Ta_3Ti_{13} (BCC SQS-16) Structure: A3B13_oC32_38_ac_a2bcdef-001

This structure originally had the label `A3B13_oC32_38_ac_a2bcdef`. Calls to that address will be redirected here.

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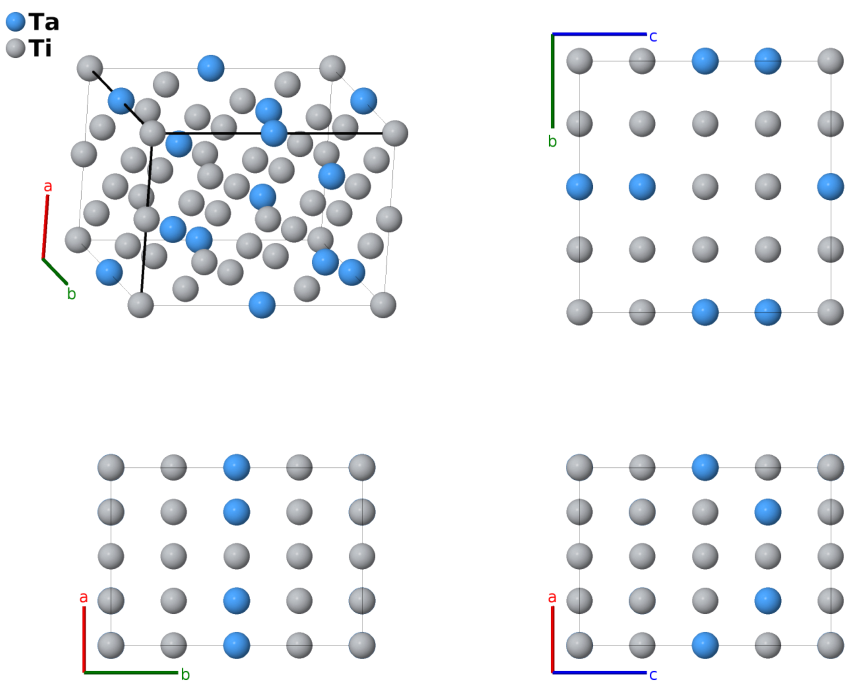
https://aflow.org/p/A2U8

https://aflow.org/p/A3B13_oC32_38_ac_a2bcdef-001



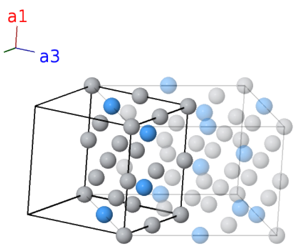
Prototype	Ta_3Ti_{13}
AFLOW prototype label	A3B13_oC32_38_ac_a2bcdef-001
ICSD	none
Pearson symbol	oC32
Space group number	38
Space group symbol	$Amm2$
AFLOW prototype command	`aflow --proto=A3B13_oC32_38_ac_a2bcdef-001` `--params=`$a, b/a, c/a, z_1, z_2, z_3, z_4, x_5, z_5, x_6, z_6, y_7, z_7, y_8, z_8, x_9, y_9, z_9$

- 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_3Ti_{13} (A3B13_oC32_38_ac_a2bcdef) (this structure),
– $TaTi_3$-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).

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = \tfrac{1}{2}b\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$



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)	Ti 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 III
$\mathbf{B_5}$	=	$x_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(4c)	Ta II
$\mathbf{B_6}$	=	$-x_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(4c)	Ta II
$\mathbf{B_7}$	=	$x_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + cz_6\,\hat{\mathbf{z}}$	(4c)	Ti IV
$\mathbf{B_8}$	=	$-x_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + cz_6\,\hat{\mathbf{z}}$	(4c)	Ti IV
$\mathbf{B_9}$	=	$(y_7 - z_7)\,\mathbf{a}_2 + (y_7 + z_7)\,\mathbf{a}_3$	=	$by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4d)	Ti V
$\mathbf{B_{10}}$	=	$-(y_7 + z_7)\,\mathbf{a}_2 - (y_7 - z_7)\,\mathbf{a}_3$	=	$-by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4d)	Ti V
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + (y_8 - z_8)\,\mathbf{a}_2 + (y_8 + z_8)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4e)	Ti VI
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - (y_8 + z_8)\,\mathbf{a}_2 - (y_8 - z_8)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4e)	Ti VI
$\mathbf{B_{13}}$	=	$x_9\,\mathbf{a}_1 + (y_9 - z_9)\,\mathbf{a}_2 + (y_9 + z_9)\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(8f)	Ti VII
$\mathbf{B_{14}}$	=	$-x_9\,\mathbf{a}_1 - (y_9 + z_9)\,\mathbf{a}_2 - (y_9 - z_9)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(8f)	Ti VII
$\mathbf{B_{15}}$	=	$x_9\,\mathbf{a}_1 - (y_9 + z_9)\,\mathbf{a}_2 - (y_9 - z_9)\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(8f)	Ti VII
$\mathbf{B_{16}}$	=	$-x_9\,\mathbf{a}_1 + (y_9 - z_9)\,\mathbf{a}_2 + (y_9 + z_9)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(8f)	Ti VII

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.