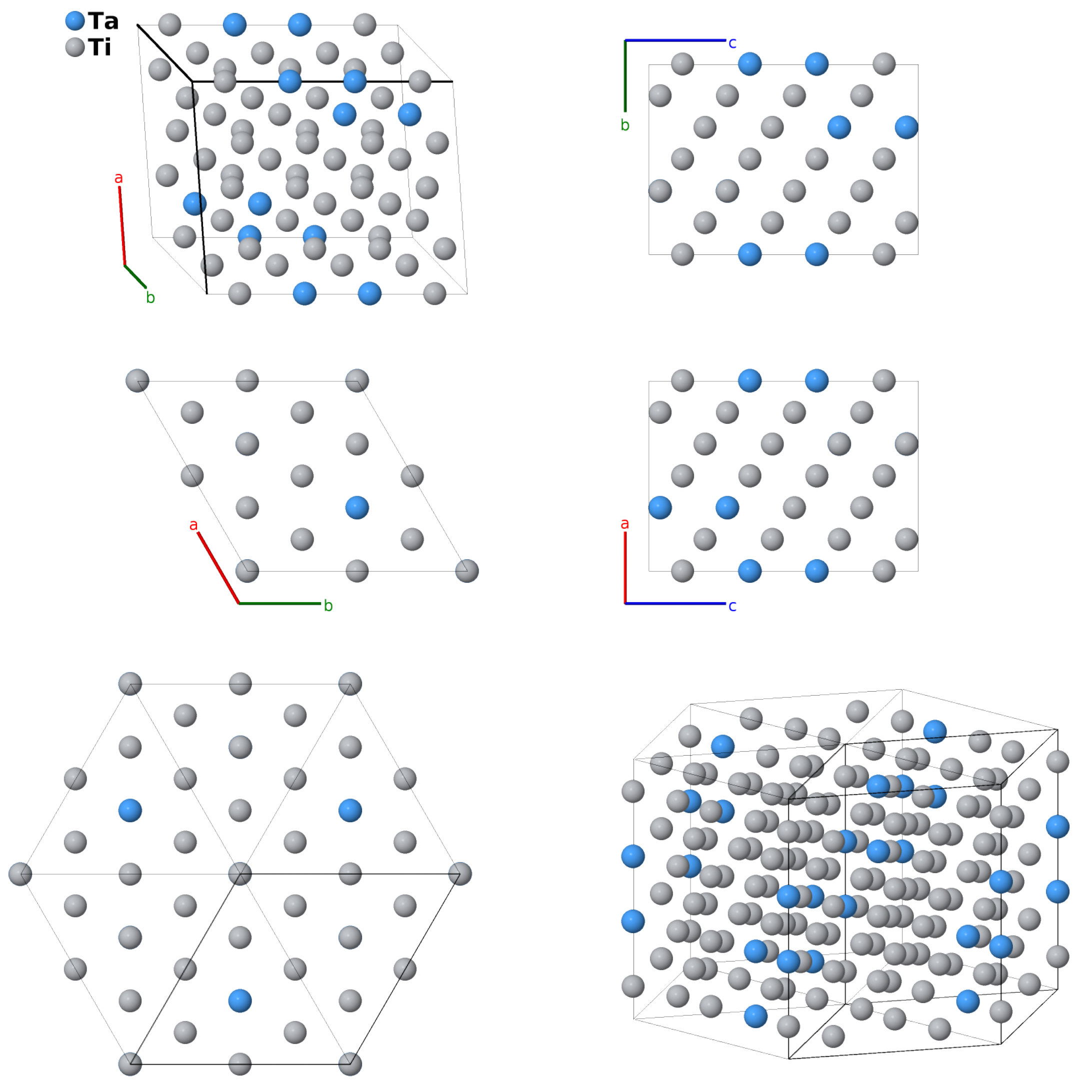
https://aflow.org/p/56NK

https://aflow.org/p/AB7_hR16_166_c_c2h-001



Prototype $TaTi_7$

AFLOW prototype label AB7_hR16_166_c_c2h-001

ICSD none

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`
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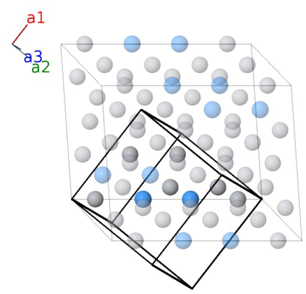
- This is a special quasirandom structure with 16 atoms per unit cell (SQS-16) for a bcc binary substitutional alloy A_xB_{1-x} (Jiang, 2004; Chakraborty, 2016)).
- Several compositions are available:
  - $TaTi_7$ (AB7_hR16_166_c_c2h) (this structure),
  - Ta_3Ti_{13} (A3B13_oC32_38_ac_a2bcdef),
  - $TaTi_3$-I (AB3_mC32_8_4a_12a) ,
  - $TaTi_3$-II (AB3_mC32_8_4a_4a4b) ,
  - Ta_5Ti_{11} (A5B11_mP16_6_2abc_2a3b3c) ,
  - Ta_3Ti_8 (A3B5_oC32_38_abce_abcdf) ,
  - TaTi (AB_aP16_2_4i_4i).

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_8}$	=	$-z_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_3 - z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(6h)	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)	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)	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)	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)	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)	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)	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)	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)	Ti III

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.