

CoNb₃S₆ Structure:

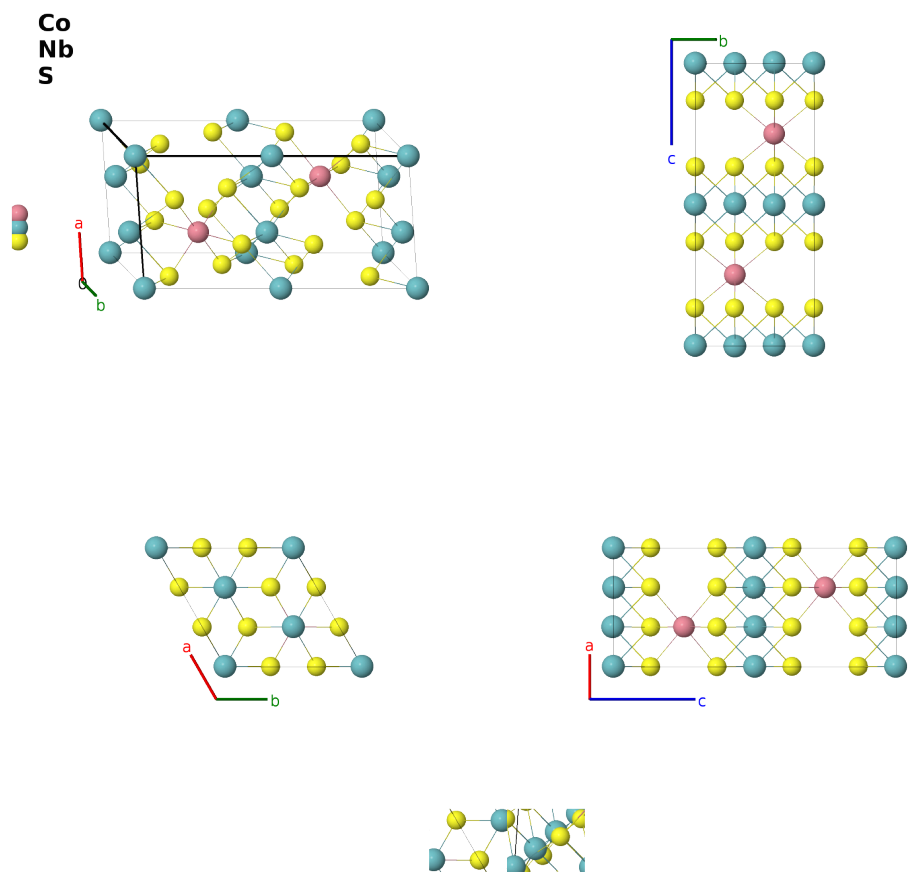
AB3C6_hP20_182_c_af_i-001

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<https://aflow.org/prototype-encyclopedia/A0VJ>

https://aflow.org/prototype-encyclopedia/AB3C6_hP20_182_c_af_i-001



Prototype	CoNb ₃ S ₆
AFLOW prototype label	AB3C6_hP20_182_c_af_i-001
ICSD	42688
CCDC	1612329
Pearson symbol	hP20
Space group number	182
Space group symbol	$P6_322$
AFLOW prototype command	<pre>aflow --proto=AB3C6_hP20_182_c_af_i-001 --params=a, c/a, z₃, x₄, y₄, z₄</pre>

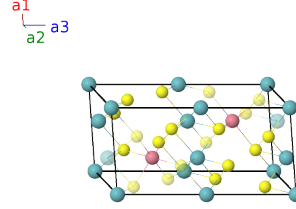
Other compounds with this structure

CoNb₃S₆, CoTa₃S₆, CrNb₃S₆, FeNb₃S₆ (edgarite), FeTa₃S₆, FeZr₃S₆, MnNb₃S₆, NiNb₃S₆, NiNb₃Se₆, NiTa₃S₆, NiTa₃Se₆, PbNb₃S₆, PbTa₃S₆, SnNb₃S₆, SnTa₃S₆, TaNb₃S₆, TiNb₃S₆, TiNb₃Se₆, VNb₃S₆

- In many cases the (2c) site is not completely occupied.
- See the discussion about the possible difference in structure between natural and synthetic edgarite, FeNb₃S₆.
- The ICSD uses FeNb₃S₆ as the prototype for both structures. Here we use CoNb₃S₆ to distinguish between the two cases.

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
$\mathbf{B}_1$	$= 0$	$=$	0	(2a)	Nb I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(2a)	Nb I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c)	Co I
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c)	Co I
$\mathbf{B}_5$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4f)	Nb II
$\mathbf{B}_6$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Nb II
$\mathbf{B}_7$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4f)	Nb II
$\mathbf{B}_8$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Nb II
$\mathbf{B}_9$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(12i)	S I
$\mathbf{B}_{10}$	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(12i)	S I
$\mathbf{B}_{11}$	$= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(12i)	S I
$\mathbf{B}_{12}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(12i)	S I
$\mathbf{B}_{13}$	$= y_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(12i)	S I
$\mathbf{B}_{14}$	$= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(12i)	S I
$\mathbf{B}_{15}$	$= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(12i)	S I
$\mathbf{B}_{16}$	$= (x_4 - y_4) \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(12i)	S I
$\mathbf{B}_{17}$	$= -x_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(12i)	S I
$\mathbf{B}_{18}$	$= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(12i)	S I

$$\mathbf{B}_{19} = \begin{matrix} -(x_4 - y_4) \mathbf{a}_1 + y_4 \mathbf{a}_2 - \\ (z_4 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}} \quad (12i) \quad \text{S I}$$

$$\mathbf{B}_{20} = x_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}} \quad (12i) \quad \text{S I}$$

References

- [1] K. Anzenhofer, J. M. V. D. Berg, P. Cossee, and J. N. Helle, *The crystal structure and magnetic susceptibilities of $MnNb_3S_6$, $FeNb_3S_6$, $CoNb_3S_6$ and $NiNb_3S_6$* , J. Phys. Chem. Solids **31**, 1057–1067 (1970), doi:10.1016/0022-3697(70)90315-X.

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