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catena-Poly[[bis(4,4′-bipyridine-κN)-cobalt(II)]-μ_3-(4,4′-dicarboxybiphenyl-3,3′-dicarboxylato-$\kappa^4O^3,O^{3'}:O^{3''}:O^{3'''}$)]

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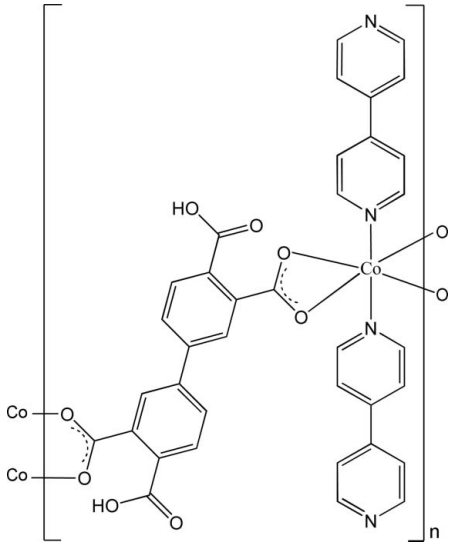
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.123; data-to-parameter ratio = 15.3.

In the title compound, $[Co(C_{16}H_8O_8)(C_{10}H_8N_2)_2]_n$, the Co^{II} atom exhibits a distorted octahedral geometry defined by four O atoms from three 4,4′-dicarboxybiphenyl-3,3′-dicarboxylate ligands and two N atoms from two 4,4′-bipyridine ligands. In the crystal structure, one-dimensional molecular chains are connected by O—H···N hydrogen bonds, forming a two-dimensional supramolecular network.

Related literature

For general background, see: Wang *et al.* (2005). For related structures, see: Hao *et al.* (2005).



Experimental

Crystal data

$[Co(C_{16}H_8O_8)(C_{10}H_8N_2)_2]$
M_r = 699.52
Triclinic, $P\overline{1}$
a = 11.045 (2) Å
b = 11.361 (2) Å
c = 12.352 (3) Å
α = 103.83 (3)°
β = 93.54 (3)°
γ = 96.84 (3)°
V = 1487.8 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.64 mm^{-1}
T = 298 (2) K
0.24 × 0.22 × 0.17 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.856, T_{max} = 0.898
14754 measured reflections
6747 independent reflections
5292 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.123
S = 1.01
6747 reflections
442 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O2^{i}	2.0369 (16)	Co1—N3	2.1716 (19)
Co1—O1^{ii}	2.0519 (17)	Co1—O7	2.1885 (18)
Co1—O8	2.1394 (18)	Co1—N2	2.2072 (19)
O2^{i}—Co1—O1^{ii}	99.25 (7)	O8—Co1—O7	60.97 (7)
O2^{i}—Co1—O8	103.34 (7)	N3—Co1—O7	89.13 (7)
O1^{ii}—Co1—O8	157.16 (7)	O2^{i}—Co1—N2	96.19 (7)
O2^{i}—Co1—N3	89.85 (7)	O1^{ii}—Co1—N2	94.62 (7)
O1^{ii}—Co1—N3	85.19 (7)	O8—Co1—N2	86.34 (7)
O8—Co1—N3	91.48 (7)	N3—Co1—N2	173.91 (7)
O2^{i}—Co1—O7	164.24 (6)	O7—Co1—N2	84.84 (7)
O1^{ii}—Co1—O7	96.34 (7)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H1···N4^{iii}	0.82	1.85	2.624 (3)	157
O5—H2···N1^{iv}	0.82	1.88	2.655 (2)	157

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Siemens, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2098).

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supplementary materials

Acta Cryst. (2007). E**63**, m3073-m3074 [**doi:10.1107/S1600536807058333**]

catena-Poly[[bis(4,4'-bipyridine-κN)cobalt(II)]-μ_3-(4,4'-dicarboxybiphenyl-3,3'-dicarboxylato-$\kappa^4O^3,O^{3'}:O^{3''}:O^{3'''}$)]

C. Qin, X.-L. Wang and E.-B. Wang

Comment

Metal–carboxylate coordination polymers have emerged as an important family in the past few years (Wang *et al.*, 2005; Hao *et al.*, 2005). We report here the structure of the title compound. The asymmetric unit contains one Co^{II} atom, one 4,4'-dicarboxybiphenyl-3,3'-dicarboxylate (bpdc) ligand and two 4,4'-bipyridine (4,4'-bpy) ligands. The Co^{II} atom has a distorted octahedral coordination geometry, defined by four O atoms from the bpdc ligands and two N atoms from the 4,4'-bpy ligands. The adjacent Co^{II} atoms are linked by the bpdc ligands to generate a one-dimensional chain running along the crystallographic *c* axis. In the crystal structure, the adjacent one-dimensional chains are further connected with O—H···N hydrogen bonds, forming a two-dimensional supramolecular network.

Experimental

The title compound was prepared by a hydrothermal method. A mixture of $Co(NO_3)_2{\cdot}6H_2O$ (0.115 g, 0.5 mmol), biphenyl-3,3',4,4'-tetracarboxylic acid (0.165 g, 0.5 mmol), 4,4'-bipyridine (0.125 g, 0.8 mmol) and water (10 ml) was stirred for 20 min and then transferred to a 23 ml Teflon-lined reactor. The reactor was kept at 433 K for 120 h under autogenous pressure. Single crystals of the title compound were obtained after cooling to room temperature.

Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93Å and O—H = 0.82 Å, and with U_{iso}(H) = 1.2U_{eq}(C) and U_{iso}(H) = 1.5U_{eq}(O).

Figures

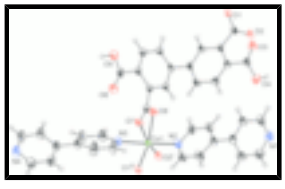

Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) −*x*, −*y*, −*z* + 1; (ii) *x*, *y*, *z* − 1.]

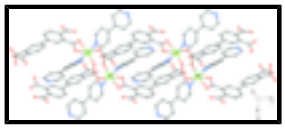

Fig. 2. The one-dimensional chain in the title compound. H atoms have been omitted for clarity.

catena-Poly[[bis(4,4'-bipyridine-κ_N_)cobalt(II)]- μ$_3$-4,4'-dicarboxybiphenyl-3,3'-dicarboxylato-κ^4_O_^{3},_O_$^{3'}$:_O_$^{3''}$:_O_$^{3'''}$)]

Crystal data

$[Co(C_{16}H_8O_8)(C_{10}H_8N_2)_2]$	$Z = 2$
$M_r = 699.52$	$F_{000} = 718$
Triclinic, $P\overline{1}$	$D_x = 1.561$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71069 Å
$a = 11.045$ (2) Å	Cell parameters from 14754 reflections
$b = 11.361$ (2) Å	θ = 3.2–27.5º
$c = 12.352$ (3) Å	μ = 0.64 mm^{-1}
α = 103.83 (3)º	$T = 298$ (2) K
β = 93.54 (3)º	Block, purple
γ = 96.84 (3)º	0.24 × 0.22 × 0.17 mm
$V = 1487.8$ (6) Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	6747 independent reflections
Radiation source: fine-focus sealed tube	5292 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.025$
$T = 298$(2) K	$\theta_{max} = 27.5$º
φ and ω scans	$\theta_{min} = 3.2$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -14\rightarrow14$
$T_{min} = 0.856$, $T_{max} = 0.898$	$k = -14\rightarrow14$
14754 measured reflections	$l = -16\rightarrow16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H-atom parameters constrained
$wR(F^2) = 0.123$	$w = 1/[\sigma^2(F_o^2) + (0.0823P)^2 + 0.1308P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.003$
6747 reflections	$\Delta\rho_{max} = 0.42$ e Å^{-3}
442 parameters	$\Delta\rho_{min} = -0.32$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.15335 (3)	0.02558 (3)	0.13743 (2)	0.02485 (10)
C1	−0.2712 (2)	−0.4174 (2)	0.4984 (2)	0.0394 (6)
H1A	−0.2746	−0.4011	0.5755	0.047*
C2	−0.1971 (2)	−0.3366 (2)	0.4554 (2)	0.0358 (5)
H2A	−0.1517	−0.2675	0.5033	0.043*
C3	−0.1905 (2)	−0.3584 (2)	0.34135 (19)	0.0305 (5)
C4	−0.2601 (3)	−0.4642 (2)	0.2740 (2)	0.0408 (6)
H4A	−0.2581	−0.4832	0.1967	0.049*
C5	−0.3324 (3)	−0.5404 (2)	0.3241 (2)	0.0445 (6)
H5A	−0.3789	−0.6104	0.2786	0.053*
C6	−0.0178 (2)	−0.0684 (2)	0.2993 (2)	0.0326 (5)
H6A	0.0000	0.0132	0.3387	0.039*
C7	−0.0854 (2)	−0.1485 (2)	0.3482 (2)	0.0343 (5)
H7A	−0.1114	−0.1206	0.4189	0.041*
C8	−0.1146 (2)	−0.2714 (2)	0.29093 (19)	0.0300 (5)
C9	−0.0714 (3)	−0.3060 (2)	0.1874 (2)	0.0411 (6)
H9A	−0.0875	−0.3872	0.1464	0.049*
C10	−0.0039 (2)	−0.2195 (2)	0.1442 (2)	0.0379 (6)
H10A	0.0236	−0.2450	0.0738	0.046*
C11	0.4115 (2)	0.1192 (3)	0.0882 (2)	0.0438 (6)
H11A	0.4308	0.0591	0.1234	0.053*
C12	0.5048 (2)	0.1784 (3)	0.0424 (2)	0.0445 (6)
H12A	0.5838	0.1583	0.0471	0.053*
C13	0.4781 (2)	0.2676 (2)	−0.0102 (2)	0.0361 (5)
C14	0.3604 (3)	0.2964 (3)	−0.0087 (3)	0.0567 (9)
H14A	0.3396	0.3588	−0.0401	0.068*
C15	0.2728 (3)	0.2327 (3)	0.0393 (3)	0.0510 (7)
H15A	0.1941	0.2540	0.0393	0.061*
C16	0.7799 (3)	0.4056 (3)	−0.0840 (3)	0.0499 (7)
H16A	0.8623	0.4185	−0.0576	0.060*
C17	0.6967 (3)	0.3472 (3)	−0.0289 (3)	0.0459 (6)
H17A	0.7230	0.3194	0.0323	0.055*
C18	0.5733 (2)	0.3304 (2)	−0.0655 (2)	0.0366 (5)
C19	0.5395 (3)	0.3744 (3)	−0.1559 (2)	0.0524 (8)
H19A	0.4574	0.3664	−0.1818	0.063*
C20	0.6290 (3)	0.4308 (3)	−0.2083 (3)	0.0584 (9)
H20A	0.6051	0.4600	−0.2694	0.070*
C21	0.22465 (19)	−0.14137 (19)	0.63711 (17)	0.0251 (4)
C22	0.20320 (19)	−0.10850 (19)	0.74957 (17)	0.0252 (4)
H22A	0.2433	−0.0351	0.7951	0.030*
C23	0.12327 (19)	−0.18306 (19)	0.79495 (17)	0.0240 (4)
C24	0.0677 (2)	−0.29749 (19)	0.72797 (17)	0.0260 (4)
C25	0.0908 (2)	−0.3316 (2)	0.61661 (19)	0.0314 (5)
H25A	0.0546	−0.4070	0.5719	0.038*
C26	0.1675 (2)	−0.2542 (2)	0.57121 (18)	0.0298 (5)

H26A	0.1810	−0.2777	0.4960	0.036*
C27	0.29693 (19)	−0.05148 (19)	0.58818 (17)	0.0255 (4)
C28	0.3919 (2)	0.0341 (2)	0.65183 (18)	0.0303 (5)
H28A	0.4156	0.0310	0.7246	0.036*
C29	0.4510 (2)	0.1239 (2)	0.60680 (19)	0.0304 (5)
H29A	0.5150	0.1795	0.6494	0.036*
C30	0.41605 (19)	0.13164 (19)	0.49935 (18)	0.0261 (4)
C31	0.32276 (19)	0.04471 (19)	0.43401 (17)	0.0266 (4)
C32	0.26553 (19)	−0.04591 (19)	0.47919 (18)	0.0269 (4)
H32A	0.2046	−0.1043	0.4352	0.032*
C33	0.08564 (19)	−0.13041 (17)	0.90973 (17)	0.0242 (4)
C34	−0.0092 (2)	−0.3814 (2)	0.78063 (19)	0.0312 (5)
C35	0.4801 (2)	0.2274 (2)	0.4504 (2)	0.0319 (5)
C36	0.2723 (2)	0.0462 (2)	0.31868 (17)	0.0281 (5)
N1	−0.3384 (2)	−0.51818 (19)	0.43373 (19)	0.0401 (5)
N2	0.02360 (18)	−0.10141 (17)	0.19870 (16)	0.0293 (4)
N3	0.29647 (18)	0.14250 (18)	0.08518 (16)	0.0330 (4)
N4	0.7468 (2)	0.4445 (2)	−0.1744 (2)	0.0491 (6)
O1	0.16807 (14)	−0.09749 (14)	0.98893 (12)	0.0299 (3)
O2	−0.02537 (14)	−0.11935 (13)	0.91601 (13)	0.0291 (3)
O3	0.01081 (18)	−0.38419 (15)	0.87748 (14)	0.0411 (4)
O4	−0.09660 (19)	−0.45426 (19)	0.71183 (16)	0.0562 (6)
H1	−0.1328	−0.5005	0.7447	0.084*
O5	0.54844 (18)	0.31614 (16)	0.52605 (15)	0.0448 (5)
H2	0.5974	0.3535	0.4947	0.067*
O6	0.47072 (19)	0.22331 (17)	0.35211 (15)	0.0484 (5)
O7	0.29338 (16)	−0.03486 (15)	0.23673 (13)	0.0345 (4)
O8	0.19877 (15)	0.12079 (14)	0.30946 (13)	0.0327 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.02672 (17)	0.02842 (16)	0.02075 (16)	−0.00082 (11)	0.00528 (11)	0.01020 (11)
C1	0.0426 (14)	0.0436 (13)	0.0367 (13)	0.0014 (11)	0.0108 (11)	0.0192 (11)
C2	0.0367 (13)	0.0370 (12)	0.0343 (13)	−0.0013 (10)	0.0073 (10)	0.0124 (10)
C3	0.0327 (11)	0.0293 (10)	0.0341 (12)	0.0032 (9)	0.0097 (9)	0.0157 (9)
C4	0.0504 (15)	0.0369 (12)	0.0357 (13)	−0.0034 (11)	0.0053 (11)	0.0141 (10)
C5	0.0497 (15)	0.0352 (12)	0.0474 (15)	−0.0095 (12)	0.0016 (12)	0.0163 (11)
C6	0.0327 (12)	0.0288 (10)	0.0372 (13)	0.0004 (9)	0.0109 (10)	0.0101 (9)
C7	0.0380 (13)	0.0335 (11)	0.0332 (12)	0.0026 (10)	0.0136 (10)	0.0106 (9)
C8	0.0313 (11)	0.0304 (10)	0.0330 (12)	0.0016 (9)	0.0092 (9)	0.0168 (9)
C9	0.0610 (17)	0.0260 (11)	0.0366 (13)	−0.0023 (11)	0.0161 (12)	0.0098 (9)
C10	0.0507 (15)	0.0342 (12)	0.0304 (12)	−0.0006 (11)	0.0156 (11)	0.0111 (9)
C11	0.0404 (14)	0.0503 (15)	0.0523 (16)	0.0076 (12)	0.0156 (12)	0.0316 (13)
C12	0.0333 (13)	0.0543 (15)	0.0556 (17)	0.0072 (11)	0.0162 (12)	0.0289 (13)
C13	0.0330 (12)	0.0383 (12)	0.0387 (13)	−0.0034 (10)	0.0114 (10)	0.0151 (10)
C14	0.0394 (15)	0.0617 (18)	0.089 (2)	0.0074 (14)	0.0188 (15)	0.0543 (18)
C15	0.0317 (13)	0.0573 (17)	0.078 (2)	0.0061 (12)	0.0166 (13)	0.0419 (16)

C16	0.0380 (14)	0.0544 (16)	0.0610 (18)	−0.0032 (13)	0.0138 (13)	0.0238 (14)
C17	0.0388 (14)	0.0515 (15)	0.0553 (17)	0.0042 (12)	0.0144 (12)	0.0267 (13)
C18	0.0359 (13)	0.0353 (12)	0.0392 (13)	−0.0051 (10)	0.0104 (10)	0.0137 (10)
C19	0.0391 (14)	0.0689 (18)	0.0499 (17)	−0.0149 (14)	0.0027 (12)	0.0274 (15)
C20	0.0585 (19)	0.075 (2)	0.0430 (16)	−0.0173 (16)	0.0041 (14)	0.0294 (15)
C21	0.0247 (10)	0.0301 (10)	0.0243 (10)	0.0007 (8)	0.0081 (8)	0.0141 (8)
C22	0.0261 (10)	0.0278 (10)	0.0218 (10)	−0.0016 (8)	0.0055 (8)	0.0081 (8)
C23	0.0238 (10)	0.0301 (10)	0.0206 (10)	0.0009 (8)	0.0053 (8)	0.0116 (8)
C24	0.0272 (10)	0.0268 (10)	0.0247 (10)	−0.0029 (8)	0.0059 (8)	0.0103 (8)
C25	0.0359 (12)	0.0273 (10)	0.0279 (11)	−0.0058 (9)	0.0064 (9)	0.0050 (8)
C26	0.0348 (12)	0.0334 (11)	0.0214 (10)	−0.0007 (9)	0.0085 (9)	0.0082 (8)
C27	0.0253 (10)	0.0299 (10)	0.0240 (10)	−0.0001 (8)	0.0099 (8)	0.0119 (8)
C28	0.0306 (11)	0.0393 (12)	0.0224 (10)	−0.0016 (9)	0.0043 (9)	0.0133 (9)
C29	0.0291 (11)	0.0323 (11)	0.0286 (11)	−0.0067 (9)	0.0027 (9)	0.0109 (9)
C30	0.0251 (10)	0.0289 (10)	0.0263 (10)	−0.0013 (8)	0.0069 (8)	0.0119 (8)
C31	0.0261 (10)	0.0312 (10)	0.0243 (10)	−0.0011 (9)	0.0076 (8)	0.0118 (8)
C32	0.0251 (10)	0.0318 (10)	0.0247 (10)	−0.0035 (8)	0.0056 (8)	0.0115 (8)
C33	0.0298 (11)	0.0209 (9)	0.0249 (10)	−0.0001 (8)	0.0100 (8)	0.0109 (8)
C34	0.0342 (12)	0.0288 (10)	0.0312 (12)	−0.0026 (9)	0.0093 (9)	0.0103 (9)
C35	0.0285 (11)	0.0344 (11)	0.0349 (12)	−0.0033 (9)	0.0074 (9)	0.0155 (9)
C36	0.0278 (11)	0.0338 (11)	0.0232 (10)	−0.0081 (9)	0.0044 (8)	0.0136 (9)
N1	0.0394 (12)	0.0381 (11)	0.0468 (13)	−0.0028 (9)	0.0088 (9)	0.0215 (9)
N2	0.0314 (10)	0.0299 (9)	0.0291 (10)	0.0013 (8)	0.0056 (8)	0.0130 (7)
N3	0.0318 (10)	0.0367 (10)	0.0327 (10)	−0.0005 (8)	0.0078 (8)	0.0143 (8)
N4	0.0441 (13)	0.0528 (13)	0.0494 (14)	−0.0132 (11)	0.0161 (11)	0.0174 (11)
O1	0.0298 (8)	0.0388 (8)	0.0208 (7)	0.0028 (6)	0.0047 (6)	0.0070 (6)
O2	0.0276 (8)	0.0310 (8)	0.0322 (8)	0.0037 (6)	0.0097 (6)	0.0134 (6)
O3	0.0549 (11)	0.0380 (9)	0.0319 (9)	−0.0068 (8)	0.0074 (8)	0.0173 (7)
O4	0.0526 (12)	0.0673 (13)	0.0427 (11)	−0.0335 (10)	−0.0005 (9)	0.0235 (10)
O5	0.0527 (11)	0.0393 (9)	0.0391 (10)	−0.0201 (8)	0.0045 (8)	0.0162 (8)
O6	0.0568 (12)	0.0530 (11)	0.0345 (10)	−0.0184 (9)	0.0026 (8)	0.0222 (8)
O7	0.0388 (9)	0.0409 (9)	0.0245 (8)	0.0020 (7)	0.0055 (7)	0.0107 (7)
O8	0.0385 (9)	0.0331 (8)	0.0275 (8)	0.0018 (7)	0.0024 (7)	0.0108 (6)

Geometric parameters (Å, °)

Co1—O2^{i}	2.0369 (16)	C17—C18	1.385 (4)
Co1—O1^{ii}	2.0519 (17)	C17—H17A	0.9300
Co1—O8	2.1394 (18)	C18—C19	1.376 (4)
Co1—N3	2.1716 (19)	C19—C20	1.391 (4)
Co1—O7	2.1885 (18)	C19—H19A	0.9300
Co1—N2	2.2072 (19)	C20—N4	1.321 (4)
Co1—C36	2.471 (2)	C20—H20A	0.9300
C1—N1	1.337 (3)	C21—C22	1.392 (3)
C1—C2	1.378 (3)	C21—C26	1.396 (3)
C1—H1A	0.9300	C21—C27	1.485 (3)
C2—C3	1.380 (3)	C22—C23	1.386 (3)
C2—H2A	0.9300	C22—H22A	0.9300
C3—C4	1.397 (3)	C23—C24	1.408 (3)

C3—C8	1.494 (3)	C23—C33	1.506 (3)
C4—C5	1.387 (3)	C24—C25	1.385 (3)
C4—H4A	0.9300	C24—C34	1.492 (3)
C5—N1	1.324 (3)	C25—C26	1.386 (3)
C5—H5A	0.9300	C25—H25A	0.9300
C6—N2	1.335 (3)	C26—H26A	0.9300
C6—C7	1.381 (3)	C27—C32	1.387 (3)
C6—H6A	0.9300	C27—C28	1.397 (3)
C7—C8	1.395 (3)	C28—C29	1.391 (3)
C7—H7A	0.9300	C28—H28A	0.9300
C8—C9	1.377 (3)	C29—C30	1.385 (3)
C9—C10	1.390 (3)	C29—H29A	0.9300
C9—H9A	0.9300	C30—C31	1.401 (3)
C10—N2	1.339 (3)	C30—C35	1.494 (3)
C10—H10A	0.9300	C31—C32	1.391 (3)
C11—N3	1.329 (3)	C31—C36	1.502 (3)
C11—C12	1.386 (3)	C32—H32A	0.9300
C11—H11A	0.9300	C33—O1	1.249 (3)
C12—C13	1.378 (3)	C33—O2	1.253 (3)
C12—H12A	0.9300	C34—O3	1.212 (3)
C13—C14	1.378 (4)	C34—O4	1.308 (3)
C13—C18	1.492 (3)	C35—O6	1.201 (3)
C14—C15	1.386 (4)	C35—O5	1.319 (3)
C14—H14A	0.9300	C36—O7	1.250 (3)
C15—N3	1.328 (3)	C36—O8	1.261 (3)
C15—H15A	0.9300	O1—Co1^{iii}	2.0519 (17)
C16—N4	1.342 (4)	O2—Co1^{i}	2.0369 (16)
C16—C17	1.378 (3)	O4—H1	0.8200
C16—H16A	0.9300	O5—H2	0.8200
O2^{i}—Co1—O1^{ii}	99.25 (7)	C19—C18—C13	119.9 (2)
O2^{i}—Co1—O8	103.34 (7)	C17—C18—C13	122.2 (2)
O1^{ii}—Co1—O8	157.16 (7)	C18—C19—C20	119.6 (3)
O2^{i}—Co1—N3	89.85 (7)	C18—C19—H19A	120.2
O1^{ii}—Co1—N3	85.19 (7)	C20—C19—H19A	120.2
O8—Co1—N3	91.48 (7)	N4—C20—C19	122.4 (3)
O2^{i}—Co1—O7	164.24 (6)	N4—C20—H20A	118.8
O1^{ii}—Co1—O7	96.34 (7)	C19—C20—H20A	118.8
O8—Co1—O7	60.97 (7)	C22—C21—C26	118.49 (18)
N3—Co1—O7	89.13 (7)	C22—C21—C27	119.44 (19)
O2^{i}—Co1—N2	96.19 (7)	C26—C21—C27	121.79 (19)
O1^{ii}—Co1—N2	94.62 (7)	C23—C22—C21	121.28 (19)
O8—Co1—N2	86.34 (7)	C23—C22—H22A	119.4
N3—Co1—N2	173.91 (7)	C21—C22—H22A	119.4
O7—Co1—N2	84.84 (7)	C22—C23—C24	119.57 (19)
O2^{i}—Co1—C36	134.01 (8)	C22—C23—C33	117.84 (18)
O1^{ii}—Co1—C36	126.68 (8)	C24—C23—C33	122.03 (17)

O8—Co1—C36	30.67 (7)	C25—C24—C23	119.23 (18)
N3—Co1—C36	91.59 (7)	C25—C24—C34	121.77 (19)
O7—Co1—C36	30.34 (7)	C23—C24—C34	118.92 (19)
N2—Co1—C36	83.63 (7)	C24—C25—C26	120.6 (2)
N1—C1—C2	122.7 (2)	C24—C25—H25A	119.7
N1—C1—H1A	118.6	C26—C25—H25A	119.7
C2—C1—H1A	118.6	C25—C26—C21	120.8 (2)
C3—C2—C1	119.9 (2)	C25—C26—H26A	119.6
C3—C2—H2A	120.1	C21—C26—H26A	119.6
C1—C2—H2A	120.1	C32—C27—C28	118.43 (18)
C2—C3—C4	117.3 (2)	C32—C27—C21	119.95 (19)
C2—C3—C8	121.7 (2)	C28—C27—C21	121.48 (18)
C4—C3—C8	121.0 (2)	C29—C28—C27	120.23 (19)
C5—C4—C3	119.0 (2)	C29—C28—H28A	119.9
C5—C4—H4A	120.5	C27—C28—H28A	119.9
C3—C4—H4A	120.5	C30—C29—C28	121.0 (2)
N1—C5—C4	123.1 (2)	C30—C29—H29A	119.5
N1—C5—H5A	118.5	C28—C29—H29A	119.5
C4—C5—H5A	118.5	C29—C30—C31	119.22 (18)
N2—C6—C7	123.8 (2)	C29—C30—C35	121.1 (2)
N2—C6—H6A	118.1	C31—C30—C35	119.62 (19)
C7—C6—H6A	118.1	C32—C31—C30	119.32 (19)
C6—C7—C8	119.6 (2)	C32—C31—C36	116.05 (18)
C6—C7—H7A	120.2	C30—C31—C36	124.49 (17)
C8—C7—H7A	120.2	C27—C32—C31	121.76 (19)
C9—C8—C7	116.82 (19)	C27—C32—H32A	119.1
C9—C8—C3	122.9 (2)	C31—C32—H32A	119.1
C7—C8—C3	120.2 (2)	O1—C33—O2	126.0 (2)
C8—C9—C10	119.9 (2)	O1—C33—C23	117.37 (19)
C8—C9—H9A	120.0	O2—C33—C23	116.58 (19)
C10—C9—H9A	120.0	O3—C34—O4	123.4 (2)
N2—C10—C9	123.3 (2)	O3—C34—C24	122.6 (2)
N2—C10—H10A	118.3	O4—C34—C24	113.95 (19)
C9—C10—H10A	118.3	O6—C35—O5	123.6 (2)
N3—C11—C12	124.4 (2)	O6—C35—C30	123.3 (2)
N3—C11—H11A	117.8	O5—C35—C30	113.08 (19)
C12—C11—H11A	117.8	O7—C36—O8	122.0 (2)
C13—C12—C11	118.7 (2)	O7—C36—C31	119.0 (2)
C13—C12—H12A	120.6	O8—C36—C31	118.4 (2)
C11—C12—H12A	120.6	O7—C36—Co1	62.22 (12)
C14—C13—C12	117.2 (2)	O8—C36—Co1	59.96 (11)
C14—C13—C18	121.8 (2)	C31—C36—Co1	168.81 (14)
C12—C13—C18	121.1 (2)	C5—N1—C1	117.9 (2)
C13—C14—C15	120.2 (2)	C6—N2—C10	116.49 (19)
C13—C14—H14A	119.9	C6—N2—Co1	121.34 (15)
C15—C14—H14A	119.9	C10—N2—Co1	121.53 (16)
N3—C15—C14	122.8 (3)	C15—N3—C11	116.5 (2)
N3—C15—H15A	118.6	C15—N3—Co1	122.41 (17)
C14—C15—H15A	118.6	C11—N3—Co1	120.75 (16)

N4—C16—C17	122.6 (3)	C20—N4—C16	118.2 (2)
N4—C16—H16A	118.7	C33—O1—Co1^{iii}	124.20 (15)
C17—C16—H16A	118.7	C33—O2—Co1^{i}	139.83 (13)
C16—C17—C18	119.3 (3)	C34—O4—H1	109.2
C16—C17—H17A	120.4	C35—O5—H2	109.2
C18—C17—H17A	120.4	C36—O7—Co1	87.44 (14)
C19—C18—C17	117.8 (2)	C36—O8—Co1	89.37 (13)

Symmetry codes: (i) −*x*, −*y*, −*z*+1; (ii) *x*, *y*, *z*−1; (iii) *x*, *y*, *z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H1···N4^{iv}	0.82	1.85	2.624 (3)	157
O5—H2···N1^{v}	0.82	1.88	2.655 (2)	157

Symmetry codes: (iv) *x*−1, *y*−1, *z*+1; (v) *x*+1, *y*+1, *z*.

Fig. 1

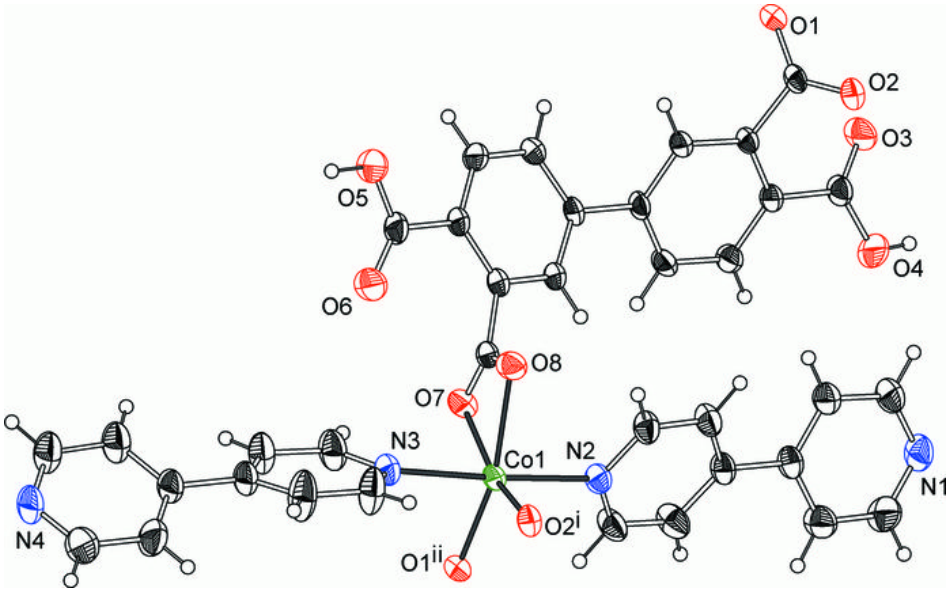

Fig. 2