

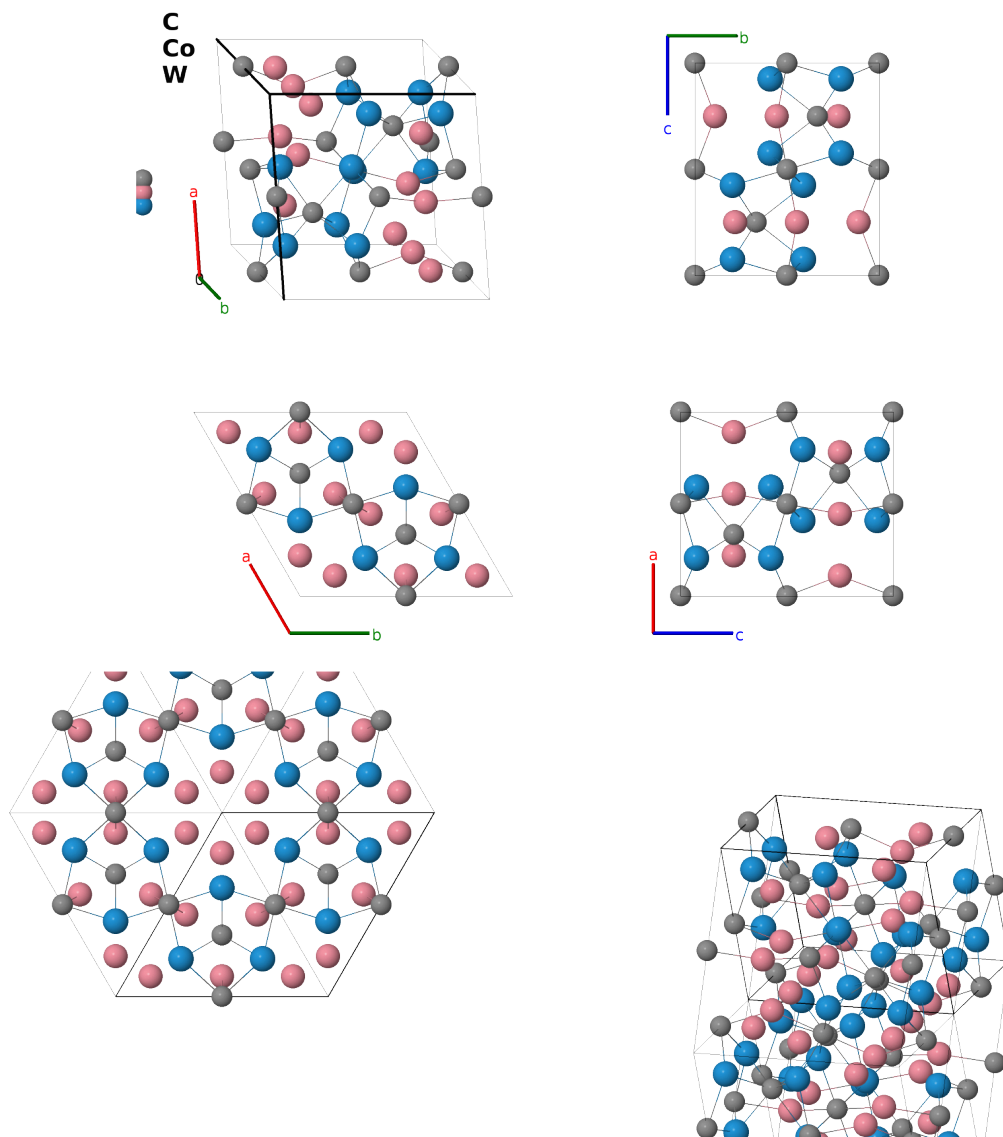
Co₃W₉C₄ Structure: A2B3C3_hP32_194_cg_2h_k-001

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

https://aflow.org/prototype-encyclopedia/A2B3C3_hP32_194_cg_2h_k-001



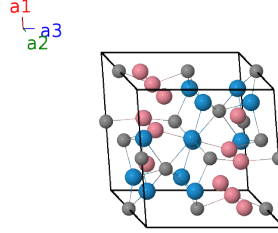
Prototype	C ₄ Co ₃ W ₉
AFLOW prototype label	A2B3C3_hP32_194_cg_2h_k-001
ICSD	16888
CCDC	1597407

Pearson symbol	hP32
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>aflow --proto=A2B3C3_hP32_194_cg_2h_k-001</code> <code>--params=a,c/a,x₃,x₄,x₅,z₅</code>

- 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

$$\begin{aligned}
\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) & \text{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) & \text{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) & \text{W I} \\
\mathbf{B}_{24} &= -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}_{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}$$

References

- [1] N. Schönberg, *The Structure of the $\text{Co}_3\text{W}_9\text{C}_4$ Phase*, Acta Metall. **2**, 837–840 (1954), doi:10.1016/0001-6160(54)90037-1.

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- [1] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys, Volume 2, International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 8 (Pergamon Press, Oxford, London, Edinburgh, New York, Toronto, Sydney, Paris, Braunschweig, 1967).

First cited in

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