Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[aqua(dipyrido[3,2-*a*:2′,3′-*c*]phenazine)cobalt(II)]-μ-benzene-1,4-dicarboxylato]

Fang-Wei and Ze-Min Mei*

Department of Chemistry, Baicheng Normal College, Baicheng 137000, People's Republic of China
Correspondence e-mail: fangwei1026@yahoo.com.cn

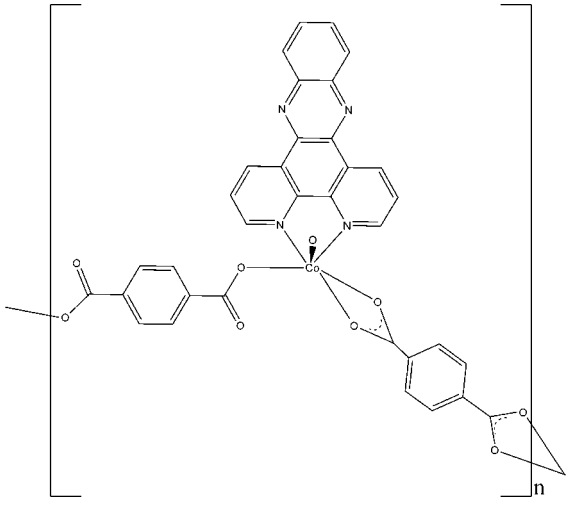
Received 2 November 2007; accepted 7 November 2007

Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.006 Å; R factor = 0.047; wR factor = 0.114; data-to-parameter ratio = 12.4.

In the title compound, $[Co(C_8H_4O_4)(C_{18}H_{10}N_4)(H_2O)]_n$, the Co^{II} atom is six-coordinated by three O atoms from two benzene-1,4-dicarboxylate (1,4-BDC) dianions (one bidentate and one monodentate), one water molecule and two N atoms from a bidentate dipyrido[3,2-*a*:2′,3′-*c*]phenazine ligand, resulting in a distorted *cis*-CoO_4N_2 octahedral geometry. The Co^{II} atoms are bridged by the 1,4-BDC ligands, forming a single-chain polymer structure. Both BDC ligands are centrosymmetric. Neighbouring chains interact through π–π interactions [minimum centroid–centroid separation = 3.459 (2) Å] and O—H···O hydrogen bonds.

Related literature

For related structures, see: Li *et al.* (2006, 2007). For the ligand synthesis, see: Dickeson & Summers (1970).



Experimental

Crystal data

$[Co(C_8H_4O_4)(C_{18}H_{10}N_4)(H_2O)]$
M_r = 523.36
Monoclinic, $P2_1/n$
a = 10.5218 (19) Å
b = 11.742 (2) Å
c = 18.077 (3) Å
β = 101.281 (4)°
V = 2190.2 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.83 mm^{-1}
T = 292 (2) K
0.47 × 0.21 × 0.10 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.815, T_{max} = 0.924
11590 measured reflections
4317 independent reflections
2417 reflections with $I > 2\sigma(I)$
R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.114
S = 0.88
4317 reflections
349 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.70 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O4	2.020 (3)	Co1—N2	2.122 (3)
Co1—O3	2.080 (3)	Co1—N1	2.182 (3)
Co1—O1	2.119 (3)	Co1—O2	2.250 (3)
N2—Co1—N1	75.79 (12)	O1—Co1—O2	60.22 (10)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3*WA*···O1^{i}	0.96 (5)	2.00 (5)	2.877 (4)	151 (4)
O3—H3*WB*···O5^{i}	0.73 (5)	1.94 (5)	2.666 (4)	179 (6)

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2002); 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, 1998); software used to prepare material for publication: *SHELXTL-Plus*.

The authors thank BaiCheng Normal College for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2627).

References

Bruker (1998). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2002). *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2006). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dickeson, J. E. & Summers, L. A. (1970). *Aust. J. Chem.* **23**, 1023–1027.
Li, C.-B., Fang, W., Dong, E.-J., Liu, B. & Li, Y.-W. (2007). *Acta Cryst.* E**63**, m150–m152.

  doi:10.1107/S1600536807056826

Li, C.-B., Fang, W., Gao, G.-G. & Liu, B. (2006). *Acta Cryst.* E**62**, m1312–m1314.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

supplementary materials

Acta Cryst. (2007). E**63**, m3098-m3099 [**doi:10.1107/S1600536807056826**]

catena-Poly[[aqua(dipyrido[3,2-*a*:2',3'-*c*]phenazine)cobalt(II)]-μ-benzene-1,4-dicarboxylato]

Fang-Wei and Z.-M. Mei

Comment

1,10-Phenanthroline (phen) and its derivatives are important ligands with numerous uses in the constructon of metal-organic complexes. Supramolecular architectures based on the dipydo[3,2 − a:2',3'-c]phenazine (Dppz) molecule have considerably less attention (Li *et al.*, 2006) As part of our ongoing studies in this area (Li *et al.*, 2007), we now report the sythesis and structure of the title compound,(I), containing Co_{II} ions, 1,4-BDC anions and phe-derived dipydo[3,2 − a:2',3'-c]phenazine ($C_{18}H_{10}N_4$) ligands.

In compound (I), the Co^{II} atom is six-coordinated by two N atoms from one Dppz molecule, three O atoms from two 1,4-BDC dianions (one monodentate, one bidentate) and one water molecule (Fig. 1, Table 1): a distorted octahedral *cis*-CoN_2O_4 arrangement is formed.

Neighboring Co^{II} atoms are bridged by the centrosymmetric 1,4-BDC ligands forming a one-dimensional chain structure (Fig. 2). In the crystal structure, adjacent chains are connected through π-π interactions between dppz and 1,4-BDC ligands with a minimum centroid-centroid stacking distance of 3.459 (2) Å. O—H···O hydrogen bonds involving the water molecules and carboxylate O atom acceptors (Table 2) complete the structure of (I).

Experimental

The Dppz ligand was synthesized by the literature method of Dickeson & Summers (1970). A mixture of $CoCl_2{\cdot}2H_2O$ (0.3 mmol), Dppz (0.1 mmol) and benzene-1,4-dicarboxylic acid (0.3 mmol) in 30 ml of distilled water was stirred thoroughly for 1 h at ambient temperature. The pH value was adjusted to about 7.5 with NaOH aqueous solution. The suspension was sealed in a Teflon-lined stainless reaction vessel (40 ml) and heated at 443 K for 5 days. The vessel was cooled slowly to room temperature at a rate of 10 K h^{-1} before opening, and purple blocks of (I) were recovered.

Refinement

The water H atoms were located in a difference map and freely refined. The C-bound H atoms were placed geometrically (C—H = 0.93 Å) and refined as riding with U_{iso}(H)= 1.2U_{eq}(carrier). The highest difference peak is 1.05Å from H2B.

Figures

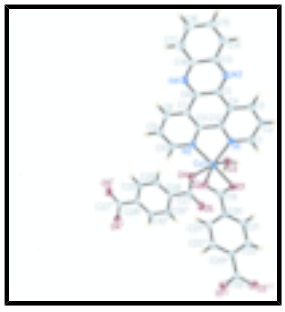


Fig. 1. The asymmetric unit of (I), together with additional atoms to complete the coordination of Co1 with displacement ellipsoids drawn at the 30% probability level (arbitrary spheres for the H atoms). [Symmetry codes: (i) 1 − *x*, 1 − *y*, 1 − *z*; (ii) −*x*, −*y*, 1 − *z*.

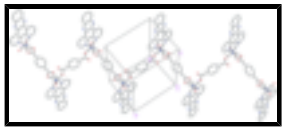


Fig. 2. A view of the polymeric chain structure of (I). H atoms have been omitted for clarity.

catena-Poly[[aqua(dipyrido[3,2 − a:2',3'-c]phenazine)cobalt(II)]-μ-benzene- 1,4-dicarboxylato]

Crystal data

$[Co(C_8H_4O_4)(C_{18}H_{10}N_4)(H_2O)]$	F_{000} = 1068.0
M_r = 523.36	D_x = 1.587 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 1368 reflections
a = 10.5218 (19) Å	θ = 2.3–26.1º
b = 11.742 (2) Å	μ = 0.83 mm^{-1}
c = 18.077 (3) Å	*T* = 292 (2) K
β = 101.281 (4)º	Block, purple
V = 2190.2 (7) Å^3	0.47 × 0.21 × 0.10 mm
Z = 4	

Data collection

Bruker APEXII diffractometer	4317 independent reflections
Radiation source: fine-focus sealed tube	2417 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.059
Detector resolution: 0 pixels mm^{-1}	θ_{max} = 26.0º
T = 292(2) K	θ_{min} = 2.1º
ω scans	*h* = −12→10
Absorption correction: multi-scan (SADABS; Bruker, 2002)	*k* = −14→11
T_{min} = 0.815, T_{max} = 0.924	*l* = −20→22
11590 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.114$	$w = 1/[\sigma^2(F_o^2) + (0.0475P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.88$	$(\Delta/\sigma)_{max} = 0.001$
4317 reflections	$\Delta\rho_{max} = 1.70$ e Å^{-3}
349 parameters	$\Delta\rho_{min} = -0.40$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.49412 (5)	0.06855 (4)	0.63798 (3)	0.03467 (18)
O1	0.3496 (3)	−0.0366 (2)	0.57392 (15)	0.0440 (7)
O2	0.2835 (3)	0.1061 (2)	0.63506 (15)	0.0487 (8)
O3	0.6371 (3)	0.0100 (3)	0.58260 (19)	0.0450 (8)
N1	0.5516 (3)	−0.0670 (3)	0.72031 (16)	0.0367 (8)
C5	0.6497 (3)	−0.0620 (3)	0.9301 (2)	0.0363 (9)
N3	0.6541 (3)	0.1013 (3)	1.01155 (18)	0.0431 (9)
N4	0.6879 (3)	−0.1346 (3)	0.98703 (19)	0.0451 (9)
N2	0.5349 (3)	0.1544 (3)	0.74323 (17)	0.0380 (8)
C6	0.7111 (4)	−0.0898 (4)	1.0577 (2)	0.0437 (11)
C4	0.6252 (4)	−0.1065 (3)	0.8530 (2)	0.0367 (10)
C18	0.5825 (3)	−0.0328 (3)	0.7924 (2)	0.0326 (9)
C12	0.6338 (3)	0.0564 (3)	0.9431 (2)	0.0368 (9)
C10	0.7204 (4)	0.0719 (4)	1.1443 (2)	0.0578 (13)
H10A	0.7108	0.1493	1.1527	0.069*
C13	0.5971 (4)	0.1338 (3)	0.8784 (2)	0.0373 (10)
C17	0.5705 (3)	0.0889 (3)	0.8059 (2)	0.0337 (9)

C19	0.2598 (4)	0.0287 (4)	0.5870 (2)	0.0401 (10)
C11	0.6939 (4)	0.0280 (4)	1.0695 (2)	0.0447 (11)
C1	0.5651 (4)	−0.1773 (3)	0.7058 (2)	0.0471 (11)
H1B	0.5425	−0.2025	0.6562	0.057*
C3	0.6421 (4)	−0.2206 (4)	0.8354 (2)	0.0489 (11)
H3B	0.6739	−0.2724	0.8734	0.059*
C14	0.5886 (4)	0.2511 (4)	0.8866 (2)	0.0520 (12)
H14A	0.6084	0.2842	0.9342	0.062*
C8	0.7748 (4)	−0.1170 (5)	1.1915 (3)	0.0652 (15)
H8A	0.8001	−0.1649	1.2327	0.078*
C2	0.6120 (4)	−0.2560 (4)	0.7623 (2)	0.0564 (13)
H2B	0.6225	−0.3319	0.7502	0.068*
C16	0.5236 (4)	0.2654 (3)	0.7536 (2)	0.0490 (12)
H16A	0.4958	0.3109	0.7115	0.059*
C9	0.7600 (4)	0.0000 (5)	1.2033 (3)	0.0633 (14)
H9A	0.7773	0.0288	1.2522	0.076*
C7	0.7525 (4)	−0.1619 (4)	1.1197 (2)	0.0551 (12)
H7A	0.7647	−0.2392	1.1124	0.066*
C15	0.5509 (5)	0.3175 (4)	0.8239 (2)	0.0578 (13)
H15A	0.5436	0.3960	0.8283	0.069*
O4	0.5077 (3)	0.2196 (2)	0.58662 (15)	0.0508 (8)
O5	0.3983 (3)	0.2030 (2)	0.46817 (16)	0.0588 (9)
C27	0.4606 (4)	0.2578 (3)	0.5222 (2)	0.0405 (10)
C30	0.5377 (4)	0.4530 (3)	0.5701 (2)	0.0384 (10)
C29	0.4429 (4)	0.4323 (4)	0.4403 (2)	0.0388 (10)
C28	0.4816 (4)	0.3832 (3)	0.5108 (2)	0.0344 (9)
C21	0.0943 (4)	−0.0796 (4)	0.4949 (2)	0.0406 (10)
C20	0.1242 (4)	0.0122 (3)	0.5429 (2)	0.0342 (9)
C22	0.0299 (4)	0.0927 (4)	0.5484 (2)	0.0408 (11)
H30	0.565 (3)	0.424 (3)	0.613 (2)	0.040 (12)*
H22	0.049 (3)	0.156 (3)	0.5768 (19)	0.036 (11)*
H21	0.161 (3)	−0.133 (3)	0.4907 (18)	0.033 (10)*
H3WA	0.631 (4)	0.045 (4)	0.534 (3)	0.075 (16)*
H3WB	0.628 (5)	−0.048 (4)	0.568 (3)	0.08 (2)*
H29	0.404 (4)	0.391 (3)	0.401 (2)	0.051 (13)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0429 (3)	0.0306 (3)	0.0290 (3)	−0.0023 (3)	0.0033 (2)	0.0023 (3)
O1	0.0375 (17)	0.0438 (17)	0.0486 (18)	0.0018 (14)	0.0032 (14)	0.0048 (14)
O2	0.0464 (19)	0.059 (2)	0.0369 (17)	−0.0066 (15)	−0.0003 (14)	−0.0121 (15)
O3	0.056 (2)	0.037 (2)	0.045 (2)	−0.0058 (16)	0.0153 (16)	−0.0020 (17)
N1	0.049 (2)	0.0328 (18)	0.0278 (18)	−0.0049 (17)	0.0053 (15)	−0.0004 (16)
C5	0.032 (2)	0.047 (2)	0.029 (2)	−0.003 (2)	0.0049 (17)	0.009 (2)
N3	0.041 (2)	0.059 (2)	0.030 (2)	−0.0001 (17)	0.0070 (16)	0.0010 (17)
N4	0.042 (2)	0.057 (2)	0.035 (2)	−0.0023 (17)	0.0052 (17)	0.0077 (18)
N2	0.042 (2)	0.036 (2)	0.034 (2)	0.0000 (16)	0.0029 (16)	0.0030 (16)

C6	0.037 (2)	0.063 (3)	0.031 (2)	−0.004 (2)	0.0061 (19)	0.010 (2)
C4	0.036 (2)	0.037 (2)	0.038 (2)	−0.0012 (18)	0.0081 (19)	0.0047 (19)
C18	0.033 (2)	0.031 (2)	0.033 (2)	−0.0046 (17)	0.0043 (18)	0.0020 (17)
C12	0.034 (2)	0.049 (3)	0.027 (2)	−0.002 (2)	0.0035 (17)	0.004 (2)
C10	0.054 (3)	0.084 (4)	0.035 (3)	−0.002 (3)	0.009 (2)	−0.001 (3)
C13	0.038 (3)	0.043 (3)	0.030 (2)	−0.0001 (19)	0.0029 (19)	0.0008 (18)
C17	0.032 (2)	0.039 (2)	0.029 (2)	−0.0021 (18)	0.0024 (17)	0.0018 (18)
C19	0.044 (3)	0.046 (3)	0.030 (2)	−0.008 (2)	0.007 (2)	0.013 (2)
C11	0.033 (2)	0.070 (3)	0.030 (2)	−0.002 (2)	0.0035 (19)	0.002 (2)
C1	0.071 (3)	0.035 (3)	0.034 (2)	0.000 (2)	0.009 (2)	−0.003 (2)
C3	0.063 (3)	0.039 (3)	0.043 (3)	0.003 (2)	0.008 (2)	0.013 (2)
C14	0.066 (3)	0.048 (3)	0.039 (3)	0.001 (2)	0.003 (2)	−0.008 (2)
C8	0.060 (3)	0.093 (4)	0.038 (3)	−0.006 (3)	0.000 (2)	0.021 (3)
C2	0.096 (4)	0.031 (2)	0.040 (3)	0.001 (2)	0.007 (3)	0.004 (2)
C16	0.068 (3)	0.036 (3)	0.041 (3)	0.003 (2)	0.006 (2)	0.005 (2)
C9	0.061 (3)	0.092 (4)	0.034 (3)	−0.011 (3)	0.006 (2)	0.001 (3)
C7	0.053 (3)	0.069 (3)	0.040 (3)	−0.005 (2)	0.001 (2)	0.012 (2)
C15	0.090 (4)	0.032 (3)	0.049 (3)	0.006 (2)	0.006 (3)	−0.004 (2)
O4	0.075 (2)	0.0348 (16)	0.0403 (17)	−0.0023 (15)	0.0061 (15)	0.0125 (14)
O5	0.096 (2)	0.0325 (17)	0.0463 (19)	−0.0056 (17)	0.0109 (18)	−0.0029 (15)
C27	0.050 (3)	0.035 (2)	0.041 (3)	0.002 (2)	0.019 (2)	0.004 (2)
C30	0.044 (3)	0.036 (3)	0.034 (2)	0.003 (2)	0.007 (2)	0.012 (2)
C29	0.047 (3)	0.035 (2)	0.035 (2)	−0.005 (2)	0.007 (2)	0.000 (2)
C28	0.037 (2)	0.030 (2)	0.037 (2)	0.0043 (18)	0.0109 (19)	0.0021 (18)
C21	0.039 (3)	0.040 (3)	0.043 (2)	0.004 (2)	0.008 (2)	−0.003 (2)
C20	0.037 (2)	0.037 (2)	0.028 (2)	−0.0051 (19)	0.0049 (18)	0.0017 (18)
C22	0.044 (3)	0.040 (3)	0.038 (3)	−0.006 (2)	0.006 (2)	−0.008 (2)

Geometric parameters (Å, °)

Co1—O4	2.020 (3)	C19—C20	1.505 (5)
Co1—O3	2.080 (3)	C1—C2	1.394 (5)
Co1—O1	2.119 (3)	C1—H1B	0.9300
Co1—N2	2.122 (3)	C3—C2	1.362 (5)
Co1—N1	2.182 (3)	C3—H3B	0.9300
Co1—O2	2.250 (3)	C14—C15	1.369 (5)
Co1—C19	2.501 (4)	C14—H14A	0.9300
O1—C19	1.275 (5)	C8—C7	1.377 (6)
O2—C19	1.248 (5)	C8—C9	1.404 (7)
O3—H3WA	0.96 (5)	C8—H8A	0.9300
O3—H3WB	0.73 (5)	C2—H2B	0.9300
N1—C1	1.335 (4)	C16—C15	1.389 (5)
N1—C18	1.340 (4)	C16—H16A	0.9300
C5—N4	1.336 (4)	C9—H9A	0.9300
C5—C12	1.426 (5)	C7—H7A	0.9300
C5—C4	1.462 (5)	C15—H15A	0.9300
N3—C12	1.323 (5)	O4—C27	1.257 (4)
N3—C11	1.358 (5)	O5—C27	1.243 (4)
N4—C6	1.358 (5)	C27—C28	1.509 (5)

N2—C16	1.325 (5)	C30—C29^{i}	1.381 (5)
N2—C17	1.360 (4)	C30—C28	1.386 (5)
C6—C7	1.404 (5)	C30—H30	0.85 (3)
C6—C11	1.416 (6)	C29—C30^{i}	1.381 (5)
C4—C3	1.397 (5)	C29—C28	1.386 (5)
C4—C18	1.401 (5)	C29—H29	0.89 (4)
C18—C17	1.460 (5)	C21—C20	1.380 (5)
C12—C13	1.471 (5)	C21—C22^{ii}	1.394 (5)
C10—C9	1.360 (6)	C21—H21	0.96 (3)
C10—C11	1.422 (5)	C20—C22	1.389 (5)
C10—H10A	0.9300	C22—C21^{ii}	1.394 (5)
C13—C17	1.389 (5)	C22—H22	0.91 (3)
C13—C14	1.390 (5)		
O4—Co1—O3	86.90 (14)	O2—C19—O1	120.9 (4)
O4—Co1—O1	111.62 (10)	O2—C19—C20	120.2 (4)
O3—Co1—O1	93.07 (12)	O1—C19—C20	118.9 (4)
O4—Co1—N2	88.55 (12)	O2—C19—Co1	63.9 (2)
O3—Co1—N2	123.37 (12)	O1—C19—Co1	57.9 (2)
O1—Co1—N2	139.90 (12)	C20—C19—Co1	169.5 (3)
O4—Co1—N1	156.75 (11)	N3—C11—C6	122.1 (4)
O3—Co1—N1	87.56 (13)	N3—C11—C10	118.5 (4)
O1—Co1—N1	91.21 (11)	C6—C11—C10	119.4 (4)
N2—Co1—N1	75.79 (12)	N1—C1—C2	122.4 (4)
O4—Co1—O2	88.58 (11)	N1—C1—H1B	118.8
O3—Co1—O2	148.78 (12)	C2—C1—H1B	118.8
O1—Co1—O2	60.22 (10)	C2—C3—C4	119.9 (4)
N2—Co1—O2	87.34 (11)	C2—C3—H3B	120.1
N1—Co1—O2	107.40 (11)	C4—C3—H3B	120.1
O4—Co1—C19	98.53 (12)	C15—C14—C13	119.4 (4)
O3—Co1—C19	120.97 (14)	C15—C14—H14A	120.3
O1—Co1—C19	30.64 (11)	C13—C14—H14A	120.3
N2—Co1—C19	115.53 (14)	C7—C8—C9	121.0 (5)
N1—Co1—C19	103.67 (12)	C7—C8—H8A	119.5
O2—Co1—C19	29.85 (11)	C9—C8—H8A	119.5
C19—O1—Co1	91.5 (2)	C3—C2—C1	119.4 (4)
C19—O2—Co1	86.3 (2)	C3—C2—H2B	120.3
Co1—O3—H3WA	112 (3)	C1—C2—H2B	120.3
Co1—O3—H3WB	115 (4)	N2—C16—C15	123.7 (4)
H3WA—O3—H3WB	95 (5)	N2—C16—H16A	118.1
C1—N1—C18	117.8 (3)	C15—C16—H16A	118.1
C1—N1—Co1	126.9 (3)	C10—C9—C8	120.9 (5)
C18—N1—Co1	115.2 (2)	C10—C9—H9A	119.6
N4—C5—C12	121.4 (4)	C8—C9—H9A	119.6
N4—C5—C4	118.5 (4)	C8—C7—C6	119.4 (5)
C12—C5—C4	120.1 (3)	C8—C7—H7A	120.3
C12—N3—C11	116.0 (4)	C6—C7—H7A	120.3
C5—N4—C6	116.7 (4)	C14—C15—C16	118.7 (4)
C16—N2—C17	117.1 (3)	C14—C15—H15A	120.6

C16—N2—Co1	125.9 (3)	C16—C15—H15A	120.6
C17—N2—Co1	116.9 (2)	C27—O4—Co1	133.5 (3)
N4—C6—C7	119.2 (4)	O5—C27—O4	126.5 (4)
N4—C6—C11	121.0 (4)	O5—C27—C28	117.9 (4)
C7—C6—C11	119.8 (4)	O4—C27—C28	115.6 (4)
C3—C4—C18	116.7 (4)	C29^{i}—C30—C28	121.5 (4)
C3—C4—C5	123.6 (4)	C29^{i}—C30—H30	119 (3)
C18—C4—C5	119.6 (4)	C28—C30—H30	120 (3)
N1—C18—C4	123.7 (3)	C30^{i}—C29—C28	120.4 (4)
N1—C18—C17	116.4 (3)	C30^{i}—C29—H29	118 (3)
C4—C18—C17	119.9 (3)	C28—C29—H29	121 (3)
N3—C12—C5	122.7 (3)	C30—C28—C29	118.0 (4)
N3—C12—C13	117.8 (4)	C30—C28—C27	121.6 (4)
C5—C12—C13	119.5 (3)	C29—C28—C27	120.4 (4)
C9—C10—C11	119.6 (5)	C20—C21—C22^{ii}	120.8 (4)
C9—C10—H10A	120.2	C20—C21—H21	119 (2)
C11—C10—H10A	120.2	C22^{ii}—C21—H21	120 (2)
C17—C13—C14	118.1 (4)	C21—C20—C22	119.9 (4)
C17—C13—C12	119.2 (3)	C21—C20—C19	120.7 (4)
C14—C13—C12	122.7 (4)	C22—C20—C19	119.4 (4)
N2—C17—C13	122.9 (3)	C20—C22—C21^{ii}	119.3 (4)
N2—C17—C18	115.6 (3)	C20—C22—H22	122 (2)
C13—C17—C18	121.5 (3)	C21^{ii}—C22—H22	119 (2)
O4—Co1—O1—C19	−69.1 (2)	Co1—O2—C19—O1	10.2 (4)
O3—Co1—O1—C19	−157.0 (2)	Co1—O2—C19—C20	−169.0 (3)
N2—Co1—O1—C19	46.2 (3)	Co1—O1—C19—O2	−10.9 (4)
N1—Co1—O1—C19	115.4 (2)	Co1—O1—C19—C20	168.4 (3)
O2—Co1—O1—C19	5.9 (2)	O4—Co1—C19—O2	−71.8 (2)
O4—Co1—O2—C19	110.0 (2)	O3—Co1—C19—O2	−163.3 (2)
O3—Co1—O2—C19	28.3 (4)	O1—Co1—C19—O2	169.6 (4)
O1—Co1—O2—C19	−6.1 (2)	N2—Co1—C19—O2	20.6 (3)
N2—Co1—O2—C19	−161.4 (2)	N1—Co1—C19—O2	101.2 (2)
N1—Co1—O2—C19	−87.2 (2)	O4—Co1—C19—O1	118.6 (2)
O4—Co1—N1—C1	−127.2 (4)	O3—Co1—C19—O1	27.0 (3)
O3—Co1—N1—C1	−50.9 (3)	N2—Co1—C19—O1	−149.0 (2)
O1—Co1—N1—C1	42.2 (3)	N1—Co1—C19—O1	−68.4 (2)
N2—Co1—N1—C1	−176.2 (3)	O2—Co1—C19—O1	−169.6 (4)
O2—Co1—N1—C1	101.2 (3)	O4—Co1—C19—C20	43.3 (18)
C19—Co1—N1—C1	70.5 (4)	O3—Co1—C19—C20	−48.2 (18)
O4—Co1—N1—C18	49.1 (5)	O1—Co1—C19—C20	−75.2 (17)
O3—Co1—N1—C18	125.4 (3)	N2—Co1—C19—C20	135.8 (17)
O1—Co1—N1—C18	−141.6 (3)	N1—Co1—C19—C20	−143.6 (17)
N2—Co1—N1—C18	0.1 (3)	O2—Co1—C19—C20	115.2 (18)
O2—Co1—N1—C18	−82.5 (3)	C12—N3—C11—C6	−0.8 (6)
C19—Co1—N1—C18	−113.3 (3)	C12—N3—C11—C10	178.4 (4)
C12—C5—N4—C6	−0.2 (5)	N4—C6—C11—N3	−0.1 (6)
C4—C5—N4—C6	179.3 (3)	C7—C6—C11—N3	180.0 (4)

O4—Co1—N2—C16	18.7 (3)	N4—C6—C11—C10	−179.4 (4)
O3—Co1—N2—C16	104.0 (4)	C7—C6—C11—C10	0.7 (6)
O1—Co1—N2—C16	−104.1 (4)	C9—C10—C11—N3	179.7 (4)
N1—Co1—N2—C16	−178.6 (4)	C9—C10—C11—C6	−1.0 (6)
O2—Co1—N2—C16	−69.9 (3)	C18—N1—C1—C2	−1.2 (6)
C19—Co1—N2—C16	−80.0 (4)	Co1—N1—C1—C2	175.0 (3)
O4—Co1—N2—C17	−164.4 (3)	C18—C4—C3—C2	−2.8 (6)
O3—Co1—N2—C17	−79.0 (3)	C5—C4—C3—C2	177.3 (4)
O1—Co1—N2—C17	72.8 (3)	C17—C13—C14—C15	2.0 (6)
N1—Co1—N2—C17	−1.7 (3)	C12—C13—C14—C15	−178.5 (4)
O2—Co1—N2—C17	107.0 (3)	C4—C3—C2—C1	0.4 (7)
C19—Co1—N2—C17	96.9 (3)	N1—C1—C2—C3	1.8 (7)
C5—N4—C6—C7	−179.5 (4)	C17—N2—C16—C15	2.7 (6)
C5—N4—C6—C11	0.7 (6)	Co1—N2—C16—C15	179.6 (3)
N4—C5—C4—C3	−1.4 (6)	C11—C10—C9—C8	0.0 (7)
C12—C5—C4—C3	178.1 (4)	C7—C8—C9—C10	1.4 (7)
N4—C5—C4—C18	178.6 (3)	C9—C8—C7—C6	−1.6 (7)
C12—C5—C4—C18	−1.9 (6)	N4—C6—C7—C8	−179.3 (4)
C1—N1—C18—C4	−1.5 (6)	C11—C6—C7—C8	0.5 (6)
Co1—N1—C18—C4	−178.1 (3)	C13—C14—C15—C16	−0.8 (7)
C1—N1—C18—C17	178.1 (3)	N2—C16—C15—C14	−1.7 (7)
Co1—N1—C18—C17	1.5 (4)	O3—Co1—O4—C27	82.1 (4)
C3—C4—C18—N1	3.4 (6)	O1—Co1—O4—C27	−10.0 (4)
C5—C4—C18—N1	−176.6 (3)	N2—Co1—O4—C27	−154.4 (4)
C3—C4—C18—C17	−176.1 (4)	N1—Co1—O4—C27	158.6 (4)
C5—C4—C18—C17	3.9 (5)	O2—Co1—O4—C27	−67.0 (4)
C11—N3—C12—C5	1.3 (6)	C19—Co1—O4—C27	−38.8 (4)
C11—N3—C12—C13	−176.9 (3)	Co1—O4—C27—O5	−7.5 (7)
N4—C5—C12—N3	−0.8 (6)	Co1—O4—C27—C28	171.8 (3)
C4—C5—C12—N3	179.7 (3)	$C29^{i}$—C30—C28—C29	−1.2 (7)
N4—C5—C12—C13	177.4 (3)	$C29^{i}$—C30—C28—C27	179.9 (4)
C4—C5—C12—C13	−2.1 (5)	$C30^{i}$—C29—C28—C30	1.2 (7)
N3—C12—C13—C17	−177.7 (4)	$C30^{i}$—C29—C28—C27	−179.9 (4)
C5—C12—C13—C17	4.1 (5)	O5—C27—C28—C30	173.0 (4)
N3—C12—C13—C14	2.8 (6)	O4—C27—C28—C30	−6.3 (6)
C5—C12—C13—C14	−175.4 (4)	O5—C27—C28—C29	−5.9 (6)
C16—N2—C17—C13	−1.3 (6)	O4—C27—C28—C29	174.8 (4)
Co1—N2—C17—C13	−178.5 (3)	$C22^{ii}$—C21—C20—C22	0.0 (7)
C16—N2—C17—C18	−179.8 (3)	$C22^{ii}$—C21—C20—C19	−177.4 (4)
Co1—N2—C17—C18	3.0 (4)	O2—C19—C20—C21	−173.8 (4)
C14—C13—C17—N2	−1.0 (6)	O1—C19—C20—C21	7.0 (5)
C12—C13—C17—N2	179.5 (3)	Co1—C19—C20—C21	76.3 (18)
C14—C13—C17—C18	177.4 (4)	O2—C19—C20—C22	8.8 (6)
C12—C13—C17—C18	−2.2 (6)	O1—C19—C20—C22	−170.5 (4)
N1—C18—C17—N2	−2.9 (5)	Co1—C19—C20—C22	−101.2 (18)
C4—C18—C17—N2	176.6 (3)	C21—C20—C22—$C21^{ii}$	0.0 (7)
N1—C18—C17—C13	178.6 (4)	C19—C20—C22—$C21^{ii}$	177.4 (4)

C4—C18—C17—C13	−1.9 (6)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3WA···O1^{iii}	0.96 (5)	2.00 (5)	2.877 (4)	151 (4)
O3—H3WB···O5^{iii}	0.73 (5)	1.94 (5)	2.666 (4)	179 (6)

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

Fig. 1

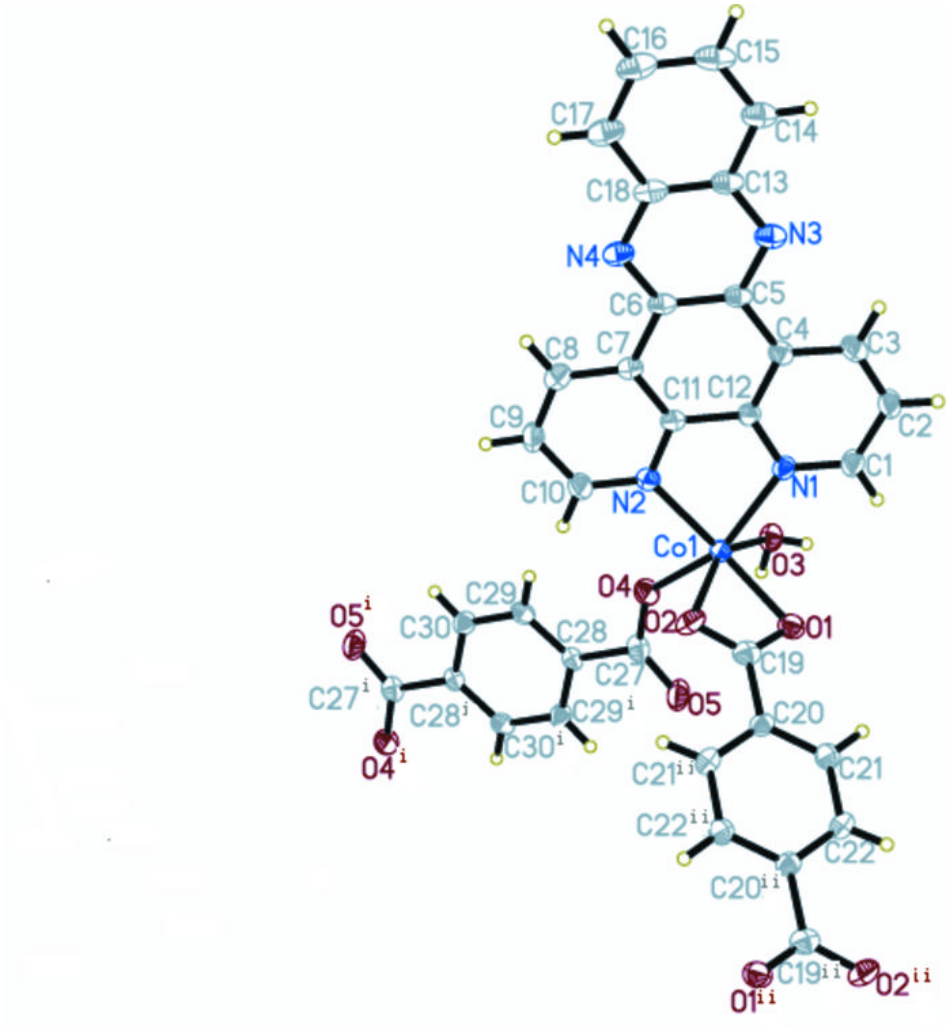

C16
C15
C17
C14
C18
C13
N4
N3
C6
C5
C8
C7
C4
C3
C11
C12
C9
C2
C10
N2
N1
C1
Co1
O3
O4
O2
O1
C29
O5i
C30
C28
C19
C27i
C27
O5
C28i
C29i
C20
O4i
C30i
C21ii
C21
C22ii
C22
C20ii
C19ii
O2ii
O1ii

Fig. 2