

VCo₃ Structure:

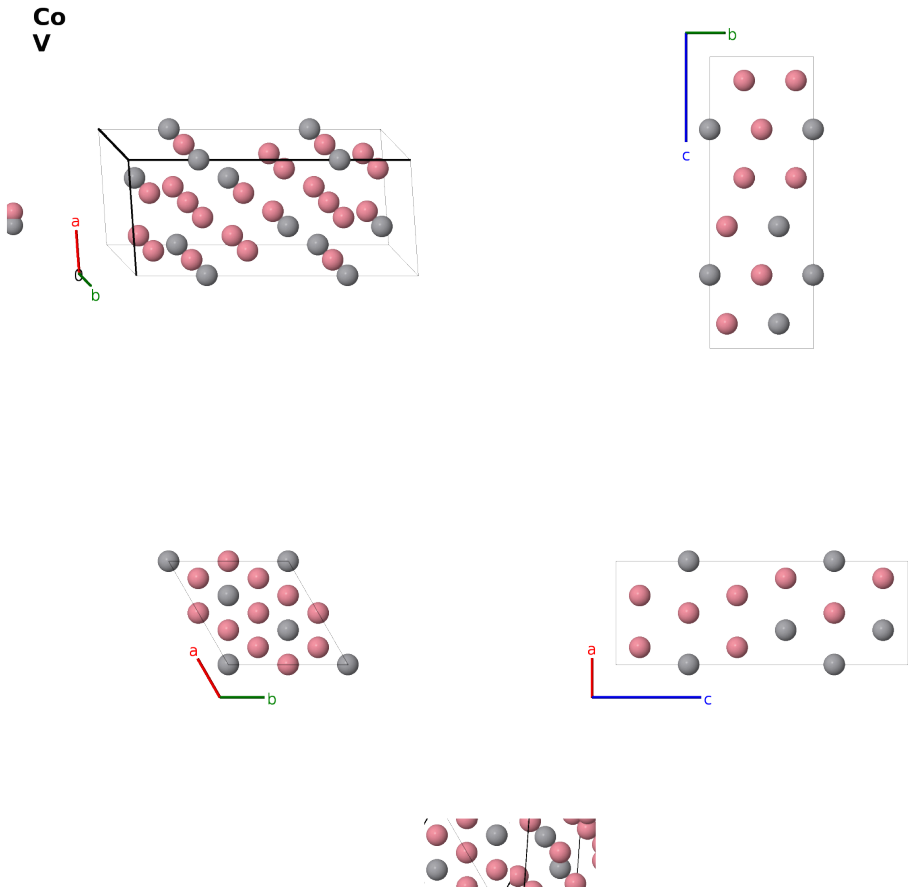
A3B_hP24_194_hk_bf-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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/XEL5>

https://aflow.org/prototype-encyclopedia/A3B_hP24_194_hk_bf-001



Prototype	Co ₃ V
AFLOW prototype label	A3B_hP24_194_hk_bf-001
ICSD	102718
CCDC	1660688
Pearson symbol	hP24
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>aflow --proto=A3B_hP24_194_hk_bf-001</code> <code>--params=a, c/a, z₂, x₃, x₄, z₄</code>

Other compounds with this structure

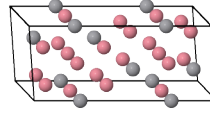
NbRh₃

- (Saito, 1959) states that this is the hexagonal analog of the cubic Cu₃Au (*L*₁₂) structure. He placed it in space group *P* $\bar{6}m2$ #187, but (Cenzual, 1991) showed that the given structure actually is in space group *P*6₃/*mmc* #194.
- VCo₃ and hexagonal PuAl₃ have the same AFLOW prototype label, A3B_hP24_194_hk_bf. They are generated by the same symmetry operations with different sets of parameters (**--params**) specified in their corresponding CIF files.

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
$\mathbf{B}_1$	$= \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}c\hat{\mathbf{z}}$	(2b)	V I
$\mathbf{B}_2$	$= \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}c\hat{\mathbf{z}}$	(2b)	V I
$\mathbf{B}_3$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + z_2\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(4f)	V II
$\mathbf{B}_4$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + (z_2 + \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + c(z_2 + \frac{1}{2})\hat{\mathbf{z}}$	(4f)	V II
$\mathbf{B}_5$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 - z_2\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - cz_2\hat{\mathbf{z}}$	(4f)	V II
$\mathbf{B}_6$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 - (z_2 - \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - c(z_2 - \frac{1}{2})\hat{\mathbf{z}}$	(4f)	V II
$\mathbf{B}_7$	$= x_3\mathbf{a}_1 + 2x_3\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{3}{2}ax_3\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(6h)	Co I
$\mathbf{B}_8$	$= -2x_3\mathbf{a}_1 - x_3\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_3\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(6h)	Co I
$\mathbf{B}_9$	$= x_3\mathbf{a}_1 - x_3\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$-\sqrt{3}ax_3\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(6h)	Co I
$\mathbf{B}_{10}$	$= -x_3\mathbf{a}_1 - 2x_3\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_3\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(6h)	Co I
$\mathbf{B}_{11}$	$= 2x_3\mathbf{a}_1 + x_3\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{2}ax_3\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(6h)	Co I
$\mathbf{B}_{12}$	$= -x_3\mathbf{a}_1 + x_3\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\sqrt{3}ax_3\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(6h)	Co I
$\mathbf{B}_{13}$	$= x_4\mathbf{a}_1 + 2x_4\mathbf{a}_2 + z_4\mathbf{a}_3$	$=$	$\frac{3}{2}ax_4\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(12k)	Co II
$\mathbf{B}_{14}$	$= -2x_4\mathbf{a}_1 - x_4\mathbf{a}_2 + z_4\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(12k)	Co II
$\mathbf{B}_{15}$	$= x_4\mathbf{a}_1 - x_4\mathbf{a}_2 + z_4\mathbf{a}_3$	$=$	$-\sqrt{3}ax_4\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(12k)	Co II
$\mathbf{B}_{16}$	$= -x_4\mathbf{a}_1 - 2x_4\mathbf{a}_2 + (z_4 + \frac{1}{2})\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\hat{\mathbf{y}} + c(z_4 + \frac{1}{2})\hat{\mathbf{z}}$	(12k)	Co II
$\mathbf{B}_{17}$	$= 2x_4\mathbf{a}_1 + x_4\mathbf{a}_2 + (z_4 + \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{3}{2}ax_4\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\hat{\mathbf{y}} + c(z_4 + \frac{1}{2})\hat{\mathbf{z}}$	(12k)	Co II
$\mathbf{B}_{18}$	$= -x_4\mathbf{a}_1 + x_4\mathbf{a}_2 + (z_4 + \frac{1}{2})\mathbf{a}_3$	$=$	$\sqrt{3}ax_4\hat{\mathbf{y}} + c(z_4 + \frac{1}{2})\hat{\mathbf{z}}$	(12k)	Co II
$\mathbf{B}_{19}$	$= 2x_4\mathbf{a}_1 + x_4\mathbf{a}_2 - z_4\mathbf{a}_3$	$=$	$\frac{3}{2}ax_4\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\hat{\mathbf{y}} - cz_4\hat{\mathbf{z}}$	(12k)	Co II
$\mathbf{B}_{20}$	$= -x_4\mathbf{a}_1 - 2x_4\mathbf{a}_2 - z_4\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\hat{\mathbf{y}} - cz_4\hat{\mathbf{z}}$	(12k)	Co II
$\mathbf{B}_{21}$	$= -x_4\mathbf{a}_1 + x_4\mathbf{a}_2 - z_4\mathbf{a}_3$	$=$	$\sqrt{3}ax_4\hat{\mathbf{y}} - cz_4\hat{\mathbf{z}}$	(12k)	Co II

$$\mathbf{B}_{22} = -2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 = -\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} \quad (12k) \quad \text{Co II}$$

$$\mathbf{B}_{23} = x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 = \frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} \quad (12k) \quad \text{Co II}$$

$$\mathbf{B}_{24} = x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 = -\sqrt{3}ax_4 \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} \quad (12k) \quad \text{Co II}$$

References

- [1] S. Saito, *The Crystal Structure of VCo₃*, Acta Cryst. **12**, 500–502 (1959), doi:10.1107/S0365110X59001517.

Found in

- [1] K. Cenzual, L. M. Gelato, M. Penzo, and E. Parthé, *Inorganic structure types with revised space groups. I*, Acta Crystallogr. Sect. B **47**, 433–439 (1991), doi:10.1107/S0108768191000903.

First cited in

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