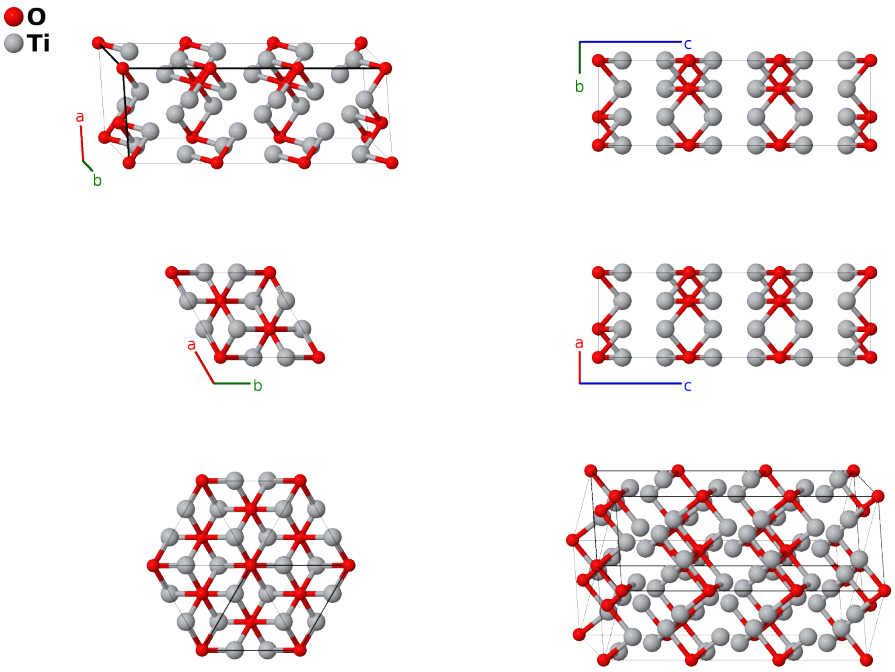
Ti_3O (Room-Temperature) Structure: AB3_hP24_149_acgi_3l-001

This structure originally had the label `AB3_hP24_149_acgi_3l`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

https://aflow.org/p/9DMX

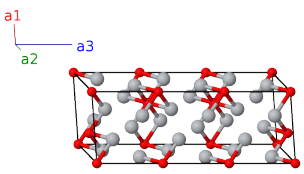
https://aflow.org/p/AB3_hP24_149_acgi_3l-001



Prototype	OTi_3
AFLOW prototype label	AB3_hP24_149_acgi_3l-001
ICSD	36055
Pearson symbol	hP24
Space group number	149
Space group symbol	$P312$
AFLOW prototype command	`aflow --proto=AB3_hP24_149_acgi_3l-001 --params=`$a, c/a, z_3, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

Trigonal (Hexagonal) primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	O I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(1c)	O II
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(2g)	O III
$\mathbf{B_4}$	=	$-z_3\,\mathbf{a}_3$	=	$-cz_3\,\hat{\mathbf{z}}$	(2g)	O III
$\mathbf{B_5}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2i)	O IV
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(2i)	O IV
$\mathbf{B_7}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6l)	Ti I
$\mathbf{B_8}$	=	$-y_5\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - 2y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6l)	Ti I
$\mathbf{B_9}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6l)	Ti I
$\mathbf{B_{10}}$	=	$-y_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(6l)	Ti I
$\mathbf{B_{11}}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_5 + 2y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(6l)	Ti I
$\mathbf{B_{12}}$	=	$x_5\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(6l)	Ti I
$\mathbf{B_{13}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6l)	Ti II
$\mathbf{B_{14}}$	=	$-y_6\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - 2y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6l)	Ti II
$\mathbf{B_{15}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6l)	Ti II
$\mathbf{B_{16}}$	=	$-y_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6l)	Ti II
$\mathbf{B_{17}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_6 + 2y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6l)	Ti II
$\mathbf{B_{18}}$	=	$x_6\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6l)	Ti II
$\mathbf{B_{19}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 + y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_7 - y_7)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(6l)	Ti III
$\mathbf{B_{20}}$	=	$-y_7\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - 2y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(6l)	Ti III
$\mathbf{B_{21}}$	=	$-(x_7 - y_7)\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_7 - y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(6l)	Ti III
$\mathbf{B_{22}}$	=	$-y_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7 + y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_7 - y_7)\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(6l)	Ti III
$\mathbf{B_{23}}$	=	$-(x_7 - y_7)\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_7 + 2y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(6l)	Ti III
$\mathbf{B_{24}}$	=	$x_7\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_7 - y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(6l)	Ti III

References

[1] A. Jostsons and A. S. Malin, *The Ordered Structure of Ti_3O*, Acta Crystallogr. Sect. B **24**, 211–213 (1968), doi:10.1107/S0567740868001974.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.