Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{4-Chloro-2-[(2-hydroxyethyl)iminomethyl]phenolato}{4-chloro-2-[(2-oxidoethyl)iminomethyl]phenolato}cobalt(III)

Li-Jun Liu

Experimental Center, Linyi Normal University, Linyi Shandong 276005, People's Republic of China
Correspondence e-mail: xiaoerduoaa@hotmail.com

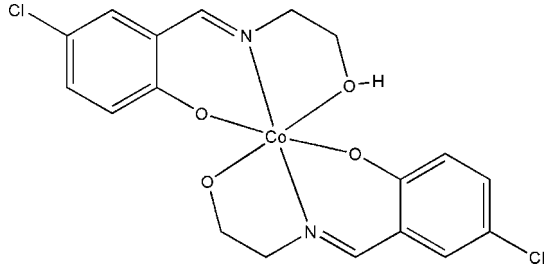
Received 10 August 2010; accepted 17 August 2010

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; disorder in main residue; R factor = 0.049; wR factor = 0.135; data-to-parameter ratio = 15.7.

In the title mononuclear cobalt(III) compound, [Co($C_9H_8ClNO_2$)($C_9H_9ClNO_2$)], the Co^{II} atom is six-coordinated by two imine N atoms, two phenolate O atoms, and one hydroxy and one oxide O atom from two Schiff base ligands, forming an octahedral geometry. In the crystal structure, adjacent molecules are linked through intermolecular O—H···O hydrogen bonds. The 2-oxidoethyl group is disordered over two positions in a 0.638 (3):0.362 (3) ratio.

Related literature

For general background to Schiff base cobalt(III) complexes, see: Zhang *et al.* (2010); Rodriguez *et al.* (2010); Khalaji *et al.* (2010); Luo & Luo (2010). For related cobalt complexes with octahedral coordination, see: De *et al.* (2001); Sun (2005); Zhu *et al.* (2003); Yuan (2006).



Experimental

Crystal data

[Co($C_9H_8ClNO_2$)($C_9H_9ClNO_2$)]
M_r = 455.17
Hexagonal, $R\overline{3}$
a = 18.675 (2) Å
c = 27.595 (3) Å
V = 8334.6 (16) Å^3
Z = 18
Mo $K\alpha$ radiation
μ = 1.24 mm^{-1}
T = 298 K
0.32 × 0.30 × 0.27 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.692, T_{max} = 0.730
13818 measured reflections
4045 independent reflections
2390 reflections with $I > 2\sigma(I)$
R_{int} = 0.126

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.135
S = 1.00
4045 reflections
257 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—O1	1.874 (2)	Co1—N2	1.897 (3)
Co1—O3	1.877 (3)	Co1—O4	1.916 (3)
Co1—N1	1.887 (3)	Co1—O2	1.918 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O4^{i}	0.86 (1)	1.59 (1)	2.436 (4)	173 (5)

Symmetry code: (i) $y-\frac{1}{3}, -x+y+\frac{1}{3}, -z+\frac{1}{3}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The author acknowledges the Linyi Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2699).

References

Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
De, R. L., Samanta, K., Maiti, K. & Keller, E. (2001). *Inorg. Chim. Acta*, **316**, 113–116.
Khalaji, A. D., Hadadzadeh, H., Fejfarova, K. & Dušek, M. (2010). *Polyhedron*, **29**, 807–812.
Luo, F. & Luo, M.-B. (2010). *Inorg. Chem. Commun.* **13**, 319–321.
Rodriguez, L., Labisbal, E., Sousa-Pedrares, A., Garcia-Vazquez, J. A., Romero, J. & Sousa, A. (2010). *Inorg. Chim. Acta*, **363**, 1284–1288.
Sheldrick, G. M. (2004). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sun, Y.-X. (2005). *Acta Cryst.* E**61**, m335–m337.
Yuan, C.-L. (2006). *Acta Cryst.* E**62**, m2257–m2259.
Zhang, J.-S., Pan, F.-D., Cheng, H. & Du, W.-J. (2010). *Synth. React. Inorg. Met. Org. Nano-Met. Chem.* **40**, 211–215.
Zhu, H.-L., Lin, Y.-S., Meng, F.-J., Zou, Y. & Wang, D.-Q. (2003). *Acta Cryst.* E**59**, m878–m879.

supporting information

Acta Cryst. (2010). E**66**, m1143 [https://doi.org/10.1107/S1600536810033088]

{4-Chloro-2-[(2-hydroxyethyl)iminomethyl]phenolato}{4-chloro-2-[(2-oxidoethyl)iminomethyl]phenolato}cobalt(III)

Li-Jun Liu

S1. Comment

Cobalt(III) complexes with Schiff bases have been widely investigated in coordination chemistry and biological chemistry (Zhang *et al.*, 2010; Rodriguez *et al.*, 2010; Khalaji *et al.*, 2010; Luo & Luo, 2010). In the present paper, the title new cobalt(III) complex with the Schiff base ligand 4-chloro-2-[(2-hydroxyethylimino)methyl]phenol, is reported.

The Co^{III} atom in the title complex (Fig. 1) is six-coordinated by two imine N atoms, two phenolate O atoms, and two hydroxy O atoms from two Schiff base ligands, forming an octahedral geometry. The mainly difference in the two ligands is that one of the hydroxy groups is deprotonated. The bond lengths and angles (Table 1) related to the Co atom are comparable with those observed in similar cobalt complexes with octahedral geometry (De *et al.*, 2001; Sun, 2005; Zhu *et al.*, 2003; Yuan, 2006). In the crystal structure, the adjacent molecules are linked through intermolecular O—H···O hydrogen bonds (Table 2, Fig. 2).

S2. Experimental

5-Chlorosalicylaldehyde (0.1 mmol, 15.6 mg), 2-(2-aminoethylamino)ethanol (0.1 mmol, 10.4 mg), and cobalt acetate tetrahydrate (0.1 mmol, 24.9 mg) were mixed and stirred in methanol (20 ml) at reflux for 2 h, to give a red solution. The solution was cooled to room temperature, and red block-shaped single crystals were formed by slow evaporation of the solution in air. The characteristic IR absorption for the hydroxy group is at 3327 cm^{-1}.

S3. Refinement

Atom H2 attached to O2 was located in a difference Fourier map and refined isotropically, with the O–H distance restrained to 0.85 (1) Å. The remaining H atoms were positioned geometrically (C–H = 0.93–0.97 Å) and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C). The C8 atom is disordered over two distinct sites, with occupancies of 0.638 (3) and 0.362 (3).

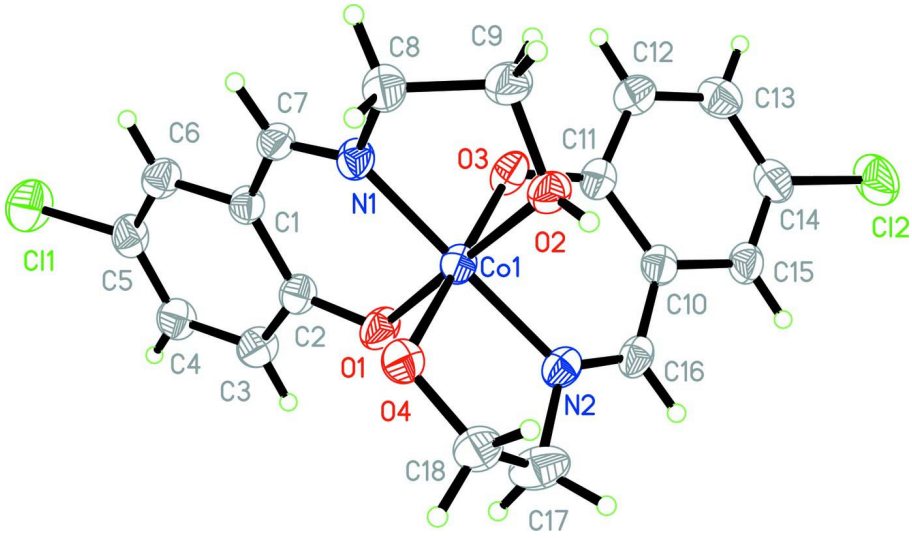


Figure 1

The molecular structure of the title complex with 30% probability displacement ellipsoids.

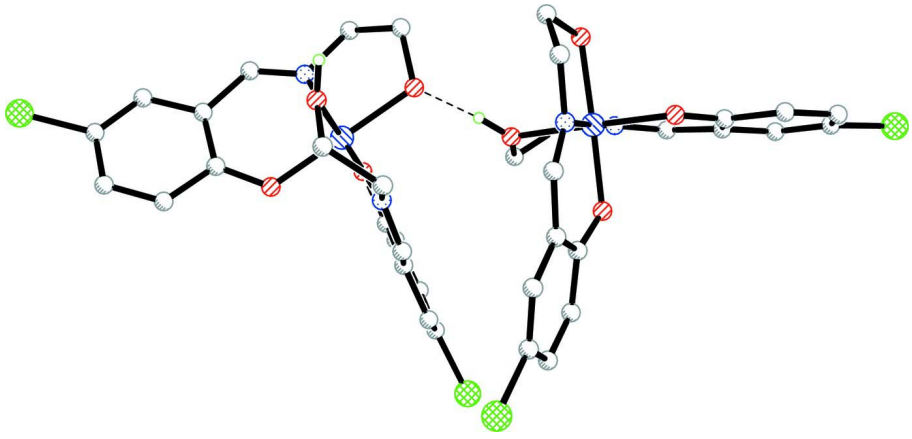


Figure 2

The crystal packing of the title complex, viewed along the *c* axis. Hydrogen bonds are shown as dashed lines.

{4-Chloro-2-[(2-hydroxyethyl)iminomethyl]phenolato}{4-chloro-2-[(2-oxidoethyl)iminomethyl]phenolato}cobalt(III)

Crystal data

$[Co(C_9H_8ClNO_2)(C_9H_9ClNO_2)]$
$M_r = 455.17$
Hexagonal, $R\overline{3}$
Hall symbol: -R 3
$a = 18.675$ (2) Å
$c = 27.595$ (3) Å
$V = 8334.6$ (16) Å^3
$Z = 18$
$F(000) = 4176$
$D_x = 1.632$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2130 reflections
$\theta = 2.5$–24.5°
$\mu = 1.24$ mm^{-1}
$T = 298$ K
Block, red
0.32 × 0.30 × 0.27 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.692, T_{max} = 0.730
13818 measured reflections
4045 independent reflections
2390 reflections with $I > 2\sigma(I)$
R_{int} = 0.126
θ_{max} = 27.0°, θ_{min} = 2.2°
h = −19→22
k = −23→23
l = −35→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.135
S = 1.00
4045 reflections
257 parameters
9 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0437P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Co1	0.55643 (3)	0.59070 (3)	0.127819 (16)	0.04116 (18)	
Cl1	0.98997 (7)	0.87669 (9)	0.09447 (5)	0.0861 (4)	
Cl2	0.41025 (9)	0.19824 (7)	0.01276 (5)	0.0928 (5)	
N1	0.63370 (19)	0.63087 (18)	0.17903 (10)	0.0430 (7)	
N2	0.47432 (18)	0.5496 (2)	0.07872 (10)	0.0453 (8)	
O1	0.63160 (15)	0.65983 (16)	0.08074 (9)	0.0539 (7)	
O2	0.47877 (16)	0.51745 (17)	0.17488 (9)	0.0503 (7)	
O3	0.58854 (15)	0.51130 (16)	0.11779 (8)	0.0514 (7)	
C1	0.7546 (2)	0.7142 (2)	0.12998 (13)	0.0433 (9)	
C2	0.7114 (2)	0.7059 (2)	0.08620 (13)	0.0455 (9)	
C3	0.7592 (2)	0.7521 (3)	0.04638 (14)	0.0538 (10)	
H3	0.7327	0.7476	0.0171	0.065*	
C4	0.8429 (2)	0.8033 (2)	0.04895 (15)	0.0536 (10)	
H4	0.8723	0.8338	0.0220	0.064*	
C5	0.8833 (2)	0.8092 (2)	0.09172 (16)	0.0540 (11)	

C6	0.8408 (2)	0.7664 (2)	0.13157 (14)	0.0505 (10)	
H6	0.8691	0.7716	0.1603	0.061*	
C7	0.7118 (2)	0.6768 (2)	0.17474 (13)	0.0436 (9)	
H7	0.7437	0.6871	0.2025	0.052*	
C8	0.5941 (3)	0.5974 (2)	0.22574 (12)	0.0543 (10)	
H8A	0.5756	0.6328	0.2402	0.065*	
H8B	0.6326	0.5939	0.2478	0.065*	
C9	0.5219 (3)	0.5132 (3)	0.21629 (14)	0.0587 (11)	
H9A	0.5410	0.4742	0.2106	0.070*	
H9B	0.4854	0.4945	0.2442	0.070*	
C10	0.4806 (2)	0.4271 (2)	0.06097 (12)	0.0459 (9)	
C11	0.5442 (2)	0.4424 (2)	0.09464 (13)	0.0446 (9)	
C12	0.5605 (3)	0.3772 (3)	0.10272 (14)	0.0549 (11)	
H12	0.5999	0.3841	0.1257	0.066*	
C13	0.5200 (3)	0.3042 (3)	0.07785 (15)	0.0608 (11)	
H13	0.5324	0.2626	0.0838	0.073*	
C14	0.4608 (3)	0.2926 (2)	0.04396 (14)	0.0575 (11)	
C15	0.4415 (2)	0.3523 (2)	0.03509 (13)	0.0518 (10)	
H15	0.4022	0.3438	0.0117	0.062*	
C16	0.4515 (2)	0.4846 (2)	0.05371 (13)	0.0458 (9)	
H16	0.4134	0.4735	0.0290	0.055*	
O4	0.52234 (16)	0.67011 (15)	0.14056 (9)	0.0524 (7)	0.638 (18)
C17	0.4410 (3)	0.6051 (3)	0.07147 (16)	0.0722 (14)	0.638 (18)
H17A	0.3836	0.5734	0.0615	0.087*	0.638 (18)
H17B	0.4717	0.6446	0.0460	0.087*	0.638 (18)
C18	0.4473 (6)	0.6495 (6)	0.1169 (4)	0.061 (3)	0.638 (18)
H18A	0.4455	0.6994	0.1098	0.073*	0.638 (18)
H18B	0.4010	0.6148	0.1378	0.073*	0.638 (18)
O4′	0.52234 (16)	0.67011 (15)	0.14056 (9)	0.0524 (7)	0.362 (18)
C17′	0.4410 (3)	0.6051 (3)	0.07147 (16)	0.0722 (14)	0.362 (18)
H17C	0.4407	0.6163	0.0372	0.087*	0.362 (18)
H17D	0.3844	0.5787	0.0831	0.087*	0.362 (18)
C18′	0.4876 (12)	0.6776 (8)	0.0957 (6)	0.062 (5)	0.362 (18)
H18C	0.4536	0.7022	0.1024	0.074*	0.362 (18)
H18D	0.5324	0.7153	0.0747	0.074*	0.362 (18)
H2	0.4293 (12)	0.507 (3)	0.1794 (16)	0.080*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0373 (3)	0.0420 (3)	0.0389 (3)	0.0159 (3)	−0.0011 (2)	−0.0015 (2)
Cl1	0.0381 (7)	0.0883 (10)	0.1121 (10)	0.0166 (6)	0.0011 (6)	0.0099 (8)
Cl2	0.1280 (12)	0.0464 (7)	0.0801 (8)	0.0257 (7)	−0.0243 (8)	−0.0136 (6)
N1	0.046 (2)	0.0418 (18)	0.0354 (16)	0.0175 (16)	−0.0015 (14)	−0.0045 (13)
N2	0.0376 (18)	0.055 (2)	0.0399 (17)	0.0202 (16)	−0.0004 (13)	−0.0005 (15)
O1	0.0357 (16)	0.0643 (18)	0.0447 (14)	0.0121 (14)	−0.0010 (11)	0.0086 (13)
O2	0.0366 (15)	0.0582 (17)	0.0497 (15)	0.0188 (14)	0.0006 (12)	0.0096 (12)
O3	0.0427 (16)	0.0563 (18)	0.0551 (15)	0.0246 (14)	−0.0131 (12)	−0.0166 (13)

C1	0.043 (2)	0.040 (2)	0.046 (2)	0.0194 (19)	−0.0029 (17)	−0.0037 (16)
C2	0.039 (2)	0.048 (2)	0.048 (2)	0.021 (2)	0.0018 (17)	−0.0018 (17)
C3	0.047 (3)	0.062 (3)	0.049 (2)	0.025 (2)	0.0038 (18)	0.0041 (19)
C4	0.040 (2)	0.054 (3)	0.062 (3)	0.019 (2)	0.0103 (19)	0.009 (2)
C5	0.033 (2)	0.047 (2)	0.077 (3)	0.017 (2)	0.004 (2)	0.000 (2)
C6	0.044 (2)	0.055 (3)	0.058 (2)	0.029 (2)	−0.0064 (19)	−0.009 (2)
C7	0.047 (3)	0.043 (2)	0.042 (2)	0.024 (2)	−0.0092 (17)	−0.0067 (16)
C8	0.062 (3)	0.052 (3)	0.035 (2)	0.018 (2)	0.0011 (18)	−0.0012 (17)
C9	0.055 (3)	0.065 (3)	0.048 (2)	0.024 (2)	−0.0023 (19)	0.011 (2)
C10	0.045 (2)	0.047 (2)	0.036 (2)	0.016 (2)	0.0040 (17)	0.0027 (17)
C11	0.039 (2)	0.048 (2)	0.041 (2)	0.0180 (19)	0.0028 (16)	−0.0037 (17)
C12	0.056 (3)	0.061 (3)	0.050 (2)	0.032 (2)	−0.0057 (19)	−0.005 (2)
C13	0.075 (3)	0.055 (3)	0.057 (3)	0.036 (3)	0.003 (2)	0.002 (2)
C14	0.072 (3)	0.044 (2)	0.045 (2)	0.020 (2)	0.004 (2)	0.0004 (18)
C15	0.051 (3)	0.045 (2)	0.043 (2)	0.012 (2)	−0.0058 (17)	−0.0031 (18)
C16	0.034 (2)	0.052 (3)	0.0365 (19)	0.0104 (19)	0.0005 (15)	0.0010 (18)
O4	0.0542 (17)	0.0457 (17)	0.0576 (16)	0.0252 (14)	−0.0065 (13)	−0.0045 (12)
C17	0.080 (3)	0.102 (4)	0.065 (3)	0.067 (3)	−0.009 (2)	−0.008 (3)
C18	0.047 (5)	0.064 (6)	0.080 (6)	0.034 (5)	−0.002 (4)	0.003 (4)
O4′	0.0542 (17)	0.0457 (17)	0.0576 (16)	0.0252 (14)	−0.0065 (13)	−0.0045 (12)
C17′	0.080 (3)	0.102 (4)	0.065 (3)	0.067 (3)	−0.009 (2)	−0.008 (3)
C18′	0.063 (9)	0.051 (7)	0.073 (8)	0.030 (6)	−0.006 (6)	−0.001 (6)

Geometric parameters (Å, º)

Co1—O1	1.874 (2)	C7—H7	0.9300
Co1—O3	1.877 (3)	C8—C9	1.496 (5)
Co1—N1	1.887 (3)	C8—H8A	0.9700
Co1—N2	1.897 (3)	C8—H8B	0.9700
Co1—O4	1.916 (3)	C9—H9A	0.9700
Co1—O2	1.918 (3)	C9—H9B	0.9700
Cl1—C5	1.747 (4)	C10—C15	1.405 (5)
Cl2—C14	1.753 (4)	C10—C11	1.420 (5)
N1—C7	1.275 (4)	C10—C16	1.440 (5)
N1—C8	1.462 (4)	C11—C12	1.413 (5)
N2—C16	1.270 (4)	C12—C13	1.367 (5)
N2—C17	1.465 (5)	C12—H12	0.9300
O1—C2	1.305 (4)	C13—C14	1.380 (6)
O2—C9	1.423 (4)	C13—H13	0.9300
O2—H2	0.855 (10)	C14—C15	1.356 (6)
O3—C11	1.298 (4)	C15—H15	0.9300
C1—C6	1.404 (5)	C16—H16	0.9300
C1—C2	1.418 (5)	O4—C18	1.414 (7)
C1—C7	1.447 (5)	C17—C18	1.474 (8)
C2—C3	1.406 (5)	C17—H17A	0.9700
C3—C4	1.368 (5)	C17—H17B	0.9700
C3—H3	0.9300	C18—H18A	0.9700
C4—C5	1.375 (5)	C18—H18B	0.9700

C4—H4	0.9300	C18′—H18C	0.9700
C5—C6	1.359 (5)	C18′—H18D	0.9700
C6—H6	0.9300		

O1—Co1—O3	90.97 (12)	N1—C8—C9	107.0 (3)
O1—Co1—N1	94.87 (12)	N1—C8—H8A	110.3
O3—Co1—N1	86.66 (12)	C9—C8—H8A	110.3
O1—Co1—N2	87.65 (12)	N1—C8—H8B	110.3
O3—Co1—N2	95.06 (12)	C9—C8—H8B	110.3
N1—Co1—N2	176.94 (12)	H8A—C8—H8B	108.6
O1—Co1—O4	91.05 (11)	O2—C9—C8	108.6 (3)
O3—Co1—O4	177.77 (11)	O2—C9—H9A	110.0
N1—Co1—O4	92.22 (12)	C8—C9—H9A	110.0
N2—Co1—O4	85.98 (12)	O2—C9—H9B	110.0
O1—Co1—O2	178.46 (12)	C8—C9—H9B	110.0
O3—Co1—O2	87.87 (12)	H9A—C9—H9B	108.4
N1—Co1—O2	86.08 (12)	C15—C10—C11	119.9 (4)
N2—Co1—O2	91.44 (12)	C15—C10—C16	118.0 (4)
O4—Co1—O2	90.13 (12)	C11—C10—C16	122.0 (3)
C7—N1—C8	122.3 (3)	O3—C11—C12	118.1 (3)
C7—N1—Co1	126.0 (2)	O3—C11—C10	125.2 (4)
C8—N1—Co1	111.5 (2)	C12—C11—C10	116.7 (3)
C16—N2—C17	122.9 (3)	C13—C12—C11	122.0 (4)
C16—N2—Co1	126.3 (3)	C13—C12—H12	119.0
C17—N2—Co1	110.8 (3)	C11—C12—H12	119.0
C2—O1—Co1	126.1 (2)	C12—C13—C14	119.9 (4)
C9—O2—Co1	109.7 (2)	C12—C13—H13	120.1
C9—O2—H2	117 (3)	C14—C13—H13	120.1
Co1—O2—H2	127 (3)	C15—C14—C13	120.9 (4)
C11—O3—Co1	123.9 (2)	C15—C14—Cl2	120.5 (3)
C6—C1—C2	119.6 (3)	C13—C14—Cl2	118.6 (4)
C6—C1—C7	118.2 (3)	C14—C15—C10	120.5 (4)
C2—C1—C7	121.8 (3)	C14—C15—H15	119.8
O1—C2—C3	118.6 (3)	C10—C15—H15	119.8
O1—C2—C1	124.8 (3)	N2—C16—C10	124.5 (3)
C3—C2—C1	116.6 (3)	N2—C16—H16	117.8
C4—C3—C2	122.7 (4)	C10—C16—H16	117.8
C4—C3—H3	118.6	C18—O4—Co1	111.8 (3)
C2—C3—H3	118.6	N2—C17—C18	109.8 (4)
C3—C4—C5	119.4 (4)	N2—C17—H17A	109.7
C3—C4—H4	120.3	C18—C17—H17A	109.7
C5—C4—H4	120.3	N2—C17—H17B	109.7
C6—C5—C4	120.8 (4)	C18—C17—H17B	109.7
C6—C5—Cl1	120.6 (3)	H17A—C17—H17B	108.2
C4—C5—Cl1	118.5 (3)	O4—C18—C17	109.6 (5)
C5—C6—C1	120.9 (4)	O4—C18—H18A	109.7
C5—C6—H6	119.6	C17—C18—H18A	109.7
C1—C6—H6	119.6	O4—C18—H18B	109.7

N1—C7—C1	125.1 (3)	C17—C18—H18B	109.7
N1—C7—H7	117.5	H18A—C18—H18B	108.2
C1—C7—H7	117.5	H18C—C18′—H18D	107.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O4^{i}	0.86 (1)	1.59 (1)	2.436 (4)	173 (5)

Symmetry code: (i) $y-1/3, -x+y+1/3, -z+1/3$.