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Poly[aqua{μ_3-5-[(pyridin-2-ylmethyl)amino]isophthalato-$\kappa^5N,N':O^1,O^{1'}:O^3$}cobalt(II)]

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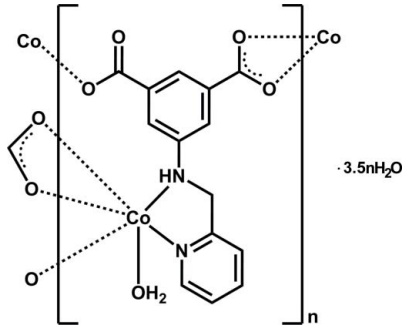
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.045; wR factor = 0.124; data-to-parameter ratio = 21.4.

In the title polymer, $\{[Co(C_{14}H_{10}N_2O_4)(H_2O)]\cdot 3.5H_2O\}_n$, the Co^{2+} ion is coordinated by three carboxylate O atoms from two 5-[(pyridin-2-ylmethyl)amino]isophthalate anions, two N atoms from a (pyridin-2-ylmethyl)amino group and an O atom from a water molecule, furnishing a distorted CoO_4N_2 octahedral geometry. Each anion acts as a μ_3-bridge, linking cobalt ions into a two-dimensional layer parallel to (100). The asymmetric unit also contains three and a half solvent water molecules, which could not be modeled. Therefore, the diffraction contribution of the solvent water molecules was removed by the subroutine SQUEEZE in *PLATON* [Spek (2009). *Acta Cryst.* D**65**, 148–155]. The crystal structure is stabilized by O—H···O hydrogen bonds in which the coordinated water molecule acts as donor and the carboxylate O atoms as acceptors.

Related literature

For related structures, see: Kuai *et al.* (2011).



Experimental

Crystal data

$[Co(C_{14}H_{10}N_2O_4)(H_2O)]\cdot 3.5H_2O$
M_r = 410.24
Monoclinic, $P2_1/c$
a = 11.0926 (11) Å
b = 9.8735 (10) Å
c = 17.4317 (15) Å
β = 116.533 (5)°
V = 1708.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.05 mm^{-1}
T = 293 K
0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.821, T_{max} = 0.821
11993 measured reflections
4259 independent reflections
3809 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.124
S = 1.11
4259 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.81 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—O3^{i}	1.9999 (19)	Co1—O1	2.132 (2)
Co1—N2^{ii}	2.090 (2)	Co1—O2	2.195 (2)
Co1—O5	2.110 (2)	Co1—N1^{ii}	2.275 (2)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5*WA*···O4^{i}	0.87	2.25	2.946 (3)	137
O5—H5*WA*···O1^{iii}	0.87	2.42	3.047 (3)	130
O5—H5*W*···O4^{iv}	0.93	1.90	2.819 (3)	168

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2000); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2477).

References

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supplementary materials

Acta Cryst. (2011). E**67**, m1862 [**doi:10.1107/S1600536811050318**]

Poly[aqua{μ_3-5-[(pyridin-2-ylmethyl)amino]isophthalato-$\kappa^5N,N':O^1,O^{1'}:O^3$}cobalt(II)]

X.-H. Zhu and X.-C. Cheng

Comment

5-(Pyridin-2-ylmethyl)aminoisophthalic acid possesses some peculiar features in the assembly of coordination compounds due to its unique molecular structure. Herein, we report the crystal structure of the title complex. The asymmetric unit consists of one cobalt ion, one 5-(pyridin-2-ylmethyl)aminoisophthalate anion, one coordinated water molecule, and 3.5 lattice water molecules. However, the solvent water molecules could not be modeled as discrete atomic sites. We employed SQUEEZE subroutine in PLATON (Spek, 2009) to exclude the diffraction contribution of the solvent water molecules.

In the title polymer, each Co ion is coordinated by three carboxylate O atoms from two different 5-(pyridin-2-ylmethyl)aminoisophthalate anions, two N atoms from (pyridin-2-ylmethyl)amino group and one O atom from a coordinated water molecule, to furnish a distorted CoO_4N_2 octahedral geometry (Fig. 1). Each anion acts as a μ_3-bridge, linking cobalt ions to form a two-dimensional layer. In the crystal structure, there exist O—H···O hydrogen bonds (Table 1). Coordinated water molecule and carboxylate oxygen atoms act as donors or acceptors in the formation of these hydrogen bonding interactions.

Experimental

A mixture of cobalt nitrate hexahydrate (58.2 mg, 0.2 mmol), 5-(pyridin-2-ylmethyl)aminoisophthalic acid (54.4 mg, 0.2 mmol), and 3 ml *N*,*N*-dimethylformamide in H_2O (12 ml) was sealed in a 16 ml Teflon-lined stainless steel container and heated to 373 K for 3 days. After cooling the container to the room temperature, red block crystals of the title complex were obtained.

Refinement

The hydrogen atoms bonded to C atoms were included in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 and 0.97 Å for aryl and methylene H-atoms with $U_{iso}(H) = 1.2U_{eq}(C)$. The hydrogen atoms bonded to N1 and O5 were located from a difference Fourier map and fixed at those positions with $U_{iso}(H) = 1.2U_{eq}(N \text{ or } O)$]. The structure contains three and a half molecules of water of hydration, which could not be modeled as discrete atomic sites. We employed SQUEEZE in PLATON (Spek, 2009) to remove the diffraction contribution of the solvent water molecules.

Figures

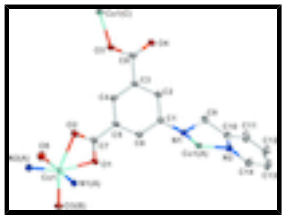


Fig. 1. : The coordination environment of Co ion in the title complex with the ellipsoids drawn at the 30% probability level. The hydrogen atoms have been omitted for clarity. Symmetry codes: A = -*x* + 2, -*y* + 1, -*z* + 1; B = *x*, -*y* + 1/2, *z* - 1/2; C = *x*, -*y* + 1/2, *z* + 1/2.

Poly[aqua{μ$_3$-5-[(pyridin-2-ylmethyl)amino]isophthalato- κ^5*N*,*N*':*O*^{1},*O*$^{1'}$:*O*^{3}}cobalt(II)]

Crystal data

$[Co(C_{14}H_{10}N_2O_4)(H_2O)]\cdot 3.5H_2O$	$F(000) = 846$
$M_r = 410.24$	$D_x = 1.593$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 6314 reflections
$a = 11.0926$ (11) Å	θ = 2.4–28.4°
$b = 9.8735$ (10) Å	μ = 1.05 mm^{-1}
$c = 17.4317$ (15) Å	$T = 293$ K
β = 116.533 (5)°	Block, red
$V = 1708.1$ (3) Å^3	0.20 × 0.20 × 0.20 mm
$Z = 4$	

Data collection

Bruker SMART APEXII CCD diffractometer	4259 independent reflections
Radiation source: fine-focus sealed tube	3809 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.021$
φ and ω scans	$\theta_{max} = 28.4°$, $\theta_{min} = 2.1°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -14\rightarrow12$
$T_{min} = 0.821$, $T_{max} = 0.821$	$k = -13\rightarrow10$
11993 measured reflections	$l = -22\rightarrow23$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.045$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.124$	H-atom parameters constrained
$S = 1.11$	$w = 1/[\sigma^2(F_o^2) + (0.0407P)^2 + 3.8921P]$ where $P = (F_o^2 + 2F_c^2)/3$
4259 reflections	$(\Delta/\sigma)_{max} = 0.001$

199 parameters	$\Delta\rho_{max} = 0.81$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.43$ e Å^{-3}

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}
C1	0.8386 (3)	0.5358 (3)	0.59337 (16)	0.0210 (5)
C2	0.8790 (3)	0.5330 (3)	0.68135 (17)	0.0225 (5)
H2	0.8344	0.5858	0.7048	0.027*
C3	0.9868 (3)	0.4503 (3)	0.73445 (16)	0.0217 (5)
C4	1.0543 (3)	0.3722 (3)	0.70059 (16)	0.0214 (5)
H4	1.1273	0.3195	0.7364	0.026*
C5	1.0122 (3)	0.3726 (3)	0.61166 (16)	0.0216 (5)
C6	0.9043 (3)	0.4529 (3)	0.55925 (17)	0.0231 (5)
H6	0.8752	0.4514	0.5003	0.028*
C7	1.0840 (3)	0.2913 (3)	0.57301 (17)	0.0232 (5)
C8	1.0286 (3)	0.4465 (3)	0.82983 (17)	0.0242 (5)
C9	0.6291 (3)	0.6616 (3)	0.55952 (19)	0.0291 (6)
H9A	0.6685	0.7056	0.6151	0.035*
H9B	0.5806	0.5819	0.5630	0.035*
C10	0.5346 (3)	0.7568 (3)	0.49261 (18)	0.0261 (5)
C11	0.3962 (3)	0.7546 (3)	0.4660 (2)	0.0375 (7)
H11	0.3587	0.6926	0.4894	0.045*
C12	0.3154 (3)	0.8459 (4)	0.4045 (3)	0.0453 (9)
H12	0.2226	0.8456	0.3856	0.054*
C13	0.3740 (3)	0.9382 (4)	0.3709 (2)	0.0419 (8)
H13	0.3216	1.0010	0.3297	0.050*
C14	0.5124 (3)	0.9341 (3)	0.4002 (2)	0.0333 (6)
H14	0.5523	0.9954	0.3781	0.040*
Co1	1.20146 (4)	0.17514 (4)	0.49770 (2)	0.02074 (11)
N1	0.7352 (2)	0.6226 (2)	0.53540 (15)	0.0239 (5)
H1N	0.6876	0.5862	0.4822	0.029*
N2	0.5908 (2)	0.8448 (2)	0.45967 (15)	0.0243 (5)
O1	1.0210 (2)	0.2537 (2)	0.49556 (13)	0.0298 (4)
O2	1.2068 (2)	0.2644 (2)	0.61450 (14)	0.0318 (5)
O3	1.1274 (2)	0.3701 (2)	0.87308 (12)	0.0270 (4)

O4	0.9694 (3)	0.5200 (3)	0.86000 (15)	0.0454 (6)
O5	1.1716 (2)	−0.0155 (2)	0.54116 (15)	0.0337 (5)
H5WA	1.1069	−0.0587	0.4995	0.040*
H5W	1.1367	−0.0012	0.5799	0.040*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0250 (12)	0.0200 (12)	0.0202 (12)	0.0001 (10)	0.0119 (10)	0.0011 (9)
C2	0.0271 (13)	0.0227 (12)	0.0222 (12)	0.0027 (10)	0.0151 (10)	0.0014 (10)
C3	0.0277 (13)	0.0225 (12)	0.0175 (11)	−0.0013 (10)	0.0123 (10)	−0.0010 (9)
C4	0.0258 (12)	0.0208 (12)	0.0190 (11)	0.0020 (10)	0.0113 (10)	0.0015 (9)
C5	0.0289 (13)	0.0210 (12)	0.0196 (12)	−0.0015 (10)	0.0150 (10)	−0.0012 (9)
C6	0.0297 (13)	0.0236 (12)	0.0182 (11)	−0.0003 (10)	0.0127 (10)	−0.0004 (10)
C7	0.0330 (14)	0.0202 (12)	0.0232 (12)	0.0004 (10)	0.0187 (11)	0.0002 (10)
C8	0.0338 (14)	0.0241 (13)	0.0202 (12)	−0.0003 (11)	0.0170 (11)	0.0002 (10)
C9	0.0282 (14)	0.0330 (15)	0.0322 (15)	0.0032 (12)	0.0188 (12)	0.0063 (12)
C10	0.0263 (13)	0.0258 (13)	0.0275 (13)	0.0020 (11)	0.0133 (11)	−0.0011 (11)
C11	0.0260 (14)	0.0339 (16)	0.051 (2)	−0.0013 (12)	0.0157 (14)	0.0028 (14)
C12	0.0244 (15)	0.0425 (19)	0.064 (2)	0.0062 (14)	0.0155 (15)	0.0073 (17)
C13	0.0323 (16)	0.0419 (18)	0.0445 (19)	0.0135 (14)	0.0110 (14)	0.0100 (15)
C14	0.0347 (15)	0.0333 (15)	0.0318 (15)	0.0097 (13)	0.0149 (13)	0.0072 (12)
Co1	0.02195 (19)	0.0267 (2)	0.01563 (17)	0.00285 (14)	0.01024 (13)	0.00087 (13)
N1	0.0257 (11)	0.0274 (11)	0.0203 (10)	0.0046 (9)	0.0117 (9)	0.0020 (9)
N2	0.0241 (11)	0.0259 (11)	0.0234 (11)	0.0032 (9)	0.0110 (9)	0.0016 (9)
O1	0.0366 (11)	0.0365 (11)	0.0191 (9)	0.0087 (9)	0.0150 (8)	−0.0012 (8)
O2	0.0298 (10)	0.0399 (12)	0.0307 (11)	−0.0009 (9)	0.0179 (9)	−0.0085 (9)
O3	0.0306 (10)	0.0348 (11)	0.0181 (9)	0.0023 (9)	0.0131 (8)	0.0022 (8)
O4	0.0668 (16)	0.0505 (15)	0.0279 (11)	0.0300 (13)	0.0293 (12)	0.0095 (10)
O5	0.0338 (11)	0.0296 (11)	0.0398 (12)	−0.0010 (9)	0.0183 (10)	0.0026 (9)

Geometric parameters (Å, °)

C1—C2	1.393 (4)	C10—C11	1.391 (4)
C1—C6	1.394 (4)	C11—C12	1.381 (5)
C1—N1	1.427 (3)	C11—H11	0.9300
C2—C3	1.402 (4)	C12—C13	1.392 (5)
C2—H2	0.9300	C12—H12	0.9300
C3—C4	1.377 (4)	C13—C14	1.384 (5)
C3—C8	1.514 (3)	C13—H13	0.9300
C4—C5	1.405 (3)	C14—N2	1.343 (4)
C4—H4	0.9300	C14—H14	0.9300
C5—C6	1.385 (4)	Co1—O3^{i}	1.9999 (19)
C5—C7	1.488 (3)	Co1—N2^{ii}	2.090 (2)
C6—H6	0.9300	Co1—O5	2.110 (2)
C7—O2	1.252 (4)	Co1—O1	2.132 (2)
C7—O1	1.267 (3)	Co1—O2	2.195 (2)
C8—O4	1.242 (3)	Co1—N1^{ii}	2.275 (2)

C8—O3	1.265 (3)	N1—Co1^{ii}	2.275 (2)
C9—N1	1.468 (3)	N1—H1N	0.9118
C9—C10	1.500 (4)	N2—Co1^{ii}	2.090 (2)
C9—H9A	0.9700	O3—Co1^{iii}	1.9999 (19)
C9—H9B	0.9700	O5—H5WA	0.8710
C10—N2	1.339 (4)	O5—H5W	0.9279
C2—C1—C6	119.1 (2)	C13—C12—H12	120.3
C2—C1—N1	123.6 (2)	C14—C13—C12	118.3 (3)
C6—C1—N1	117.3 (2)	C14—C13—H13	120.8
C1—C2—C3	119.9 (2)	C12—C13—H13	120.8
C1—C2—H2	120.1	N2—C14—C13	122.3 (3)
C3—C2—H2	120.1	N2—C14—H14	118.9
C4—C3—C2	120.7 (2)	C13—C14—H14	118.9
C4—C3—C8	119.9 (2)	O3^{i}—Co1—N2^{ii}	102.58 (9)
C2—C3—C8	119.4 (2)	O3^{i}—Co1—O5	97.84 (9)
C3—C4—C5	119.6 (2)	N2^{ii}—Co1—O5	96.50 (9)
C3—C4—H4	120.2	O3^{i}—Co1—O1	97.79 (8)
C5—C4—H4	120.2	N2^{ii}—Co1—O1	156.61 (9)
C6—C5—C4	119.5 (2)	O5—Co1—O1	91.96 (8)
C6—C5—C7	119.3 (2)	O3^{i}—Co1—O2	157.69 (8)
C4—C5—C7	121.1 (2)	N2^{ii}—Co1—O2	98.01 (9)
C5—C6—C1	121.1 (2)	O5—Co1—O2	88.21 (9)
C5—C6—H6	119.4	O1—Co1—O2	60.40 (8)
C1—C6—H6	119.4	O3^{i}—Co1—N1^{ii}	86.81 (8)
O2—C7—O1	119.6 (2)	N2^{ii}—Co1—N1^{ii}	75.91 (9)
O2—C7—C5	121.1 (2)	O5—Co1—N1^{ii}	171.88 (9)
O1—C7—C5	119.2 (2)	O1—Co1—N1^{ii}	94.02 (8)
O4—C8—O3	125.3 (3)	O2—Co1—N1^{ii}	89.96 (8)
O4—C8—C3	119.4 (3)	C1—N1—C9	116.7 (2)
O3—C8—C3	115.3 (2)	C1—N1—Co1^{ii}	117.72 (17)
N1—C9—C10	108.2 (2)	C9—N1—Co1^{ii}	102.74 (17)
N1—C9—H9A	110.1	C1—N1—H1N	113.6
C10—C9—H9A	110.1	C9—N1—H1N	102.8
N1—C9—H9B	110.1	Co1^{ii}—N1—H1N	101.1
C10—C9—H9B	110.1	C10—N2—C14	119.4 (3)
H9A—C9—H9B	108.4	C10—N2—Co1^{ii}	115.93 (18)
N2—C10—C11	121.6 (3)	C14—N2—Co1^{ii}	124.6 (2)
N2—C10—C9	116.2 (2)	C7—O1—Co1	91.19 (17)
C11—C10—C9	122.2 (3)	C7—O2—Co1	88.71 (16)
C12—C11—C10	119.0 (3)	C8—O3—Co1^{iii}	127.34 (17)
C12—C11—H11	120.5	Co1—O5—H5WA	110.0
C10—C11—H11	120.5	Co1—O5—H5W	108.0
C11—C12—C13	119.4 (3)	H5WA—O5—H5W	103.0
C11—C12—H12	120.3		

C6—C1—C2—C3	1.8 (4)	C6—C1—N1—C9	153.4 (3)
N1—C1—C2—C3	−176.3 (2)	C2—C1—N1—Co1^{ii}	94.4 (3)
C1—C2—C3—C4	0.4 (4)	C6—C1—N1—Co1^{ii}	−83.8 (3)
C1—C2—C3—C8	−179.2 (2)	C10—C9—N1—C1	177.6 (2)
C2—C3—C4—C5	−1.7 (4)	C10—C9—N1—Co1^{ii}	47.3 (3)
C8—C3—C4—C5	177.9 (2)	C11—C10—N2—C14	0.7 (4)
C3—C4—C5—C6	0.7 (4)	C9—C10—N2—C14	−179.2 (3)
C3—C4—C5—C7	179.0 (2)	C11—C10—N2—Co1^{ii}	−176.5 (2)
C4—C5—C6—C1	1.6 (4)	C9—C10—N2—Co1^{ii}	3.6 (3)
C7—C5—C6—C1	−176.7 (2)	C13—C14—N2—C10	−0.5 (5)
C2—C1—C6—C5	−2.8 (4)	C13—C14—N2—Co1^{ii}	176.4 (3)
N1—C1—C6—C5	175.4 (2)	O2—C7—O1—Co1	−3.4 (3)
C6—C5—C7—O2	149.9 (3)	C5—C7—O1—Co1	173.6 (2)
C4—C5—C7—O2	−28.4 (4)	O3^{i}—Co1—O1—C7	−173.06 (16)
C6—C5—C7—O1	−27.1 (4)	N2^{ii}—Co1—O1—C7	−22.6 (3)
C4—C5—C7—O1	154.7 (3)	O5—Co1—O1—C7	88.75 (17)
C4—C3—C8—O4	178.1 (3)	O2—Co1—O1—C7	1.93 (15)
C2—C3—C8—O4	−2.3 (4)	N1^{ii}—Co1—O1—C7	−85.74 (17)
C4—C3—C8—O3	0.9 (4)	O1—C7—O2—Co1	3.3 (3)
C2—C3—C8—O3	−179.5 (2)	C5—C7—O2—Co1	−173.6 (2)
N1—C9—C10—N2	−37.2 (4)	O3^{i}—Co1—O2—C7	11.2 (3)
N1—C9—C10—C11	142.9 (3)	N2^{ii}—Co1—O2—C7	168.46 (17)
N2—C10—C11—C12	−0.3 (5)	O5—Co1—O2—C7	−95.23 (17)
C9—C10—C11—C12	179.6 (3)	O1—Co1—O2—C7	−1.95 (16)
C10—C11—C12—C13	−0.4 (6)	N1^{ii}—Co1—O2—C7	92.69 (17)
C11—C12—C13—C14	0.5 (6)	O4—C8—O3—Co1^{iii}	9.0 (4)
C12—C13—C14—N2	−0.1 (5)	C3—C8—O3—Co1^{iii}	−174.00 (17)
C2—C1—N1—C9	−28.5 (4)		

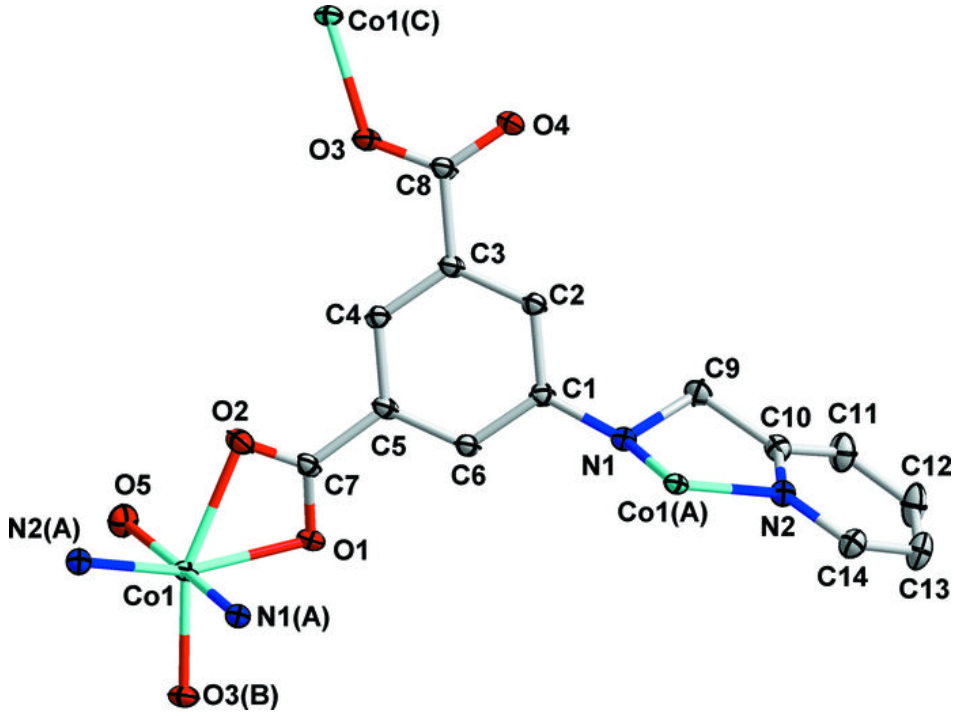
Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2; (ii) −*x*+2, −*y*+1, −*z*+1; (iii) *x*, −*y*+1/2, *z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5WA···O4^{i}	0.87	2.25	2.946 (3)	137.
O5—H5WA···O1^{iv}	0.87	2.42	3.047 (3)	130.
O5—H5W···O4^{v}	0.93	1.90	2.819 (3)	168.

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2; (iv) −*x*+2, −*y*, −*z*+1; (v) −*x*+2, *y*−1/2, −*z*+3/2.

Fig. 1


Co1(C)
O3
O4
C8
C3
C2
C4
C1
C9
O2
C5
C6
N1
C10
C11
C12
O5
C7
Co1(A)
N2
N2(A)
O1
C14
C13
Co1
N1(A)
O3(B)