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catena-Poly[[bis(*N*,*N*-dimethylformamide)-cobalt(II)]-di-μ-1,5-dicyanamido]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(N–C) = 0.005 Å
R factor = 0.029
wR factor = 0.087
Data-to-parameter ratio = 11.6

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

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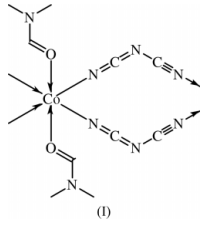
A pair of L-shaped dicyanamide anions link the bis(*N*,*N*-dimethylformamide)cobalt(II) units into a linear chain running along the *b* axis of the monoclinic crystal of $(C_2N_3)_2(DMF)_2Co$. The Co atom and the dicyanamido bridging ligand occupy special positions of symmetry 2/*m* and *m*, respectively. The coordination polyhedron of the Co atom is close to a regular octahedron.

Comment

Owing to its capacity for binding to metal atoms in different modes, the dicyanamide anion, $[N(CN)_2]^-$ (dca), is an excellent building block for the synthesis of a wide range of metal complexes. Polymeric dicyanamido complexes possess interesting magnetic properties and unusual coordination architectures (Miller & Manson, 2001). A number of one-, two- and three-dimensional coordination polymers featuring various structural motifs have been reported. One-dimensional $[M(dca)_2L]$ chains (L = neutral terminal or chelating ligand) (Manson *et al.*, 1999; Vangdal *et al.*, 2002), two-dimensional β-$M(dca)_2$ sheets and three-dimensional rutile-like α-$M(dca)_2$ networks (Miller & Manson, 2001), along with other motifs (Gao *et al.*, 2002; Shi *et al.*, 2002; Yeung *et al.*, 2002) may be mentioned as a few examples. The recently published structures of benzyltrialkylammonium tris(dicyanamido)metalates, $[C_6H_5CH_2NR_3][M(dca)_3]$ ($R = n$-C_4H_9, M = Mn, Co; $R = C_2H_5$, M = Mn, Fe) (Tong *et al.*, 2003), exhibit a three-dimensional architecture based on a cubic network of $[MN_6]$ coordination octahedra, following the motif of the α-Po type, and bridged by the dca ligand.



(I)

In the title compound, (I), the bis-DMF adduct of $Co(dca)_2$ forms one-dimensional chains in the crystal structure (Fig. 1). The Co atom lies at the 2*c* Wyckoff position ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$) of site symmetry 2/*m*. The dca occupies a special position across the mirror plane (Wyckoff 4*i*). The Co atom has an octahedral environment, formed by four N atoms belonging to four different dca groups [Co1—N1 2.123 (2) Å] and two O atoms of two DMF ligands [Co1—O1 2.096 (2) Å]; the DMF ligands, in compliance with symmetry requirements, are *trans* to each

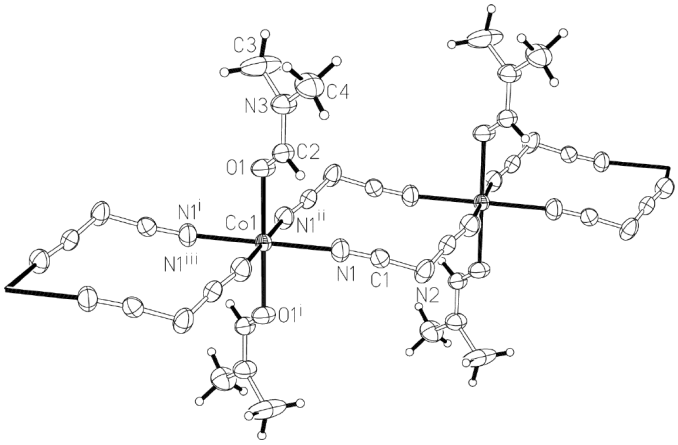


Figure 1
*ORTEP*II (Johnson, 1976) plot depicting a fragment of the structure. Displacement ellipsoids are drawn at the 50% probability level; H atoms are shown as small spheres of arbitrary radii. [Symmetry codes: (i) $1-x$, $1-y$, $1-z$; (ii) $1-x$, y, $1-z$; (iii) x, $1-y$, z.]

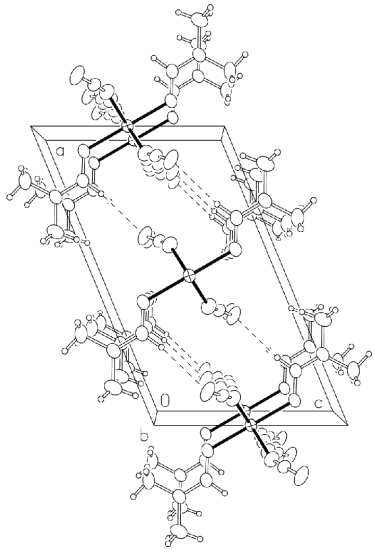


Figure 2
ORTEP (Johnson, 1976) plot of the hydrogen-bonded layer structure.

other. Adjacent chains are held together by a weak C—H···N hydrogen bond, forming layers parallel to the *ab* plane (Fig. 2; Table 2).

Experimental

Cobalt(II) chloride (0.12 g, 0.5 mmol) and sodium dicyanamide (0.09 g, 1.0 mmol) were placed in a 10:1 *v*/*v* methanol/DMF mixture and the solution was heated until the reagents dissolved. Polyhedral crystals separated from the solution in about 80% yield after 10 d.

Crystal data

$[Co(C_2N_3)(C_3H_7NO)_2]$
M_r = 337.22
Monoclinic, $C2/m$
a = 13.525 (4) Å
b = 7.383 (2) Å
c = 8.094 (3) Å
β = 112.399 (5)°
V = 747.3 (4) Å^3
Z = 2
D_x = 1.499 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 282 reflections
θ = 3.3–27.5°
μ = 1.17 mm^{-1}
T = 293 (2) K
Block, pink
0.42 × 0.36 × 0.30 mm

Data collection

Rigaku Mercury CCD diffractometer
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2002)
T_{min} = 0.528, T_{max} = 0.721
2432 measured reflections
878 independent reflections
847 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 27.5°
$h = -17 \rightarrow 12$
$k = -9 \rightarrow 9$
$l = -9 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.087
S = 1.06
878 reflections
76 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0676P)^2 + 0.0203P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.096 (2)	N2—C1	1.305 (2)
Co1—N1	2.123 (2)	N3—C2	1.318 (3)
O1—C2	1.235 (3)	N3—C3	1.446 (4)
N1—C1	1.147 (2)	N3—C4	1.455 (4)
O1—Co1—N1	91.6 (1)	N1—Co1—N1^{ii}	88.0 (1)
O1—Co1—N1^{ii}	88.5 (1)		

Symmetry code: (ii) $1-x, y, 1-z$.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···N2^{iv}	0.94 (1)	2.53 (1)	3.464 (3)	172 (3)

Symmetry code: (iv) $\frac{3}{2}-x, \frac{3}{2}-y, 1-z$.

The diffraction data were of sufficiently high quality to allow for the refinement of the H atoms, subject to bond-length restraints of C—H = 0.95 (1) Å for the methyl groups, with the H···H distance 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.

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