

Ti₄Co₂O Structure:

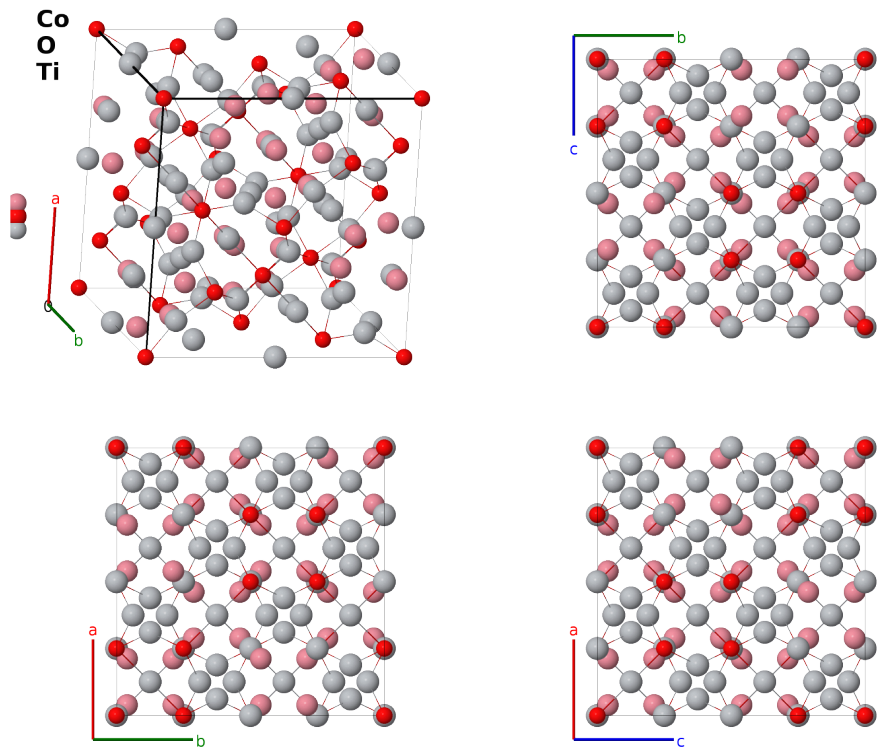
A2BC4_cF112_227_e_c_df-001

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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/U9R4>

https://aflow.org/prototype-encyclopedia/A2BC4_cF112_227_e_c_df-001



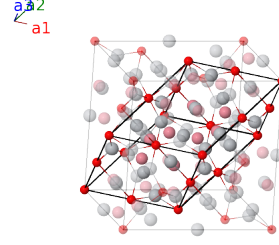
Prototype	Co ₂ OTi ₄
AFLOW prototype label	A2BC4_cF112_227_e_c_df-001
ICSD	139679
CCDC	2096554
Pearson symbol	cF112
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A2BC4_cF112_227_e_c_df-001</code> <code>--params=a, x₃, x₄</code>

- This is an ordered form of the η -carbide ($E9_3$) structure.

- AFLOW shifts the origin from the Ti I site to the O I site.

Face-centered Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(16c) O I
$\mathbf{B}_2$	$=$	$\frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}}$	(16c) O I
$\mathbf{B}_3$	$=$	$\frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16c) O I
$\mathbf{B}_4$	$=$	$\frac{1}{2}\mathbf{a}_1$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16c) O I
$\mathbf{B}_5$	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(16d) Ti I
$\mathbf{B}_6$	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(16d) Ti I
$\mathbf{B}_7$	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16d) Ti I
$\mathbf{B}_8$	$=$	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16d) Ti I
$\mathbf{B}_9$	$=$	$x_3\mathbf{a}_1 + x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$ax_3\hat{\mathbf{x}} + ax_3\hat{\mathbf{y}} + ax_3\hat{\mathbf{z}}$	(32e) Co I
$\mathbf{B}_{10}$	$=$	$x_3\mathbf{a}_1 + x_3\mathbf{a}_2 - (3x_3 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{4})\hat{\mathbf{x}} - a(x_3 - \frac{1}{4})\hat{\mathbf{y}} + ax_3\hat{\mathbf{z}}$	(32e) Co I
$\mathbf{B}_{11}$	$=$	$x_3\mathbf{a}_1 - (3x_3 - \frac{1}{2})\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{4})\hat{\mathbf{x}} + ax_3\hat{\mathbf{y}} - a(x_3 - \frac{1}{4})\hat{\mathbf{z}}$	(32e) Co I
$\mathbf{B}_{12}$	$=$	$-(3x_3 - \frac{1}{2})\mathbf{a}_1 + x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$ax_3\hat{\mathbf{x}} - a(x_3 - \frac{1}{4})\hat{\mathbf{y}} - a(x_3 - \frac{1}{4})\hat{\mathbf{z}}$	(32e) Co I
$\mathbf{B}_{13}$	$=$	$-x_3\mathbf{a}_1 - x_3\mathbf{a}_2 + (3x_3 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{4})\hat{\mathbf{x}} + a(x_3 + \frac{1}{4})\hat{\mathbf{y}} - ax_3\hat{\mathbf{z}}$	(32e) Co I
$\mathbf{B}_{14}$	$=$	$-x_3\mathbf{a}_1 - x_3\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$-ax_3\hat{\mathbf{x}} - ax_3\hat{\mathbf{y}} - ax_3\hat{\mathbf{z}}$	(32e) Co I
$\mathbf{B}_{15}$	$=$	$-x_3\mathbf{a}_1 + (3x_3 + \frac{1}{2})\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{4})\hat{\mathbf{x}} - ax_3\hat{\mathbf{y}} + a(x_3 + \frac{1}{4})\hat{\mathbf{z}}$	(32e) Co I
$\mathbf{B}_{16}$	$=$	$(3x_3 + \frac{1}{2})\mathbf{a}_1 - x_3\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$-ax_3\hat{\mathbf{x}} + a(x_3 + \frac{1}{4})\hat{\mathbf{y}} + a(x_3 + \frac{1}{4})\hat{\mathbf{z}}$	(32e) Co I
$\mathbf{B}_{17}$	$=$	$-(x_4 - \frac{1}{4})\mathbf{a}_1 + x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$ax_4\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(48f) Ti II
$\mathbf{B}_{18}$	$=$	$x_4\mathbf{a}_1 - (x_4 - \frac{1}{4})\mathbf{a}_2 - (x_4 - \frac{1}{4})\mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{4})\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(48f) Ti II
$\mathbf{B}_{19}$	$=$	$x_4\mathbf{a}_1 - (x_4 - \frac{1}{4})\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + ax_4\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(48f) Ti II
$\mathbf{B}_{20}$	$=$	$-(x_4 - \frac{1}{4})\mathbf{a}_1 + x_4\mathbf{a}_2 - (x_4 - \frac{1}{4})\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} - a(x_4 - \frac{1}{4})\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(48f) Ti II
$\mathbf{B}_{21}$	$=$	$x_4\mathbf{a}_1 + x_4\mathbf{a}_2 - (x_4 - \frac{1}{4})\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} + ax_4\hat{\mathbf{z}}$	(48f) Ti II
$\mathbf{B}_{22}$	$=$	$-(x_4 - \frac{1}{4})\mathbf{a}_1 - (x_4 - \frac{1}{4})\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} - a(x_4 - \frac{1}{4})\hat{\mathbf{z}}$	(48f) Ti II
$\mathbf{B}_{23}$	$=$	$(x_4 + \frac{3}{4})\mathbf{a}_1 - x_4\mathbf{a}_2 + (x_4 + \frac{3}{4})\mathbf{a}_3$	$=$	$\frac{3}{8}a\hat{\mathbf{x}} + a(x_4 + \frac{3}{4})\hat{\mathbf{y}} + \frac{3}{8}a\hat{\mathbf{z}}$	(48f) Ti II
$\mathbf{B}_{24}$	$=$	$-x_4\mathbf{a}_1 + (x_4 + \frac{3}{4})\mathbf{a}_2 - x_4\mathbf{a}_3$	$=$	$\frac{3}{8}a\hat{\mathbf{x}} - ax_4\hat{\mathbf{y}} + \frac{3}{8}a\hat{\mathbf{z}}$	(48f) Ti II
$\mathbf{B}_{25}$	$=$	$-x_4\mathbf{a}_1 + (x_4 + \frac{3}{4})\mathbf{a}_2 + (x_4 + \frac{3}{4})\mathbf{a}_3$	$=$	$a(x_4 + \frac{3}{4})\hat{\mathbf{x}} + \frac{3}{8}a\hat{\mathbf{y}} + \frac{3}{8}a\hat{\mathbf{z}}$	(48f) Ti II

$$\mathbf{B}_{26} = \left(x_4 + \frac{3}{4}\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3 = -ax_4 \hat{\mathbf{x}} + \frac{3}{8}a \hat{\mathbf{y}} + \frac{3}{8}a \hat{\mathbf{z}} \quad (48f) \quad \text{Ti II}$$

$$\mathbf{B}_{27} = -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(x_4 + \frac{3}{4}\right) \mathbf{a}_3 = \frac{3}{8}a \hat{\mathbf{x}} + \frac{3}{8}a \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}} \quad (48f) \quad \text{Ti II}$$

$$\mathbf{B}_{28} = \left(x_4 + \frac{3}{4}\right) \mathbf{a}_1 + \left(x_4 + \frac{3}{4}\right) \mathbf{a}_2 - x_4 \mathbf{a}_3 = \frac{3}{8}a \hat{\mathbf{x}} + \frac{3}{8}a \hat{\mathbf{y}} + a \left(x_4 + \frac{3}{4}\right) \hat{\mathbf{z}} \quad (48f) \quad \text{Ti II}$$

References

- [1] K. Ma, R. L., K. Gornicka, H. O. Jeschke, X. Zhang, Z. Guguchia, T. Klimczuk, and F. O. von Rohr, *Group-9 Transition-Metal Suboxides Adopting the Filled-Ti₂Ni Structure: A Class of Superconductors Exhibiting Exceptionally High Upper Critical Fields*, Chem. of Mater. **33**, 8722–8732 (2021), doi:10.1021/acs.chemmater.1c02683.

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