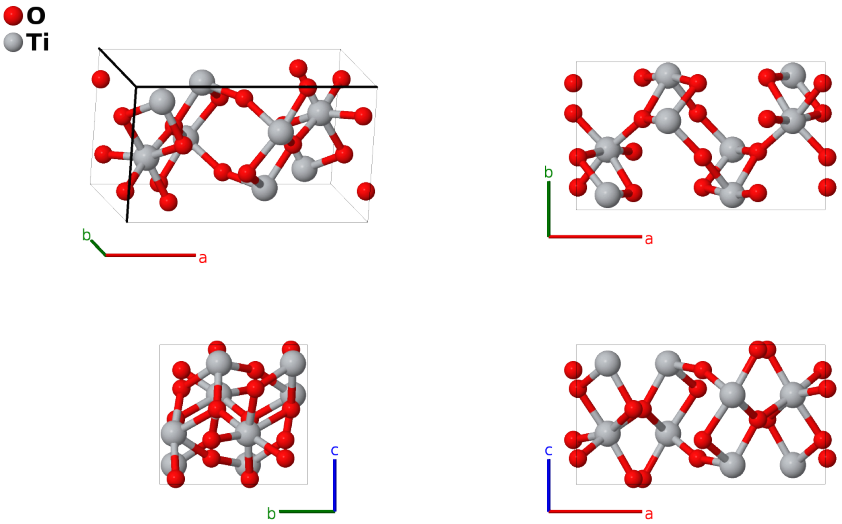
Brookite (TiO_2, $C21$) Structure: A2B_oP24_61_2c_c-001

This structure originally had the label `A2B_oP24_61_2c_c`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

https://aflow.org/p/ZJ0C

https://aflow.org/p/A2B_oP24_61_2c_c-001

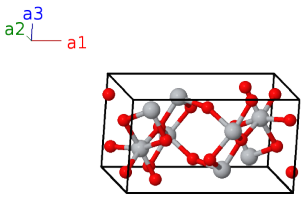


Prototype	O_2Ti
AFLOW prototype label	A2B_oP24_61_2c_c-001
***Strukturbericht* designation**	$C21$
Mineral name	brookite
ICSD	36408
Pearson symbol	oP24
Space group number	61
Space group symbol	*Pbca*
AFLOW prototype command	`aflow --proto=A2B_oP24_61_2c_c-001 --params=`$a, b/a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3$

- TiO_2 may also be found as anatase ($C5$) or rutile ($C4$).
- Our original version of this page (Mehl, 2017) misstated the value of the lattice constant b. We have corrected it here.
- Pararammelsbergite ($NiAs_2$), β-TeO_2 and brookite ($C21$, TiO_2) have the same AFLOW prototype label, A2B_oP24_61_2c_c. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_2}$	=	$-\left(x_1-\frac{1}{2}\right)\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + \left(y_1+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_1-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + b\left(y_1+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_1-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_4}$	=	$\left(x_1+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_1-\frac{1}{2}\right)\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_1-\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_6}$	=	$\left(x_1+\frac{1}{2}\right)\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 - \left(z_1-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} - c\left(z_1-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_7}$	=	$x_1\,\mathbf{a}_1 - \left(y_1-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} - b\left(y_1-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_8}$	=	$-\left(x_1-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_1+\frac{1}{2}\right)\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_1+\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_9}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_{10}}$	=	$-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_{11}}$	=	$-x_2\,\mathbf{a}_1 + \left(y_2+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + b\left(y_2+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_{12}}$	=	$\left(x_2+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2-\frac{1}{2}\right)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2-\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_{13}}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_{14}}$	=	$\left(x_2+\frac{1}{2}\right)\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 - \left(z_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} - c\left(z_2-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_{15}}$	=	$x_2\,\mathbf{a}_1 - \left(y_2-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - b\left(y_2-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_{16}}$	=	$-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2+\frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2+\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_{17}}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8c)	Ti I
$\mathbf{B_{18}}$	=	$-\left(x_3-\frac{1}{2}\right)\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Ti I
$\mathbf{B_{19}}$	=	$-x_3\,\mathbf{a}_1 + \left(y_3+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + b\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Ti I
$\mathbf{B_{20}}$	=	$\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3-\frac{1}{2}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8c)	Ti I
$\mathbf{B_{21}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8c)	Ti I
$\mathbf{B_{22}}$	=	$\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - \left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Ti I
$\mathbf{B_{23}}$	=	$x_3\,\mathbf{a}_1 - \left(y_3-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - b\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Ti I

$$\mathbf{B_{24}} = -\left(x_3 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3 = -a\left(x_3 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}} \quad \text{(8c)} \quad \text{Ti I}$$

References

[1] E. P. Meagher and G. A. Lager, *Polyhedral thermal expansion in the TiO_2 polymorphs; refinement of the crystal structures of rutile and brookite at high temperature*, Can. Mineral. **17**, 77–85 (1979).

[2] M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1–S828 (2017), doi:10.1016/j.commatsci.2017.01.017.