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catena-Poly[[dimethanolcobalt(II)]-di-μ-1,5-dicyanamido]

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Key indicators

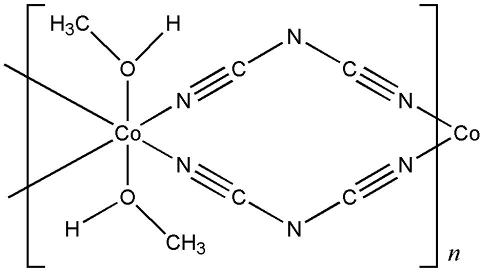
Single-crystal X-ray study
T = 293 K
Mean σ(N–C) = 0.002 Å
R factor = 0.027
wR factor = 0.075
Data-to-parameter ratio = 10.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

A pair of L-shaped dicyanamide anions link the dimethanolcobalt(II) units into a one-dimensional ribbon running along the b axis of the monoclinic crystal structure of the title compound, $[Co(C_2N_3)_2(CH_4O)_2]_n$. The Co atom occupies a special position of $2/m$ symmetry and the C_2N_3 unit lies on a mirror plane. The coordination polyhedron of the Co atom is a slightly distorted octahedron.

Comment

The dicyanamide anion, $[N(CN)_2]^-$ (dca), is a versatile building block for the synthesis of a range of metal-organic coordination polymers owing to its capacity for binding to metal atoms in different modes and stabilizing high-spin states (Miller & Manson, 2001; Batten & Murray, 2003). The polymeric dicyanamide complexes possess interesting magnetic properties and unusual coordination architectures. A number of one-, two- and three-dimensional coordination polymers with different structural features have been reported, such as one-dimensional $[M(\mathrm{dca})_2L]$ chains (L = neutral terminal ligand; Manson *et al.*, 1999; Tong, Zhou *et al.*, 2003), two-dimensional β-$M(\mathrm{dca})_2$ sheets and three-dimensional rutile-like α-$M(\mathrm{dca})_2$ networks (Miller & Manson, 2001). We recently reported a series of structures of benzyltrialkylammonium tris(dicyanamido)metalates, $[C_6H_5CH_2NR_3]$-$[M(\mathrm{dca})_3]$ (R = n-C_4H_9, M = Mn and Co; R = C_2H_5, M = Mn and Fe; Tong, Ru *et al.*, 2003), which exhibit μ-dca bridged three-dimensional architectures of the α-Po-like type.



(I)

The title compound, (I), the bis-MeOH adduct of $Co(\mathrm{dca})_2$, forms one-dimensional chains in its crystal structure (Fig. 1), similar to that of $[Co(\mathrm{dca})_2(\mathrm{DMF})_2]$ (Tong, Zhou *et al.*, 2003). The Co center resides on the twofold axis along b. The Co atom has a slightly distorted CoN_4O_2 octahedral environment formed by four N atoms belonging to four different dca groups [Co—N = 2.1149 (18) Å] and two *trans*-coordinated O atoms of two MeOH ligands [Co—O = 2.070 (2) Å]. A pair of dca bridges link the Co centers, affording rigid one-dimensional ribbons parallel to the crystallographic b axis. Adjacent chains are held together by an interchain hydrogen bond of the O—H···N type (Table 1), resulting in interesting extended two-dimensional stair-like layers (Fig. 2). The title compound is isostructural with the reported manganese(II) and iron(II) analogs, $[M(\mathrm{dca})_2(\mathrm{CH_3OH})_2]$ (M = Mn and Fe; Manson *et al.*, 1999; Batten *et al.*, 1999).

Experimental

Cobalt(II) chloride (0.12 g, 0.5 mmol) and sodium dicyanamide (0.09 g, 1.0 mmol) were added to methanol (15 ml) and the mixture was heated until the reagents dissolved. Pink crystals separated from the solution in about 75% yield after 5 d.

Crystal data

$[\mathrm{Co(C_2N_3)_2(CH_4O)_2}]$
$M_r = 255.11$
Monoclinic, $C2/m$
$a = 12.356$ (4) Å
$b = 7.309$ (2) Å
$c = 6.508$ (2) Å
$\beta = 120.796$ (5)°
$V = 504.9$ (3) Å^3
$Z = 2$
$D_x = 1.678$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 276 reflections
$\theta = 3.4$–26.0°
$\mu = 1.69$ mm^{-1}
$T = 293$ (2) K
Prism, pink
0.34 × 0.30 × 0.21 mm

Data collection

Rigaku Mercury CCD diffractometer
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2002)
$T_{\min} = 0.569$, $T_{\max} = 0.701$
989 measured reflections
531 independent reflections
522 reflections with $I > 2\sigma(I)$
$R_{\mathrm{int}} = 0.012$
$\theta_{\max} = 26.0°$
$h = -15 \rightarrow 5$
$k = -6 \rightarrow 8$
$l = -5 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.075$
$S = 1.20$
531 reflections
51 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0477P)^2 + 0.1136P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.57$ e Å^{-3}
$\Delta\rho_{\min} = -0.30$ e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2$^{\mathrm{i}}$	0.842 (10)	1.952 (12)	2.788 (3)	172 (3)

Symmetry code: (i) $\frac{1}{2}-x, \frac{1}{2}-y, 1-z$.

The diffraction data were of sufficiently high quality to allow for the refinement of the H atoms. These were refined subject to restraints of C—H = 0.95 (1) Å and O—H = 0.85 (1) Å; for the methyl groups, the H···H distance was restrained to 1.50 (1) Å.

Data collection: *CrystalClear* (Rigaku, 2002); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

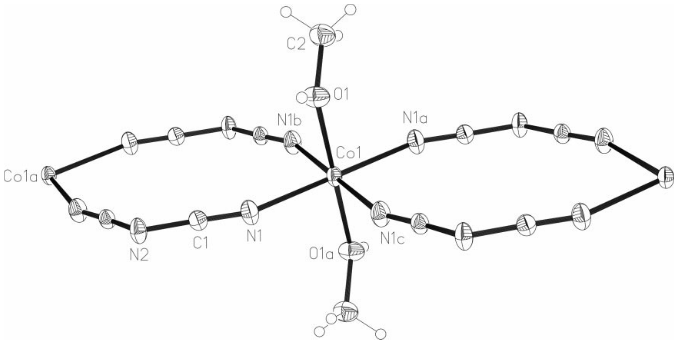


Figure 1
ORTEP (Johnson, 1976) plot depicting a fragment of the structure. Displacement ellipsoids are plotted at the 50% probability level; H atoms are shown as small spheres of arbitrary radii. [Symmetry codes: (*a*) $1-x, -y, 2-z$; (*b*) $1-x, y, 2-z$; (*c*) $x, -y, z$.]

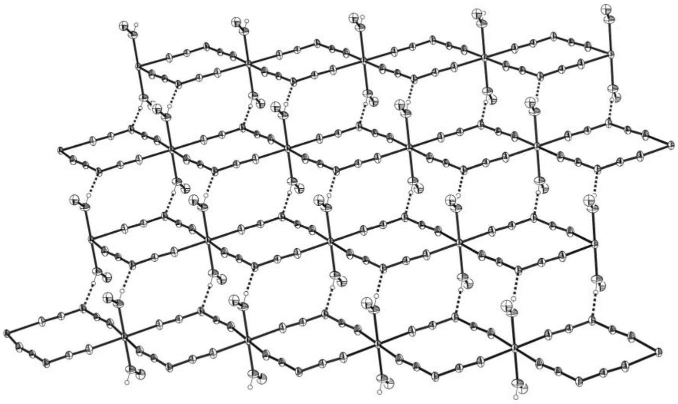


Figure 2
ORTEP (Johnson, 1976) plot of the hydrogen-bonded layer structure.

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