

Rutile (TiO₂, C4) Structure:

A2B_tP6_136_f_a-001

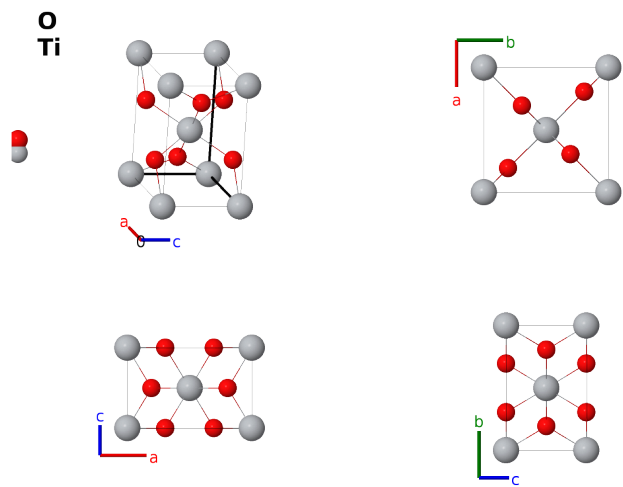
This structure previously used the label(s) **A2B_tP6_136_f_a**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/D4ZH>

https://aflow.org/prototype-encyclopedia/A2B_tP6_136_f_a-001



Prototype	O ₂ Ti
AFLOW prototype label	A2B_tP6_136_f_a-001
<i>Strukturbericht</i> designation	C4
Mineral name	rutile
ICSD	80843
CCDC	1641021
Pearson symbol	tP6
Space group number	136
Space group symbol	$P4_2/mnm$
AFLOW prototype command	<code>aflow --proto=A2B_tP6_136_f_a-001</code> <code>--params=a, c/a, x₂</code>

Other compounds with this structure

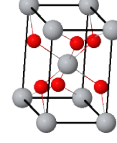
CoF₂, CrO₂, GeO₂, IrO₂, MgF₂, MnF₂, MoO₂, NTi₂, NbO₂, NiF₂, OsO₂, PbO₂, RuO₂, SiO₂ (stishovite), SnO₂ (cassiterite), TaO₂, TeO₂, VO₂ (HT), WO₂, ZnF₂

- TiO_2 can also be found as anatase ($C5$) and brookite ($C21$).

Simple Tetragonal primitive vectors

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

a1 a2 a3



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(2a) Ti I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2a) Ti I
$\mathbf{B}_3$	$=$	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}}$	(4f) O I
$\mathbf{B}_4$	$=$	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}}$	(4f) O I
$\mathbf{B}_5$	$=$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f) O I
$\mathbf{B}_6$	$=$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f) O I

References

- [1] R. J. Swope, J. R. Smyth, and A. C. Larson, *H in rutile-type compounds: I. Single-crystal neutron and X-ray diffraction study of H in rutile*, Am. Mineral. **80**, 448–453 (1995).

Found in

- [1] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, New York, 1974).

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. 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