

# Brookite (TiO<sub>2</sub>, *C*21) Structure: A2B\_oP24\_61\_2c\_c-001

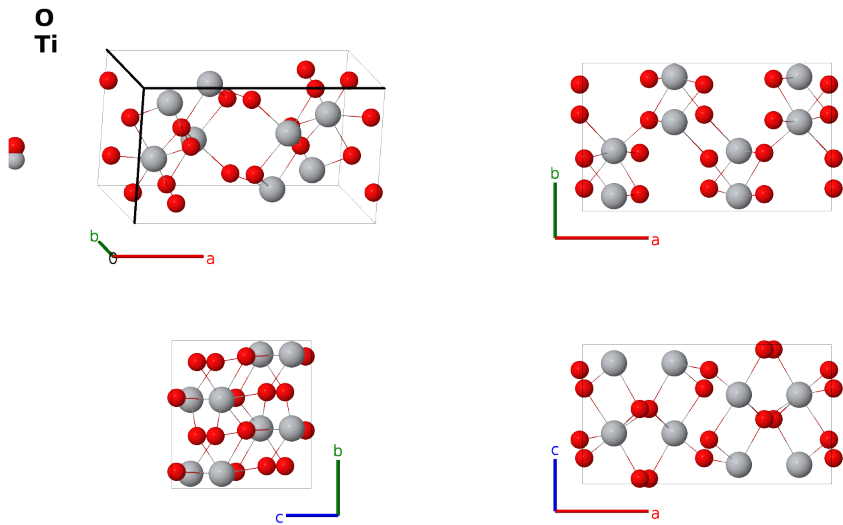
This structure previously used the label(s) **A2B\_oP24\_61\_2c\_c**. Calls to these addresses will be redirected here.

Cite this page as:

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/ZJ0C>

[https://aflow.org/prototype-encyclopedia/A2B\\_oP24\\_61\\_2c\\_c-001](https://aflow.org/prototype-encyclopedia/A2B_oP24_61_2c_c-001)



|                                    |                                                                                                                                                                                                                             |
|------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prototype                          | O <sub>2</sub> Ti                                                                                                                                                                                                           |
| AFLOW prototype label              | A2B_oP24_61_2c_c-001                                                                                                                                                                                                        |
| <i>Strukturbericht</i> designation | <i>C</i> 21                                                                                                                                                                                                                 |
| Mineral name                       | brookite                                                                                                                                                                                                                    |
| ICSD                               | 36408                                                                                                                                                                                                                       |
| CCDC                               | 1608143                                                                                                                                                                                                                     |
| Pearson symbol                     | oP24                                                                                                                                                                                                                        |
| Space group number                 | 61                                                                                                                                                                                                                          |
| Space group symbol                 | <i>Pbca</i>                                                                                                                                                                                                                 |
| AFLOW prototype command            | <code>aflow --proto=A2B_oP24_61_2c_c-001</code><br><code>--params=a, b/a, c/a, x<sub>1</sub>, y<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub></code> |

- TiO<sub>2</sub> may also be found as anatase (*C*5) or rutile (*C*4).
- Our original version of this page (Mehl, 2017) misstated the value of the lattice constant *b*. We have corrected it here.

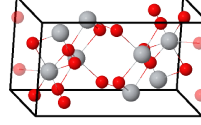
- Pararammelsbergite ( $\text{NiAs}_2$ ),  $\beta\text{-TeO}_2$  and brookite ( $C21$ ,  $\text{TiO}_2$ ) have the same AFLOW prototype label, A2B\_oP24\_61\_2c.c. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

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### Simple Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$

$\mathbf{a}_1^3$   
 $\mathbf{a}_2^3$   
 $\mathbf{a}_3^3$




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### Basis vectors

|                   | Lattice<br>coordinates                                                                                            |     | Cartesian<br>coordinates                                                                                                       | Wyckoff<br>position | Atom<br>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         |

$$\begin{aligned}
\mathbf{B}_{22} &= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + y_3 \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3 = a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{Ti I} \\
\mathbf{B}_{23} &= x_3 \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3 = ax_3 \hat{\mathbf{x}} - b \left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{Ti I} \\
\mathbf{B}_{24} &= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 + z_3 \mathbf{a}_3 = -a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}} & (8c) & \text{Ti I}
\end{aligned}$$

## References

- [1] E. P. Meagher and G. A. Lager, *Polyhedral thermal expansion in the  $\text{TiO}_2$  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.

## First cited in

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