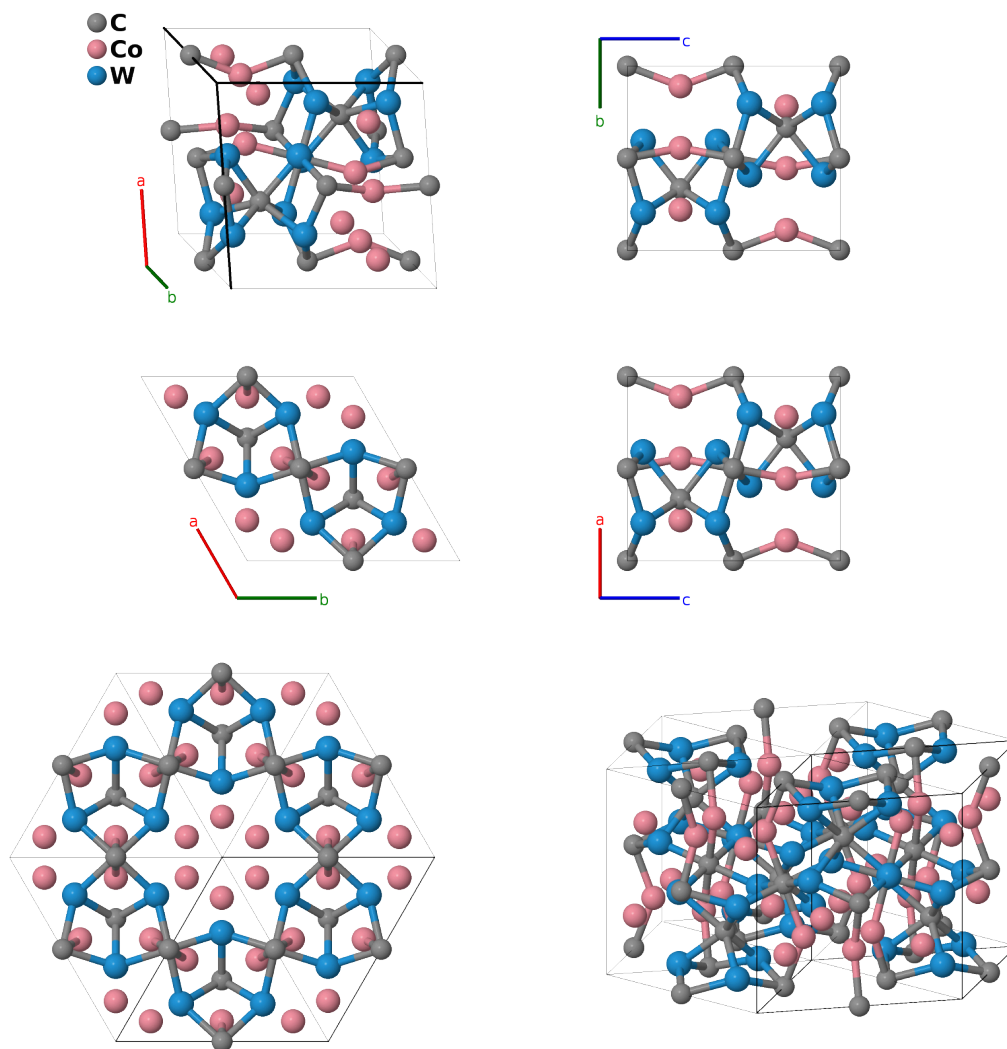


Co₃W₉C₄ Structure: A2B3C3_hP32_194_cg_2h_k-001

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<https://afLOW.org/p/JSHF>

https://afLOW.org/p/A2B3C3_hP32_194_cg_2h_k-001



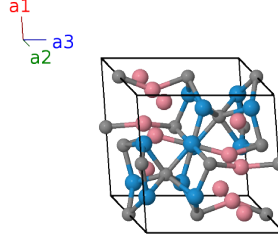
Prototype	C ₄ Co ₃ W ₉
AFLOW prototype label	A2B3C3_hP32_194_cg_2h_k-001
ICSD	16888
Pearson symbol	hP32
Space group number	194
Space group symbol	<i>P6₃/mmc</i>

AFLOW prototype command `aflow --proto=A2B3C3_hP32_194_cg_2h_k-001`
`--params=a, c/a, x3, x4, x5, z5`

- The (6h) sites we have labeled Co-I and Co-II are actually a 50-50 mixture of cobalt and tungsten, giving the observed $\text{Co}_3\text{W}_9\text{C}_4$ stoichiometry.

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c)	C I
\mathbf{B}_2	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c)	C I
\mathbf{B}_3	$= \frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}}$	(6g)	C II
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a \hat{\mathbf{y}}$	(6g)	C II
\mathbf{B}_5	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}}$	(6g)	C II
\mathbf{B}_6	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6g)	C II
\mathbf{B}_7	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6g)	C II
\mathbf{B}_8	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6g)	C II
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Co I
\mathbf{B}_{10}	$= -2x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Co I
\mathbf{B}_{11}	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Co I
\mathbf{B}_{12}	$= -x_3 \mathbf{a}_1 - 2x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Co I
\mathbf{B}_{13}	$= 2x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Co I
\mathbf{B}_{14}	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\sqrt{3}ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Co I
\mathbf{B}_{15}	$= x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Co II
\mathbf{B}_{16}	$= -2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Co II
\mathbf{B}_{17}	$= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Co II
\mathbf{B}_{18}	$= -x_4 \mathbf{a}_1 - 2x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Co II
\mathbf{B}_{19}	$= 2x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Co II
\mathbf{B}_{20}	$= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\sqrt{3}ax_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Co II
\mathbf{B}_{21}	$= x_5 \mathbf{a}_1 + 2x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{3}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(12k)	W I
\mathbf{B}_{22}	$= -2x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(12k)	W I
\mathbf{B}_{23}	$= x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-\sqrt{3}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(12k)	W I
\mathbf{B}_{24}	$= -x_5 \mathbf{a}_1 - 2x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	W I

$$\begin{aligned}
\mathbf{B}_{25} &= 2x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 &= \frac{3}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{W I} \\
\mathbf{B}_{26} &= -x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 &= \sqrt{3}ax_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{W I} \\
\mathbf{B}_{27} &= 2x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 &= \frac{3}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} &(12k) & \text{W I} \\
\mathbf{B}_{28} &= -x_5 \mathbf{a}_1 - 2x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 &= -\frac{3}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} &(12k) & \text{W I} \\
\mathbf{B}_{29} &= -x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 &= \sqrt{3}ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} &(12k) & \text{W I} \\
\mathbf{B}_{30} &= -2x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3 &= -\frac{3}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{W I} \\
\mathbf{B}_{31} &= x_5 \mathbf{a}_1 + 2x_5 \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3 &= \frac{3}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{W I} \\
\mathbf{B}_{32} &= x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3 &= -\sqrt{3}ax_5 \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{W I}
\end{aligned}$$

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