

catena-Poly[[*(2,9-dimethyl-1,10-phenanthroline-κ²N,N')*(nitrate-κ²O,O')-cobalt(II)]-μ-dicyanamido-κ²N¹:N⁵]

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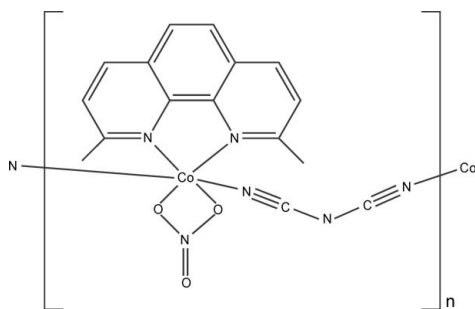
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Key indicators: single-crystal X-ray study; $T = 153$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.033; wR factor = 0.098; data-to-parameter ratio = 16.0.

The title compound, $[\text{Co}(\text{C}_2\text{N}_3)(\text{NO}_3)(\text{C}_{14}\text{H}_{12}\text{N}_2)]_n$, exhibits a zigzag chain structure. The Co^{II} atom has a slightly distorted octahedral geometry formed by two N atoms of a 2,9-dimethyl-1,10-phenanthroline ligand, two N atoms from two different dicyanamide ligands and two O atoms of a nitrate anion. A one-dimensional chain is formed through the dicyanamides, which act as end-to-end bridging ligands. The chains are linked into a three-dimensional network *via* weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For general background, see: Batten & Murray (2003); Burčák *et al.* (2004); Potočňák *et al.* (2002); Vangdal *et al.* (2002); Wu *et al.* (2003).



Experimental

Crystal data

$[\text{Co}(\text{C}_2\text{N}_3)(\text{NO}_3)(\text{C}_{14}\text{H}_{12}\text{N}_2)]_n$
 $M_r = 395.25$
Monoclinic, $P2_1/n$
 $a = 7.3481$ (15) Å
 $b = 13.925$ (3) Å
 $c = 16.531$ (3) Å
 $\beta = 101.42$ (3)°

$V = 1658.0$ (6) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 1.07$ mm⁻¹
 $T = 153$ (2) K
0.20 × 0.15 × 0.10 mm

Data collection

Bruker KappaCCD area-detector diffractometer
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.815$, $T_{\text{max}} = 0.901$

7407 measured reflections
3784 independent reflections
2450 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.098$
 $S = 0.94$
3784 reflections

237 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.44$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.32$ e Å⁻³

Table 1

Selected bond lengths (Å).

Co—N4 ⁱ	2.069 (2)	Co—N2	2.123 (2)
Co—N5	2.105 (2)	Co—O2	2.1466 (17)
Co—N6	2.1116 (18)	Co—O3	2.2268 (18)

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

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
C14—H14A ⁱⁱ ⋯O2	0.96	2.45	3.190 (4)	133
C12—H12 ⁱⁱⁱ ⋯O1 ⁱⁱ	0.93	2.54	3.455 (4)	169
C7—H7 ⁱⁱⁱ ⋯O2 ⁱⁱⁱ	0.93	2.48	3.388 (3)	167

 Symmetry codes: (ii) $-x - \frac{1}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$; (iii) $x + \frac{1}{2}, -y + \frac{3}{2}, z - \frac{1}{2}$

Data collection: COLLECT (Nonius, 1998); cell refinement: SAINT (Bruker, 2003); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2003); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2068).

References

- Batten, S. R. & Murray, K. S. (2003). *Coord. Chem. Rev.* **246**, 103–130.
Bruker (2003). SAINT and SHELXTL. Bruker AXS Inc., Madison, Wisconsin, USA.
Burčák, M., Potočňák, I., Baran, P. & Jäger, L. (2004). *Acta Cryst.* **C60**, m601–m604.
Nonius (1998). COLLECT. Nonius BV, Delft, The Netherlands.
Potočňák, I., Burčák, M., Wagner, C. & Jäger, L. (2002). *Acta Cryst.* **C58**, m327–m329.
Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.
Vangdal, B., Carranza, J., Lloret, F., Julve, M. & Sletten, J. (2002). *J. Chem. Soc. Dalton Trans.* pp. 566–574.
Wu, A.-Q., Zheng, F.-K., Cai, L.-Z., Guo, G.-C., Mao, J.-G. & Huang, J.-S. (2003). *Acta Cryst.* **E59**, m257–m259.

supplementary materials

Acta Cryst. (2007). E63, m1986 [doi:10.1107/S1600536807030279]

***catena-Poly*[[*(2,9-dimethyl-1,10-phenanthroline-κ²N,N')*(*nitrate-κ²O,O'*)cobalt(II)]-*μ*-dicyanamido-κ²N¹:N⁵]**

Y.-Y. Wang and T.-F. Liu

Comment

Due to the stabilization of relatively strong magnetic coupling, multi-dimensional coordination polymers consisting of transition metal ions and dicyanamide ligand are currently being studied (Batten & Murray, 2003). Although the addition of ancillary ligands (*e.g.* pyridine, pyrazine, pyrimidine, 2,2'-bipyrimidine, 4,4'-bipyridine and 2,2'-bipyridine, *etc.*) into these binary systems frequently alters the bridging mode of the dicyanamide ligand from μ -1,3 to μ -1,5 and therefore leads to a paramagnetic behavior, a wide variety of molecular architectures subsequently obtained conduce to establish a better understanding of the relationship between structure and magnetic behavior (Burčák *et al.*, 2004; Potočňák *et al.*, 2002; Vangdal *et al.*, 2002; Wu *et al.*, 2003). Here we describe the structure of an end-to-end dicyanamide-bridged cobalt(II) complex, (I), incorporating 2,9-dimethyl-1,10-phenanthroline (dmphen) as an ancillary ligand.

The structure of compound (I) consists of well isolated chains of Co^{II} atoms bridged by end-to-end dicyanamide ligands (Fig. 1). In the chain structure, each Co^{II} atom is coordinated by one dmphen ligand, one nitrate anion and two dicyanamide ligands in an octahedral geometry. The Co—N bond distances are in the range of 2.069 (2) to 2.123 (2) Å (Table 1). The nitrate ion binds in a bidentate fashion and the distances of Co—O are 2.1466 (17) and 2.2268 (18) Å. The shortest Co···Co distance is 7.169 (7) Å in the chain and 7.348 (2) Å between the chains.

An N1—O1···Cg(aryl ring) interaction is observed [Cg is the centroid of the ring C5, C6, C7, C8, C9 and C10 at 1/2 - x, 1/2 + y, 1/2 - z] with O1···Cg = 3.296 Å. No significant π - π interaction between the dmphen rings is observed (the shortest centroid-to-centroid distance is 4.364 Å). The weak C—H···O hydrogen bonds link the chains into a three-dimensional structure (Fig. 2, Table 2).

Experimental

Co(NO₃)₂·6H₂O (0.073 g, 0.25 mmol) and sodium dicyanamide (0.022 g, 0.25 mmol) were dissolved in water (10 ml). A methanol solution (10 ml) of dmphen (0.052 g, 0.25 mmol) was added with continuous stirring. The resulting solution was filtrated and allowed to slowly evaporate at room temperature. After one month, red single crystals suitable for X-ray diffraction appeared. The crystals were collected, washed with water and dried in air (0.059 g, yield 60%). IR (KBr, cm⁻¹): 2318 (ms), 2293 (ms), 2269 (ms), 2247 (*m*), 2211 (*s*), 2180 (*s*).

Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aromatic rings, and C—H = 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl groups.

Figures

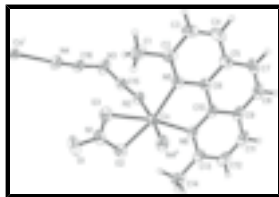


Fig. 1. The structure of (I), showing the Co^{II} coordination. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) $1/2 - x, 1/2 + y, 1/2 - z$; (ii) $1/2 - x, -1/2 + y, 1/2 - z$.]

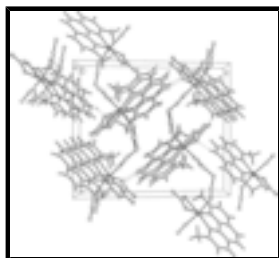


Fig. 2. Hydrogen bonds (dashed lines) between neighboring chains create a three-dimensional structure.

catena-Poly[[**(2,9-dimethyl-1,10-phenanthroline- κ^2N,N')(nitrate- κ^2O,O')cobalt(II)- μ -dicyanamido- $\kappa^2N^1:N^5$]**

Crystal data

[Co(C₂N₃)(NO₃)(C₁₄H₁₂N₂)]

$M_r = 395.25$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2yn$

$a = 7.3481$ (15) Å

$b = 13.925$ (3) Å

$c = 16.531$ (3) Å

$\beta = 101.42$ (3)°

$V = 1658.0$ (6) Å³

$Z = 4$

$F_{000} = 804$

$D_x = 1.583$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 16421 reflections

$\theta = 3.4\text{--}27.5^\circ$

$\mu = 1.07$ mm⁻¹

$T = 153$ (2) K

Block, red

$0.20 \times 0.15 \times 0.10$ mm

Data collection

Bruker KappaCCD area-detector diffractometer

3784 independent reflections

Radiation source: sealed tube

2450 reflections with $I > 2\sigma(I)$

Monochromator: graphite

$R_{\text{int}} = 0.022$

$T = 153$ (2) K

$\theta_{\text{max}} = 27.5^\circ$

ω scans

$\theta_{\text{min}} = 3.6^\circ$

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$h = -9 \rightarrow 9$

$T_{\text{min}} = 0.815, T_{\text{max}} = 0.901$

$k = -18 \rightarrow 18$

7407 measured reflections

$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.033$	H-atom parameters constrained
$wR(F^2) = 0.098$	$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2]$
$S = 0.94$	where $P = (F_o^2 + 2F_c^2)/3$
3784 reflections	$(\Delta/\sigma)_{\max} < 0.001$
237 parameters	$\Delta\rho_{\max} = 0.44 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.32 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co	0.17457 (4)	0.86364 (2)	0.203521 (18)	0.03941 (12)
C1	0.5626 (4)	0.9754 (2)	0.1736 (2)	0.0718 (8)
H1A	0.5790	0.9478	0.2278	0.108*
H1B	0.4717	1.0257	0.1684	0.108*
H1C	0.6785	1.0013	0.1653	0.108*
C2	0.4981 (3)	0.8998 (2)	0.11066 (16)	0.0550 (6)
C3	0.5930 (4)	0.8817 (2)	0.0460 (2)	0.0689 (8)
H3	0.6973	0.9178	0.0419	0.083*
C4	0.5327 (4)	0.8119 (2)	-0.01033 (18)	0.0710 (9)
H4	0.5974	0.7997	-0.0522	0.085*
C5	0.3748 (4)	0.75839 (19)	-0.00591 (15)	0.0564 (7)
C6	0.2852 (3)	0.77972 (16)	0.05976 (13)	0.0432 (5)
C7	0.3025 (5)	0.6845 (2)	-0.06323 (16)	0.0685 (9)
H7	0.3640	0.6690	-0.1055	0.082*
C8	0.1478 (5)	0.63745 (19)	-0.05684 (16)	0.0683 (9)
H8	0.1021	0.5905	-0.0956	0.082*
C9	0.0506 (4)	0.65740 (17)	0.00819 (15)	0.0544 (7)
C10	0.1201 (3)	0.72828 (15)	0.06690 (13)	0.0422 (5)
C11	-0.1105 (4)	0.60941 (19)	0.01902 (18)	0.0640 (8)
H11	-0.1647	0.5638	-0.0194	0.077*
C12	-0.1875 (4)	0.62898 (18)	0.08485 (19)	0.0644 (8)
H12	-0.2918	0.5951	0.0927	0.077*
C13	-0.1113 (3)	0.69973 (17)	0.14120 (15)	0.0498 (6)
C14	-0.1931 (4)	0.7203 (2)	0.21529 (18)	0.0675 (8)
H14A	-0.2027	0.7884	0.2219	0.101*
H14B	-0.1148	0.6936	0.2635	0.101*
H14C	-0.3144	0.6919	0.2081	0.101*
C15	0.0563 (3)	1.05722 (17)	0.12152 (13)	0.0429 (5)
C16	0.1296 (4)	1.20845 (18)	0.16598 (16)	0.0506 (6)
N1	0.1251 (3)	0.97749 (16)	0.32013 (12)	0.0586 (6)

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N2	0.0411 (3)	0.97627 (14)	0.12771 (12)	0.0497 (5)
N3	0.0722 (4)	1.14768 (15)	0.10658 (14)	0.0778 (8)
N4	0.1824 (3)	1.26809 (16)	0.21111 (13)	0.0608 (6)
N5	0.3482 (3)	0.84869 (13)	0.11715 (12)	0.0433 (5)
N6	0.0384 (2)	0.74995 (12)	0.13134 (11)	0.0398 (4)
O1	0.0919 (3)	1.03262 (17)	0.37294 (13)	0.0953 (8)
O2	0.0128 (3)	0.91132 (14)	0.29068 (11)	0.0593 (5)
O3	0.2731 (3)	0.98178 (13)	0.29219 (11)	0.0595 (5)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co	0.0450 (2)	0.03348 (18)	0.03892 (18)	-0.00008 (14)	0.00622 (13)	-0.00058 (13)
C1	0.0499 (17)	0.0674 (19)	0.098 (2)	-0.0148 (14)	0.0133 (16)	-0.0054 (17)
C2	0.0438 (15)	0.0568 (15)	0.0646 (16)	0.0035 (12)	0.0112 (13)	0.0095 (13)
C3	0.0508 (17)	0.079 (2)	0.082 (2)	0.0055 (15)	0.0261 (15)	0.0217 (17)
C4	0.076 (2)	0.084 (2)	0.0608 (18)	0.0249 (18)	0.0327 (16)	0.0142 (16)
C5	0.0659 (17)	0.0580 (16)	0.0472 (14)	0.0186 (14)	0.0160 (13)	0.0087 (12)
C6	0.0515 (14)	0.0397 (12)	0.0372 (12)	0.0117 (11)	0.0063 (11)	0.0031 (10)
C7	0.105 (3)	0.0627 (19)	0.0404 (14)	0.0280 (18)	0.0199 (16)	-0.0004 (13)
C8	0.111 (3)	0.0458 (16)	0.0421 (14)	0.0168 (17)	-0.0005 (16)	-0.0048 (12)
C9	0.077 (2)	0.0366 (13)	0.0416 (13)	0.0102 (12)	-0.0073 (13)	0.0002 (10)
C10	0.0514 (14)	0.0315 (11)	0.0399 (12)	0.0059 (10)	-0.0004 (10)	0.0000 (9)
C11	0.079 (2)	0.0379 (14)	0.0621 (17)	-0.0032 (14)	-0.0180 (16)	-0.0042 (12)
C12	0.0582 (17)	0.0427 (15)	0.084 (2)	-0.0113 (13)	-0.0060 (16)	0.0039 (14)
C13	0.0478 (15)	0.0369 (13)	0.0602 (15)	-0.0010 (11)	0.0001 (12)	0.0078 (11)
C14	0.0626 (18)	0.0605 (18)	0.084 (2)	-0.0099 (14)	0.0253 (16)	0.0085 (15)
C15	0.0458 (14)	0.0410 (14)	0.0391 (12)	-0.0005 (10)	0.0018 (10)	0.0000 (10)
C16	0.0627 (16)	0.0350 (13)	0.0492 (14)	-0.0038 (12)	-0.0003 (12)	0.0057 (11)
N1	0.0713 (17)	0.0570 (14)	0.0440 (12)	0.0149 (12)	0.0030 (12)	-0.0053 (10)
N2	0.0554 (13)	0.0367 (12)	0.0545 (12)	0.0012 (9)	0.0051 (10)	0.0024 (9)
N3	0.128 (2)	0.0393 (13)	0.0535 (14)	-0.0122 (13)	-0.0121 (15)	0.0048 (11)
N4	0.0799 (17)	0.0452 (13)	0.0506 (12)	-0.0086 (11)	-0.0034 (12)	0.0024 (10)
N5	0.0407 (11)	0.0412 (11)	0.0475 (11)	0.0039 (9)	0.0077 (9)	0.0024 (9)
N6	0.0428 (11)	0.0325 (10)	0.0419 (10)	0.0005 (8)	0.0033 (9)	0.0017 (8)
O1	0.1099 (19)	0.0995 (18)	0.0737 (14)	0.0292 (14)	0.0117 (13)	-0.0411 (13)
O2	0.0649 (12)	0.0634 (12)	0.0513 (10)	-0.0039 (10)	0.0160 (9)	-0.0018 (9)
O3	0.0559 (11)	0.0576 (12)	0.0617 (11)	0.0011 (9)	0.0039 (10)	-0.0098 (8)

Geometric parameters (\AA , $^\circ$)

Co—N4 ⁱ	2.069 (2)	C8—C9	1.431 (4)
Co—N5	2.105 (2)	C8—H8	0.9300
Co—N6	2.1116 (18)	C9—C11	1.402 (4)
Co—N2	2.123 (2)	C9—C10	1.407 (3)
Co—O2	2.1466 (17)	C10—N6	1.357 (3)
Co—O3	2.2268 (18)	C11—C12	1.350 (4)
C1—C2	1.490 (4)	C11—H11	0.9300

C1—H1A	0.9600	C12—C13	1.395 (4)
C1—H1B	0.9600	C12—H12	0.9300
C1—H1C	0.9600	C13—N6	1.340 (3)
C2—N5	1.333 (3)	C13—C14	1.495 (3)
C2—C3	1.409 (4)	C14—H14A	0.9600
C3—C4	1.359 (4)	C14—H14B	0.9600
C3—H3	0.9300	C14—H14C	0.9600
C4—C5	1.393 (4)	C15—N2	1.139 (3)
C4—H4	0.9300	C15—N3	1.293 (3)
C5—C6	1.408 (3)	C16—N4	1.132 (3)
C5—C7	1.428 (4)	C16—N3	1.302 (3)
C6—N5	1.365 (3)	N1—O1	1.223 (3)
C6—C10	1.433 (3)	N1—O3	1.264 (3)
C7—C8	1.334 (4)	N1—O2	1.268 (3)
C7—H7	0.9300	N4—Co ⁱⁱ	2.069 (2)
N4 ⁱ —Co—N5	96.01 (8)	C7—C8—H8	119.2
N4 ⁱ —Co—N6	91.33 (8)	C9—C8—H8	119.2
N5—Co—N6	79.97 (7)	C11—C9—C10	116.5 (2)
N4 ⁱ —Co—N2	172.30 (8)	C11—C9—C8	124.3 (3)
N5—Co—N2	86.78 (8)	C10—C9—C8	119.2 (3)
N6—Co—N2	96.23 (8)	N6—C10—C9	122.7 (2)
N4 ⁱ —Co—O2	90.87 (8)	N6—C10—C6	117.84 (19)
N5—Co—O2	167.53 (7)	C9—C10—C6	119.4 (2)
N6—Co—O2	110.34 (7)	C12—C11—C9	120.4 (2)
N2—Co—O2	85.14 (7)	C12—C11—H11	119.8
N4 ⁱ —Co—O3	88.35 (8)	C9—C11—H11	119.8
N5—Co—O3	110.97 (7)	C11—C12—C13	120.3 (3)
N6—Co—O3	169.04 (7)	C11—C12—H12	119.9
N2—Co—O3	83.96 (8)	C13—C12—H12	119.9
O2—Co—O3	58.71 (7)	N6—C13—C12	121.2 (2)
C2—C1—H1A	109.5	N6—C13—C14	118.2 (2)
C2—C1—H1B	109.5	C12—C13—C14	120.6 (2)
H1A—C1—H1B	109.5	C13—C14—H14A	109.5
C2—C1—H1C	109.5	C13—C14—H14B	109.5
H1A—C1—H1C	109.5	H14A—C14—H14B	109.5
H1B—C1—H1C	109.5	C13—C14—H14C	109.5
N5—C2—C3	120.4 (3)	H14A—C14—H14C	109.5
N5—C2—C1	118.3 (2)	H14B—C14—H14C	109.5
C3—C2—C1	121.3 (2)	N2—C15—N3	174.2 (3)
C4—C3—C2	120.3 (3)	N4—C16—N3	172.5 (3)
C4—C3—H3	119.9	O1—N1—O3	122.6 (3)
C2—C3—H3	119.9	O1—N1—O2	121.6 (2)
C3—C4—C5	120.6 (3)	O3—N1—O2	115.82 (19)
C3—C4—H4	119.7	C15—N2—Co	137.9 (2)
C5—C4—H4	119.7	C15—N3—C16	121.1 (2)
C4—C5—C6	116.7 (3)	C16—N4—Co ⁱⁱ	169.3 (2)
C4—C5—C7	123.7 (3)	C2—N5—C6	119.5 (2)

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C6—C5—C7	119.6 (3)	C2—N5—Co	128.54 (17)
N5—C6—C5	122.5 (2)	C6—N5—Co	111.90 (15)
N5—C6—C10	118.09 (19)	C13—N6—C10	118.8 (2)
C5—C6—C10	119.4 (2)	C13—N6—Co	129.13 (16)
C8—C7—C5	120.8 (3)	C10—N6—Co	112.11 (14)
C8—C7—H7	119.6	N1—O2—Co	94.46 (14)
C5—C7—H7	119.6	N1—O3—Co	90.83 (14)
C7—C8—C9	121.6 (3)		
N5—C2—C3—C4	-0.1 (4)	N2—Co—N5—C2	81.6 (2)
C1—C2—C3—C4	179.4 (3)	O2—Co—N5—C2	31.9 (5)
C2—C3—C4—C5	1.1 (4)	O3—Co—N5—C2	-0.7 (2)
C3—C4—C5—C6	-0.9 (4)	N4 ⁱ —Co—N5—C6	92.44 (16)
C3—C4—C5—C7	179.5 (3)	N6—Co—N5—C6	2.15 (14)
C4—C5—C6—N5	-0.4 (4)	N2—Co—N5—C6	-94.76 (16)
C7—C5—C6—N5	179.3 (2)	O2—Co—N5—C6	-144.4 (3)
C4—C5—C6—C10	179.0 (2)	O3—Co—N5—C6	-177.03 (14)
C7—C5—C6—C10	-1.4 (3)	C12—C13—N6—C10	-2.6 (3)
C4—C5—C7—C8	-178.3 (3)	C14—C13—N6—C10	176.3 (2)
C6—C5—C7—C8	2.1 (4)	C12—C13—N6—Co	177.26 (18)
C5—C7—C8—C9	-1.3 (4)	C14—C13—N6—Co	-3.8 (3)
C7—C8—C9—C11	-178.9 (3)	C9—C10—N6—C13	2.3 (3)
C7—C8—C9—C10	-0.1 (4)	C6—C10—N6—C13	-177.1 (2)
C11—C9—C10—N6	0.3 (3)	C9—C10—N6—Co	-177.60 (17)
C8—C9—C10—N6	-178.6 (2)	C6—C10—N6—Co	3.1 (2)
C11—C9—C10—C6	179.6 (2)	N4 ⁱ —Co—N6—C13	81.5 (2)
C8—C9—C10—C6	0.8 (3)	N5—Co—N6—C13	177.3 (2)
N5—C6—C10—N6	-1.3 (3)	N2—Co—N6—C13	-97.05 (19)
C5—C6—C10—N6	179.4 (2)	O2—Co—N6—C13	-9.9 (2)
N5—C6—C10—C9	179.4 (2)	O3—Co—N6—C13	-6.7 (5)
C5—C6—C10—C9	0.0 (3)	N4 ⁱ —Co—N6—C10	-98.67 (15)
C10—C9—C11—C12	-2.6 (4)	N5—Co—N6—C10	-2.80 (15)
C8—C9—C11—C12	176.2 (3)	N2—Co—N6—C10	82.81 (16)
C9—C11—C12—C13	2.4 (4)	O2—Co—N6—C10	169.91 (14)
C11—C12—C13—N6	0.3 (4)	O3—Co—N6—C10	173.2 (3)
C11—C12—C13—C14	-178.6 (3)	O1—N1—O2—Co	176.7 (2)
N5—Co—N2—C15	-89.6 (3)	O3—N1—O2—Co	-4.1 (2)
N6—Co—N2—C15	-169.1 (3)	N4 ⁱ —Co—O2—N1	90.02 (15)
O2—Co—N2—C15	80.9 (3)	N5—Co—O2—N1	-33.6 (4)
O3—Co—N2—C15	21.9 (3)	N6—Co—O2—N1	-178.24 (13)
C3—C2—N5—C6	-1.2 (4)	N2—Co—O2—N1	-83.39 (15)
C1—C2—N5—C6	179.3 (2)	O3—Co—O2—N1	2.48 (13)
C3—C2—N5—Co	-177.25 (19)	O1—N1—O3—Co	-176.8 (2)
C1—C2—N5—Co	3.2 (3)	O2—N1—O3—Co	4.0 (2)
C5—C6—N5—C2	1.4 (3)	N4 ⁱ —Co—O3—N1	-94.50 (14)
C10—C6—N5—C2	-177.9 (2)	N5—Co—O3—N1	169.70 (13)
C5—C6—N5—Co	178.11 (18)	N6—Co—O3—N1	-6.0 (4)
C10—C6—N5—Co	-1.2 (2)	N2—Co—O3—N1	85.49 (14)

N4 ⁱ —Co—N5—C2	-91.2 (2)	O2—Co—O3—N1	-2.48 (13)
N6—Co—N5—C2	178.5 (2)		

Symmetry codes: (i) $-x+1/2, y-1/2, -z+1/2$; (ii) $-x+1/2, y+1/2, -z+1/2$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C14—H14A \cdots O2	0.96	2.45	3.190 (4)	133
C12—H12 \cdots O1 ⁱⁱⁱ	0.93	2.54	3.455 (4)	169
C7—H7 \cdots O2 ^{iv}	0.93	2.48	3.388 (3)	167

Symmetry codes: (iii) $-x-1/2, y-1/2, -z+1/2$; (iv) $x+1/2, -y+3/2, z-1/2$.

Fig. 1

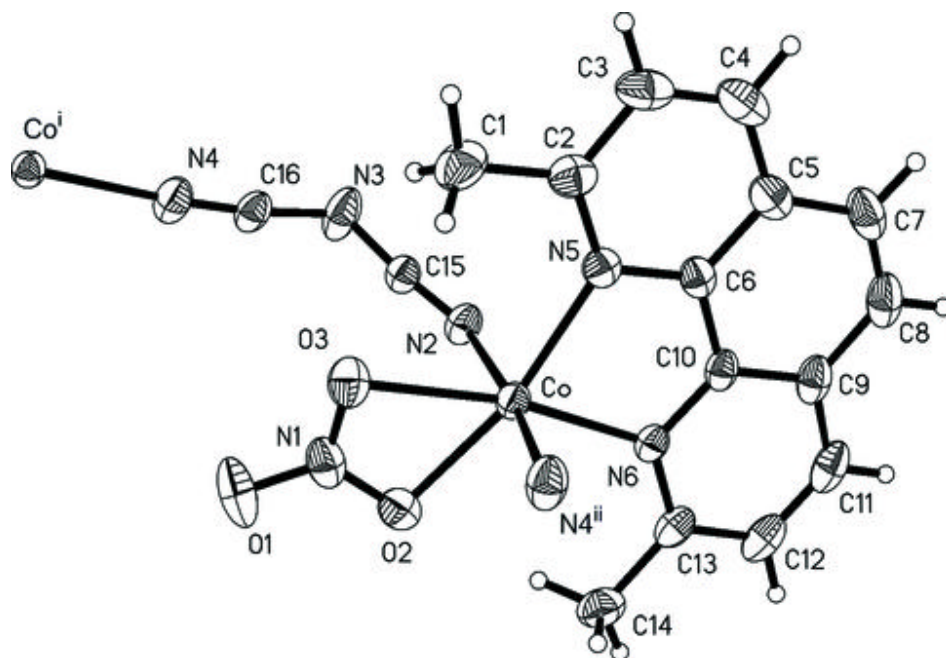


Fig. 2

