Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

A novel heptacoordinated cobalt(II) complex of 6,7-dicyanodipyridoquinoxaline (dcdpq): $[Co(NO_3)_2(CH_3CN)(dcdpq)]$

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Received 9 January 2001
Accepted 5 February 2001
Online 13 February 2001

Key indicators

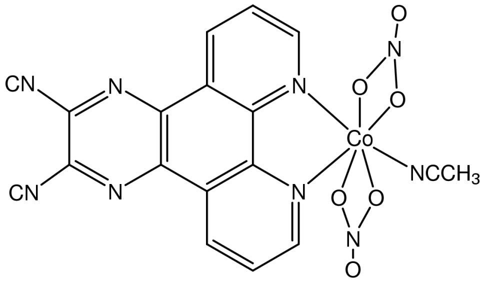
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.028
wR factor = 0.070
Data-to-parameter ratio = 11.1

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

The title complex, (acetonitrile)(6,7-dicyanodipyrido[3,2-*f*;-2,3-*h*]quinoxine)dinitrocobalt(II), $[Co(NO_3)_2(C_2H_3N)(C_{16}H_6N_6)]$, crystallizes in the monoclinic system with space group $P2_1$. The Co^{II} center is heptacoordinated by two N atoms of the pyridine moieties, four O atoms of two nitrate anions and one N atom of a CH_3CN molecule. The crystal structure reveals that the CoN_3O_4 coordination sphere has a distorted pentagonal-bipyramid geometry.

Comment

Polypyridyl ligands and their transition metal complexes have attracted great interest due to their potential as building blocks for supramolecular assemblies and ability to functionalize as optical sensors and probes for nucleic acid (Arkin *et al.*, 1996; Holmlin *et al.*, 1999). In recent years, ligands derived from appropriate modification of dipyrido[3,2-*a*:2′,3′-*c*]-phenazine (dppz) have been employed in order to suit those applications. However, most of the studies of this type of ligand have focused on metal centers such as Ru^{II} (Arounaguiri & Maiya, 1999), Os^{II} (Holmlin & Barton, 1995) and Re^{I} (Yam *et al.*, 1997), and studies on Cu^{II}, Co^{II} and Ni^{II} are still quite rare. As part of our effort to develop new functional complexes with such ligands, we report herein the crystal structure of a novel heptacoordinated Co^{II} complex, (I), with 6,7-dicyanodipyridoquinoxine (dcdpq).



(I)

Complex (I) is a neutral molecule due to the two coordinated nitrate anions (Fig. 1). The Co^{II} center has the unexpected heptacoordinated distorted pentagonal-bipyramid coordination geometry, consisting of two N atoms of the pyridine rings, four O atoms of two nitrate anions and an N atom of a CH_3CN molecule. Two N atoms of one pyridine ring, N1 and the CH_3CN molecule, N7, occupy the axial positions. The Co atom lies approximately in the pentagonal least-squares plane defined by N2, O1, O2, O4 and O5, deviating by 0.081 Å from the plane. Neither cyano group is coordinated to a Co atom. No significant intermolecular interactions were observed.

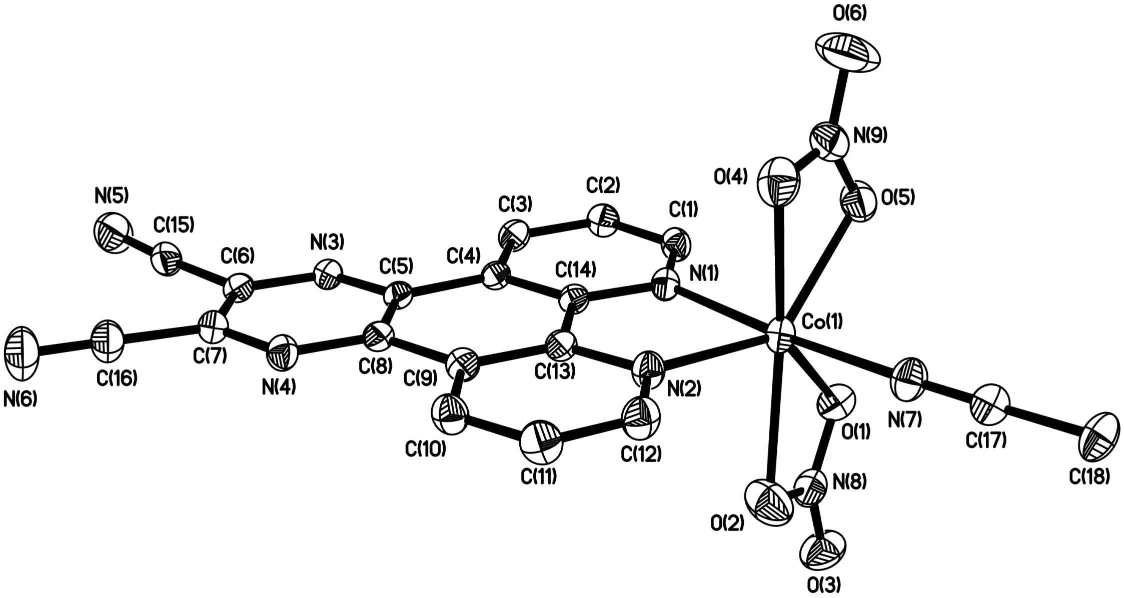


Figure 1
*ORTEP*II (Johnson, 1976) view of (I) with 30% probability displacement ellipsoids.

Experimental

The ligand 6,7-dicyanodipyridoquinoxaline (dcdpq) was prepared according to the literature method of Arounaguiri & Maiya (1999). (I) was synthesized by mixing $Co(NO_3)_2{\cdot}6H_2O$ (0.29 g, 1.0 mmol) and 6,7-dicyanodipyridoquinoxaline (0.28 g, 1.0 mmol) in CH_3CN solution (30 ml). The reaction mixture was filtered and left to stand at room temperature. Brown single crystals suitable for X-ray analysis were obtained by slow evaporation of the solvent. Yield: 350 mg (70%). FT–IR data (KBr pellet, cm^{-1}): 2934 (*w*), 2312 (*m*), 2286 (*m*), 2251 (*m*), 1767 (*m*), 1587 (*s*), 1577 (*s*), 1519 (*m*), 1472 (*vs*), 1397 (*vs*), 1383 (*vs*), 1364 (*vs*), 1302 (*s*), 1287 (*s*), 826 (*m*), 736 (s). Analysis calculated for $C_{18}H_9CoN_9O_6$: C 42.70, H 1.79, N 24.91%; found: C 42.55, H 1.93, N 24.87%.

Crystal data

$[Co(NO_3)_2(C_2H_3N)(C_{16}H_6N_6)]$
$M_r = 506.27$
Monoclinic, $P2_1$
$a = 8.3141\ (8)$ Å
$b = 14.6625\ (13)$ Å
$c = 9.0670\ (9)$ Å
$\beta = 115.154\ (2)°$
$V = 1000.50\ (16)$ Å^3
$Z = 2$

$D_x = 1.681$ Mg m$^{-3$}
Mo $K\alpha$ radiation
Cell parameters from 4702 reflections
$\theta = 2.5–26.4°$
$\mu = 0.92$ mm^{-1}
$T = 298\ (2)$ K
Prism, pink
0.35 × 0.20 × 0.20 mm

Data collection

SMART CCD diffractometer
ω scans
Absorption correction: by integration (Bruker, 1998)
$T_{min} = 0.739$, $T_{max} = 0.838$
4749 measured reflections
3809 independent reflections

3559 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 26.4°$
$h = -10 \rightarrow 10$
$k = -18 \rightarrow 17$
$l = -11 \rightarrow 7$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.070$
$S = 1.05$
3809 reflections
343 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0437P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.021$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}
Absolute structure: Flack (1983)
Flack parameter = 0.040 (11); 3809 Friedel reflections

Table 1
Selected geometric parameters (Å, °).

Co1—N7	2.083 (2)	Co1—O5	2.2090 (18)
Co1—N1	2.106 (2)	Co1—O4	2.278 (2)
Co1—N2	2.130 (2)	Co1—O2	2.310 (3)
Co1—O1	2.183 (2)		
N7—Co1—N1	175.95 (9)	N1—Co1—O4	89.42 (8)
N7—Co1—N2	105.08 (9)	N2—Co1—O4	84.05 (9)
N1—Co1—N2	77.92 (8)	O1—Co1—O4	142.52 (8)
N7—Co1—O1	93.05 (8)	O5—Co1—O4	56.51 (8)
N1—Co1—O1	86.85 (8)	N7—Co1—O2	83.20 (10)
N2—Co1—O1	131.12 (8)	N1—Co1—O2	100.08 (9)
N7—Co1—O5	91.02 (8)	N2—Co1—O2	80.66 (8)
N1—Co1—O5	84.93 (7)	O1—Co1—O2	56.53 (8)
N2—Co1—O5	137.11 (9)	O5—Co1—O2	141.50 (9)
O1—Co1—O5	86.01 (8)	O4—Co1—O2	159.83 (9)
N7—Co1—O4	88.20 (9)		

All the H atoms were located by geometry and refined. The range of bond lengths to H atoms is 0.87 (4)–1.06 (5) Å.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1998).

We gratefully acknowledge financial support from the National Natural Science Foundation of China (Nos. 29771022 and 29971019), Tianjin Natural Science Foundation and the Trans-Century Talents Training Program Foundation from the State Education Ministry of China.

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