

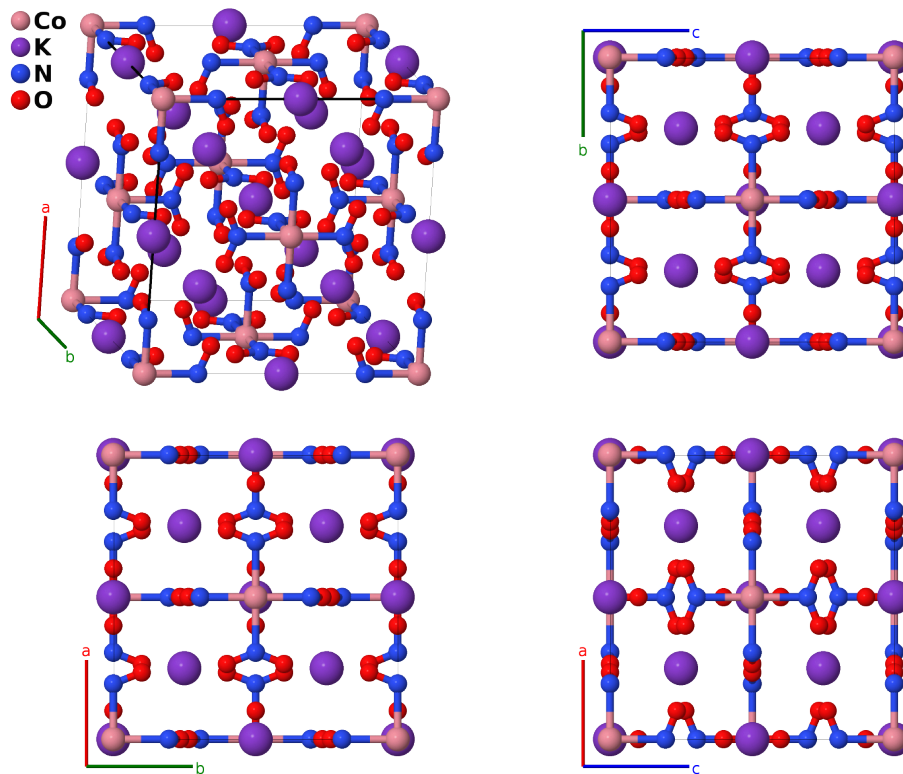
$K_3Co(NO_2)_6$ ($J2_4$) Structure: AB3C6D12_cF88_202_a_bc_e_h-001

This structure originally had the label AB3C6D12_cF88_202_a_bc_e_h. Calls to that address will be redirected here.

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<https://afLOW.org/p/G8R0>

https://afLOW.org/p/AB3C6D12_cF88_202_a_bc_e_h-001



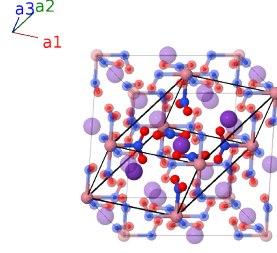
Prototype	$CoK_3N_6O_{12}$
AFLOW prototype label	AB3C6D12_cF88_202_a_bc_e_h-001
<i>Strukturbericht</i> designation	$J2_4$
ICSD	26746
Pearson symbol	cF88
Space group number	202
Space group symbol	$Fm\bar{3}$
AFLOW prototype command	<code>afLOW --proto=AB3C6D12_cF88_202_a_bc_e_h-001 --params=a, x4, y5, z5</code>

Other compounds with this structure

$(\text{NH}_4)_2\text{AgBi}(\text{NO}_2)_6$, $(\text{NH}_4)_2\text{LiBi}(\text{NO}_2)_6$, $(\text{NH}_4)_2\text{NaBi}(\text{NO}_2)_6$, $(\text{NH}_4)_2\text{NaCo}(\text{NO}_2)_6$, $(\text{NH}_4)_2\text{NaRh}(\text{NO}_2)_6$, $(\text{NH}_4)_3\text{Co}(\text{NO}_2)_6$, $\text{Cs}_2\text{AgBi}(\text{NO}_2)_6$, $\text{Cs}_2\text{LiBi}(\text{NO}_2)_6$, $\text{Cs}_2\text{NaBi}(\text{NO}_2)_6$, $\text{Cs}_3\text{Bi}(\text{NO}_2)_6$, $\text{K}_2\text{LiBi}(\text{NO}_2)_6$, $\text{K}_2\text{NaBi}(\text{NO}_2)_6$, $\text{K}_2\text{NaCo}(\text{NO}_2)_6$, $\text{K}_2\text{PbCu}(\text{NO}_2)_6$, $\text{K}_3\text{Ca}(\text{NO}_2)_6$, $\text{Rb}_2\text{AgBi}(\text{NO}_2)_6$, $\text{Rb}_2\text{NaBi}(\text{NO}_2)_6$, $\text{Tl}_2\text{AgBi}(\text{NO}_2)_6$, $\text{Tl}_2\text{LiBi}(\text{NO}_2)_6$, $\text{Tl}_2\text{NaBi}(\text{NO}_2)_6$

Face-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	$=$	0	(4a)	Co I
\mathbf{B}_2	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{y} + \frac{1}{2}a\hat{z}$	(4b)	K I
\mathbf{B}_3	$\frac{1}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{x} + \frac{1}{4}a\hat{y} + \frac{1}{4}a\hat{z}$	(8c)	K II
\mathbf{B}_4	$\frac{3}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}a\hat{x} + \frac{3}{4}a\hat{y} + \frac{3}{4}a\hat{z}$	(8c)	K II
\mathbf{B}_5	$-x_4\mathbf{a}_1 + x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$ax_4\hat{x}$	(24e)	N I
\mathbf{B}_6	$x_4\mathbf{a}_1 - x_4\mathbf{a}_2 - x_4\mathbf{a}_3$	$=$	$-ax_4\hat{x}$	(24e)	N I
\mathbf{B}_7	$x_4\mathbf{a}_1 - x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$ax_4\hat{y}$	(24e)	N I
\mathbf{B}_8	$-x_4\mathbf{a}_1 + x_4\mathbf{a}_2 - x_4\mathbf{a}_3$	$=$	$-ax_4\hat{y}$	(24e)	N I
\mathbf{B}_9	$x_4\mathbf{a}_1 + x_4\mathbf{a}_2 - x_4\mathbf{a}_3$	$=$	$ax_4\hat{z}$	(24e)	N I
\mathbf{B}_{10}	$-x_4\mathbf{a}_1 - x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$-ax_4\hat{z}$	(24e)	N I
\mathbf{B}_{11}	$(y_5 + z_5)\mathbf{a}_1 - (y_5 - z_5)\mathbf{a}_2 + (y_5 - z_5)\mathbf{a}_3$	$=$	$ay_5\hat{y} + az_5\hat{z}$	(48h)	O I
\mathbf{B}_{12}	$-(y_5 - z_5)\mathbf{a}_1 + (y_5 + z_5)\mathbf{a}_2 - (y_5 + z_5)\mathbf{a}_3$	$=$	$-ay_5\hat{y} + az_5\hat{z}$	(48h)	O I
\mathbf{B}_{13}	$(y_5 - z_5)\mathbf{a}_1 - (y_5 + z_5)\mathbf{a}_2 + (y_5 + z_5)\mathbf{a}_3$	$=$	$ay_5\hat{y} - az_5\hat{z}$	(48h)	O I
\mathbf{B}_{14}	$-(y_5 + z_5)\mathbf{a}_1 + (y_5 - z_5)\mathbf{a}_2 - (y_5 - z_5)\mathbf{a}_3$	$=$	$-ay_5\hat{y} - az_5\hat{z}$	(48h)	O I
\mathbf{B}_{15}	$(y_5 - z_5)\mathbf{a}_1 + (y_5 + z_5)\mathbf{a}_2 - (y_5 - z_5)\mathbf{a}_3$	$=$	$az_5\hat{x} + ay_5\hat{z}$	(48h)	O I
\mathbf{B}_{16}	$-(y_5 + z_5)\mathbf{a}_1 - (y_5 - z_5)\mathbf{a}_2 + (y_5 + z_5)\mathbf{a}_3$	$=$	$az_5\hat{x} - ay_5\hat{z}$	(48h)	O I
\mathbf{B}_{17}	$(y_5 + z_5)\mathbf{a}_1 + (y_5 - z_5)\mathbf{a}_2 - (y_5 + z_5)\mathbf{a}_3$	$=$	$-az_5\hat{x} + ay_5\hat{z}$	(48h)	O I
\mathbf{B}_{18}	$-(y_5 - z_5)\mathbf{a}_1 - (y_5 + z_5)\mathbf{a}_2 + (y_5 - z_5)\mathbf{a}_3$	$=$	$-az_5\hat{x} - ay_5\hat{z}$	(48h)	O I
\mathbf{B}_{19}	$-(y_5 - z_5)\mathbf{a}_1 + (y_5 - z_5)\mathbf{a}_2 + (y_5 + z_5)\mathbf{a}_3$	$=$	$ay_5\hat{x} + az_5\hat{y}$	(48h)	O I

$$\mathbf{B}_{20} = \begin{matrix} (y_5 + z_5) \mathbf{a}_1 - (y_5 + z_5) \mathbf{a}_2 - \\ (y_5 - z_5) \mathbf{a}_3 \end{matrix} = -ay_5 \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}} \quad (48h) \quad \text{O I}$$

$$\mathbf{B}_{21} = \begin{matrix} -(y_5 + z_5) \mathbf{a}_1 + (y_5 + z_5) \mathbf{a}_2 + \\ (y_5 - z_5) \mathbf{a}_3 \end{matrix} = ay_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} \quad (48h) \quad \text{O I}$$

$$\mathbf{B}_{22} = \begin{matrix} (y_5 - z_5) \mathbf{a}_1 - (y_5 - z_5) \mathbf{a}_2 - \\ (y_5 + z_5) \mathbf{a}_3 \end{matrix} = -ay_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} \quad (48h) \quad \text{O I}$$

References

- [1] M. van Driel and H. J. Verweel, *Über die Struktur der Tripelnitrite*, Z Kristallogr. **35**, 308–314 (1936), doi:10.1524/zkri.1936.95.1.308.

Found in

- [1] C. Gottfried, ed., *Strukturbericht Band IV 1936* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1938).