

{2,2'-[6,6'-Dimethoxycyclohexane-1,2-diylbis(nitrilomethylidene)]diphenolato- $\kappa^4 O^1, N, N', O^1$ }cobalt(II) monohydrate

Yan Bao, Hong-Feng Li, Peng-Fei Yan, Guang-Ming Li* and Guang-Feng Hou

Key Laboratory of Functional Inorganic Material Chemistry (Heilongjiang University), Ministry of Education, School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China
Correspondence e-mail: gmlh@hlju.edu.cn

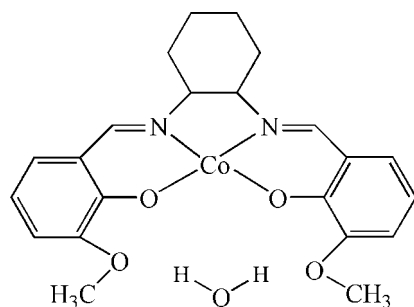
Received 23 December 2008; accepted 6 June 2009

Key indicators: single-crystal X-ray study; $T = 291$ K; mean $\sigma(C-C) = 0.003$ Å; R factor = 0.029; wR factor = 0.069; data-to-parameter ratio = 12.5.

In the title complex, $[Co(C_{22}H_{24}N_2O_4)] \cdot H_2O$, the Co^{II} atom is in an almost square-planar coordination environment involving two O and two N atoms from the Schiff base ligand. A water molecule cocrystallizes with the coordination compound and may be held in the crystal by $O-H \cdots O$ hydrogen bonds. Heteroatomic $\pi-\pi$ ring interactions may be present between symmetry-related complexes, with centroid-centroid distances of 3.5661 (8) Å.

Related literature

For related platinum complexes of a similar Schiff base, see: Lu *et al.* (2008).



Experimental

Crystal data

$[Co(C_{22}H_{24}N_2O_4)] \cdot H_2O$
 $M_r = 457.38$
Monoclinic, $P2_1/n$
 $a = 11.241$ (3) Å
 $b = 10.605$ (3) Å
 $c = 17.864$ (7) Å
 $\beta = 107.158$ (14)°

$V = 2034.9$ (12) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.88$ mm⁻¹
 $T = 291$ K
 $0.20 \times 0.19 \times 0.17$ mm

Data collection

Rigaku R-Axis RAPID diffractometer
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{min} = 0.826$, $T_{max} = 0.851$

19221 measured reflections
4647 independent reflections
3840 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.034$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$
 $wR(F^2) = 0.069$
 $S = 1.04$
4647 reflections
373 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{max} = 0.36$ e Å⁻³
 $\Delta\rho_{min} = -0.24$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O5-H25 \cdots O2$	0.90 (4)	2.11 (4)	2.916 (3)	149 (3)
$O5-H25 \cdots O1$	0.90 (4)	2.45 (4)	3.103 (2)	129 (3)
$O5-H26 \cdots O4$	0.89 (4)	2.05 (4)	2.895 (3)	159 (4)
$O5-H26 \cdots O3$	0.89 (4)	2.59 (4)	3.248 (2)	131 (3)

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; 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: *SHELXL97*.

The authors gratefully acknowledge financial support from the National Natural Science Foundation of China (grant Nos. 20572018 and 20672032), Heilongjiang Province (grant Nos. 1055HZ001, ZJG0504 and JC200605) and Heilongjiang University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CS2106).

References

- Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Lu, X. P., Wong, W. Y. & Wong, W. K. (2008). *J. Eur. Inorg. Chem.* pp. 523–528.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supplementary materials

Acta Cryst. (2009). E65, m770 [doi:10.1107/S1600536809021540]

{2,2'-[6,6'-Dimethoxycyclohexane-1,2-diylbis(nitrilomethylidene)]diphenolato- κ^4O^1,N,N',O^1' }cobalt(II) monohydrate

Y. Bao, H.-F. Li, P.-F. Yan, G.-M. Li and G.-F. Hou

Comment

As shown in Fig. 1, Co^{II} is four-coordinated in a square planar environment as the ligating Schiff base is a tetradentate ligand (Table 1). The co-crystallized water molecule does not coordinate to the Co ion. Its position is stabilized by bifurcated O—H...O hydrogen bonds (Table 2). It is also worth noting that stabilizing π – π ring interactions may occur between symmetry center related phenyl C1 \rightarrow C6 and C7 \rightarrow O1 heteroatomic rings, as show in Fig. 2. The π – π center to center distance is 3.5661 (8) Å. Together with an almost perfect rings-to-rings matching this may indicate appreciable interactions.

Experimental

The title complex was obtained by the treatment of cobalt(II) acetate tetrahydrate with the neutral Schiff base in methanol/acetone (1:2). The yellow clear mixture turned to salmon pink precipitation after stirred for 4 h; diethyl ether was allowed to diffuse slowly into the solution of the filtrate. Red single crystals were obtained after several days. Analysis calculated for C₂₂H₂₆CoN₂O₅: C, 57.77; H, 5.73; N, 6.12; Co, 12.88; found: C, 57.56; H, 5.23; N, 6.77; Co, 12.79%.

Refinement

All H atoms were located in difference Fourier maps and freely refined, but water H atoms was set $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

Figures

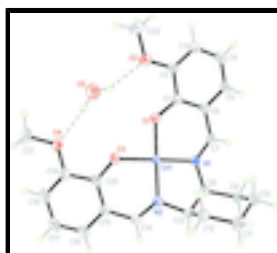


Fig. 1. The molecular structure of the title complex, showing 30% probability displacement ellipsoids for non-H atoms. Dashed lines indicate the hydrogen-bonding interactions between the water and the host.

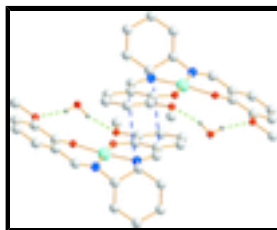


Fig. 2. Heteroatomic π – π ring interactions across an inversion center, indicated by broken lines.

{2,2'-[6,6'-Dimethoxycyclohexane-1,2-diylbis(nitrilomethylidene)]diphenolato- $\kappa^4 O^1, N, N', O^1$ }cobalt(II) monohydrate

Crystal data

[Co(C₂₂H₂₄N₂O₄)]·H₂O

$M_r = 457.38$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 11.241$ (3) Å

$b = 10.605$ (3) Å

$c = 17.864$ (7) Å

$\beta = 107.158$ (14)°

$V = 2034.9$ (12) Å³

$Z = 4$

$F_{000} = 956$

$D_x = 1.493$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 15295 reflections

$\theta = 3.1$ – 27.5 °

$\mu = 0.88$ mm⁻¹

$T = 291$ K

Block, red

$0.20 \times 0.19 \times 0.17$ mm

Data collection

Rigaku R-Axis RAPID
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 291$ K

ω scans

Absorption correction: Multi-scan
(ABSCOR; Higashi, 1995)

$T_{\min} = 0.826$, $T_{\max} = 0.851$

19221 measured reflections

4647 independent reflections

3840 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.034$

$\theta_{\max} = 27.5$ °

$\theta_{\min} = 3.1$ °

$h = -14 \rightarrow 14$

$k = -11 \rightarrow 13$

$l = -23 \rightarrow 23$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.029$

$wR(F^2) = 0.069$

$S = 1.04$

4647 reflections

373 parameters

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

$$w = 1/[\sigma^2(F_o^2) + (0.0317P)^2 + 0.4P]$$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.36$ e Å⁻³

$\Delta\rho_{\min} = -0.24$ e Å⁻³

Extinction correction: none

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.55207 (14)	0.17711 (15)	0.02619 (9)	0.0336 (3)
C2	0.47583 (15)	0.27964 (16)	-0.01173 (10)	0.0397 (4)
C3	0.46233 (17)	0.30829 (18)	-0.08877 (11)	0.0450 (4)
C4	0.52295 (17)	0.23721 (19)	-0.13239 (11)	0.0476 (4)
C5	0.59830 (16)	0.13964 (19)	-0.09779 (10)	0.0427 (4)
C6	0.61536 (14)	0.10945 (15)	-0.01824 (9)	0.0336 (3)
C7	0.69932 (14)	0.00941 (16)	0.01550 (10)	0.0346 (3)
C8	0.81705 (14)	-0.13254 (16)	0.11525 (10)	0.0349 (3)
C9	0.91820 (16)	-0.1510 (2)	0.07467 (11)	0.0448 (4)
C10	1.01669 (18)	-0.0482 (2)	0.09542 (13)	0.0548 (5)
C11	1.07198 (18)	-0.0338 (3)	0.18328 (13)	0.0588 (6)
C12	0.97012 (17)	-0.0087 (2)	0.22218 (12)	0.0462 (4)
C13	0.87250 (15)	-0.11292 (17)	0.20283 (10)	0.0364 (4)
C14	0.75527 (16)	-0.12574 (16)	0.29443 (10)	0.0385 (4)
C15	0.65495 (15)	-0.09883 (17)	0.32630 (10)	0.0386 (4)
C16	0.6452 (2)	-0.1711 (2)	0.39057 (12)	0.0509 (5)
C17	0.5519 (2)	-0.1499 (2)	0.42283 (13)	0.0629 (6)
C18	0.4652 (2)	-0.0550 (2)	0.39271 (13)	0.0602 (6)
C19	0.47299 (17)	0.01755 (19)	0.33093 (11)	0.0447 (4)
C20	0.56884 (15)	-0.00204 (16)	0.29425 (10)	0.0365 (4)
C21	0.2944 (2)	0.1401 (3)	0.33174 (16)	0.0633 (6)
C22	0.3317 (2)	0.4392 (2)	0.00145 (17)	0.0610 (6)
N1	0.73023 (11)	-0.02450 (13)	0.08792 (8)	0.0322 (3)
N2	0.76520 (12)	-0.07817 (13)	0.23028 (8)	0.0351 (3)
Co1	0.656300 (17)	0.030194 (19)	0.162807 (12)	0.02751 (7)
O1	0.55821 (10)	0.15217 (11)	0.09913 (7)	0.0371 (3)
O2	0.42054 (14)	0.34365 (13)	0.03579 (9)	0.0586 (4)
O3	0.57104 (11)	0.06922 (11)	0.23491 (7)	0.0400 (3)
O4	0.39176 (12)	0.11321 (15)	0.29806 (8)	0.0559 (4)
O5	0.30979 (18)	0.1993 (3)	0.13719 (12)	0.0994 (7)
H25	0.370 (4)	0.239 (4)	0.122 (2)	0.149*
H26	0.354 (4)	0.176 (4)	0.185 (2)	0.149*
H5	0.7650 (15)	-0.2112 (17)	0.1078 (10)	0.034 (4)*
H4	0.7370 (17)	-0.0353 (16)	-0.0216 (11)	0.042 (5)*
H15	0.8198 (16)	-0.1865 (17)	0.3229 (10)	0.038 (5)*
H14	0.9086 (16)	-0.1919 (17)	0.2269 (11)	0.039 (5)*
H6	0.8798 (17)	-0.1612 (17)	0.0162 (12)	0.047 (5)*
H1	0.4088 (17)	0.3782 (18)	-0.1147 (11)	0.047 (5)*
H13	0.9278 (18)	0.077 (2)	0.2029 (12)	0.053 (6)*
H12	1.0042 (19)	-0.0036 (18)	0.2804 (13)	0.051 (6)*
H2	0.5101 (18)	0.2573 (19)	-0.1860 (13)	0.057 (6)*
H23	0.261 (2)	0.402 (2)	-0.0407 (14)	0.062 (6)*
H16	0.704 (2)	-0.237 (2)	0.4099 (13)	0.060 (6)*
H3	0.6401 (19)	0.087 (2)	-0.1280 (12)	0.058 (6)*
H7	0.9564 (18)	-0.235 (2)	0.0946 (12)	0.054 (6)*

supplementary materials

H9	0.978 (2)	0.038 (2)	0.0714 (14)	0.065 (7)*
H19	0.329 (2)	0.168 (2)	0.3868 (16)	0.077 (7)*
H18	0.396 (2)	-0.039 (2)	0.4151 (15)	0.079 (8)*
H11	1.132 (2)	0.044 (2)	0.1943 (14)	0.071 (7)*
H17	0.541 (2)	-0.207 (2)	0.4636 (15)	0.078 (7)*
H20	0.247 (2)	0.060 (2)	0.3337 (14)	0.068 (7)*
H22	0.301 (2)	0.471 (2)	0.0463 (17)	0.087 (9)*
H8	1.082 (2)	-0.065 (2)	0.0701 (13)	0.063 (6)*
H10	1.116 (2)	-0.111 (2)	0.2077 (14)	0.064 (7)*
H24	0.368 (2)	0.504 (3)	-0.0252 (16)	0.087 (9)*
H21	0.245 (2)	0.210 (2)	0.2927 (16)	0.083 (8)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0289 (7)	0.0366 (8)	0.0335 (9)	-0.0053 (6)	0.0065 (6)	0.0020 (7)
C2	0.0366 (8)	0.0387 (9)	0.0430 (10)	-0.0011 (7)	0.0104 (7)	0.0043 (8)
C3	0.0400 (9)	0.0438 (10)	0.0466 (11)	-0.0021 (8)	0.0054 (8)	0.0121 (8)
C4	0.0482 (10)	0.0565 (12)	0.0349 (10)	-0.0083 (9)	0.0072 (8)	0.0100 (9)
C5	0.0422 (9)	0.0514 (11)	0.0341 (9)	-0.0054 (8)	0.0105 (8)	-0.0002 (8)
C6	0.0292 (7)	0.0386 (9)	0.0319 (8)	-0.0049 (7)	0.0074 (6)	0.0008 (7)
C7	0.0323 (7)	0.0409 (9)	0.0315 (8)	-0.0029 (7)	0.0110 (7)	-0.0045 (7)
C8	0.0307 (7)	0.0358 (9)	0.0381 (9)	0.0020 (7)	0.0099 (7)	-0.0035 (7)
C9	0.0385 (9)	0.0572 (12)	0.0393 (10)	0.0107 (8)	0.0125 (8)	-0.0032 (9)
C10	0.0384 (9)	0.0813 (16)	0.0489 (12)	-0.0047 (10)	0.0194 (9)	0.0004 (11)
C11	0.0355 (9)	0.0888 (17)	0.0521 (13)	-0.0097 (11)	0.0130 (9)	-0.0079 (12)
C12	0.0381 (9)	0.0593 (12)	0.0386 (10)	-0.0060 (8)	0.0075 (8)	-0.0066 (9)
C13	0.0319 (8)	0.0415 (9)	0.0360 (9)	0.0060 (7)	0.0105 (7)	0.0040 (7)
C14	0.0409 (9)	0.0395 (9)	0.0337 (9)	0.0009 (7)	0.0092 (7)	0.0034 (7)
C15	0.0404 (8)	0.0454 (10)	0.0303 (8)	-0.0045 (8)	0.0111 (7)	-0.0004 (7)
C16	0.0575 (11)	0.0561 (12)	0.0401 (11)	-0.0021 (10)	0.0162 (9)	0.0087 (9)
C17	0.0711 (14)	0.0784 (16)	0.0467 (12)	-0.0038 (12)	0.0292 (11)	0.0157 (11)
C18	0.0566 (12)	0.0860 (17)	0.0480 (12)	-0.0035 (11)	0.0309 (10)	0.0033 (11)
C19	0.0411 (9)	0.0589 (11)	0.0367 (9)	-0.0019 (8)	0.0157 (8)	-0.0045 (8)
C20	0.0385 (8)	0.0438 (9)	0.0280 (8)	-0.0046 (7)	0.0109 (7)	-0.0039 (7)
C21	0.0442 (11)	0.0938 (19)	0.0601 (15)	-0.0018 (13)	0.0281 (11)	-0.0154 (14)
C22	0.0524 (12)	0.0483 (12)	0.0757 (17)	0.0146 (10)	0.0088 (12)	0.0001 (12)
N1	0.0286 (6)	0.0357 (7)	0.0324 (7)	-0.0002 (6)	0.0091 (5)	-0.0018 (6)
N2	0.0345 (7)	0.0380 (7)	0.0335 (7)	0.0013 (6)	0.0112 (6)	0.0013 (6)
Co1	0.02730 (10)	0.03082 (12)	0.02579 (11)	0.00243 (8)	0.00995 (8)	0.00088 (8)
O1	0.0373 (6)	0.0411 (6)	0.0344 (6)	0.0063 (5)	0.0128 (5)	0.0035 (5)
O2	0.0652 (8)	0.0561 (8)	0.0584 (9)	0.0267 (7)	0.0244 (7)	0.0140 (7)
O3	0.0448 (6)	0.0445 (7)	0.0350 (6)	0.0063 (5)	0.0186 (5)	0.0036 (5)
O4	0.0476 (7)	0.0772 (10)	0.0513 (8)	0.0127 (7)	0.0277 (6)	0.0003 (7)
O5	0.0700 (12)	0.161 (2)	0.0736 (13)	0.0206 (13)	0.0315 (10)	0.0263 (14)

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

C1—O1	1.3112 (19)	C13—N2	1.477 (2)
-------	-------------	--------	-----------

C1—C6	1.409 (2)	C13—H14	0.974 (18)
C1—C2	1.426 (2)	C14—N2	1.287 (2)
C2—O2	1.371 (2)	C14—C15	1.434 (2)
C2—C3	1.373 (3)	C14—H15	0.991 (18)
C3—C4	1.398 (3)	C15—C20	1.411 (2)
C3—H1	0.980 (19)	C15—C16	1.411 (2)
C4—C5	1.364 (3)	C16—C17	1.356 (3)
C4—H2	0.95 (2)	C16—H16	0.96 (2)
C5—C6	1.413 (2)	C17—C18	1.394 (3)
C5—H3	0.99 (2)	C17—H17	0.98 (2)
C6—C7	1.430 (2)	C18—C19	1.369 (3)
C7—N1	1.288 (2)	C18—H18	0.99 (3)
C7—H4	1.005 (19)	C19—O4	1.375 (2)
C8—N1	1.491 (2)	C19—C20	1.432 (2)
C8—C13	1.518 (2)	C20—O3	1.308 (2)
C8—C9	1.531 (2)	C21—O4	1.425 (2)
C8—H5	1.005 (17)	C21—H19	0.99 (3)
C9—C10	1.519 (3)	C21—H20	1.01 (2)
C9—H6	1.01 (2)	C21—H21	1.06 (3)
C9—H7	1.01 (2)	C22—O2	1.427 (2)
C10—C11	1.516 (3)	C22—H23	1.00 (2)
C10—H9	1.05 (2)	C22—H22	1.02 (3)
C10—H8	0.98 (2)	C22—H24	0.99 (3)
C11—C12	1.528 (3)	N1—Co1	1.8635 (14)
C11—H11	1.04 (2)	N2—Co1	1.8443 (14)
C11—H10	0.99 (2)	Co1—O1	1.8556 (12)
C12—C13	1.524 (3)	Co1—O3	1.8647 (12)
C12—H13	1.04 (2)	O5—H25	0.90 (4)
C12—H12	1.00 (2)	O5—H26	0.89 (4)
O1—C1—C6	124.74 (15)	N2—C13—H14	110.1 (10)
O1—C1—C2	118.30 (15)	C8—C13—H14	109.1 (11)
C6—C1—C2	116.96 (15)	C12—C13—H14	110.2 (10)
O2—C2—C3	125.08 (16)	N2—C14—C15	124.09 (16)
O2—C2—C1	113.72 (15)	N2—C14—H15	118.0 (10)
C3—C2—C1	121.20 (16)	C15—C14—H15	117.9 (10)
C2—C3—C4	120.77 (17)	C20—C15—C16	121.09 (16)
C2—C3—H1	120.7 (11)	C20—C15—C14	120.62 (15)
C4—C3—H1	118.5 (11)	C16—C15—C14	118.29 (17)
C5—C4—C3	119.74 (18)	C17—C16—C15	120.7 (2)
C5—C4—H2	121.1 (12)	C17—C16—H16	120.3 (13)
C3—C4—H2	119.2 (12)	C15—C16—H16	118.9 (13)
C4—C5—C6	120.62 (17)	C16—C17—C18	119.7 (2)
C4—C5—H3	121.0 (12)	C16—C17—H17	119.7 (14)
C6—C5—H3	118.3 (12)	C18—C17—H17	120.3 (14)
C1—C6—C5	120.65 (16)	C19—C18—C17	120.92 (18)
C1—C6—C7	121.38 (15)	C19—C18—H18	118.5 (15)
C5—C6—C7	117.96 (15)	C17—C18—H18	120.6 (14)
N1—C7—C6	125.43 (15)	C18—C19—O4	124.51 (17)
N1—C7—H4	119.3 (11)	C18—C19—C20	121.53 (19)

supplementary materials

C6—C7—H4	115.2 (11)	O4—C19—C20	113.96 (16)
N1—C8—C13	105.21 (13)	O3—C20—C15	125.06 (14)
N1—C8—C9	116.68 (14)	O3—C20—C19	118.93 (16)
C13—C8—C9	111.66 (14)	C15—C20—C19	116.01 (15)
N1—C8—H5	107.2 (9)	O4—C21—H19	110.8 (14)
C13—C8—H5	107.2 (10)	O4—C21—H20	108.8 (13)
C9—C8—H5	108.5 (9)	H19—C21—H20	105.9 (19)
C10—C9—C8	112.49 (16)	O4—C21—H21	100.6 (14)
C10—C9—H6	112.8 (11)	H19—C21—H21	115 (2)
C8—C9—H6	110.6 (10)	H20—C21—H21	115.9 (19)
C10—C9—H7	110.1 (11)	O2—C22—H23	109.8 (13)
C8—C9—H7	104.1 (11)	O2—C22—H22	104.5 (15)
H6—C9—H7	106.1 (16)	H23—C22—H22	110.4 (19)
C11—C10—C9	111.82 (18)	O2—C22—H24	111.5 (15)
C11—C10—H9	109.3 (13)	H23—C22—H24	105 (2)
C9—C10—H9	110.1 (12)	H22—C22—H24	116 (2)
C11—C10—H8	111.3 (13)	C7—N1—C8	120.01 (13)
C9—C10—H8	110.0 (13)	C7—N1—Co1	126.08 (11)
H9—C10—H8	104.2 (17)	C8—N1—Co1	113.06 (10)
C10—C11—C12	110.80 (17)	C14—N2—C13	119.46 (14)
C10—C11—H11	108.6 (13)	C14—N2—Co1	127.67 (12)
C12—C11—H11	108.0 (13)	C13—N2—Co1	112.85 (11)
C10—C11—H10	111.9 (14)	N2—Co1—O1	174.19 (6)
C12—C11—H10	106.9 (13)	N2—Co1—N1	85.67 (6)
H11—C11—H10	110.6 (18)	O1—Co1—N1	95.00 (6)
C13—C12—C11	110.88 (17)	N2—Co1—O3	93.68 (6)
C13—C12—H13	109.3 (11)	O1—Co1—O3	86.28 (5)
C11—C12—H13	109.5 (11)	N1—Co1—O3	173.66 (5)
C13—C12—H12	107.7 (11)	C1—O1—Co1	126.68 (10)
C11—C12—H12	112.0 (12)	C2—O2—C22	118.21 (17)
H13—C12—H12	107.3 (16)	C20—O3—Co1	124.61 (11)
N2—C13—C8	104.42 (13)	C19—O4—C21	117.60 (18)
N2—C13—C12	110.35 (14)	H25—O5—H26	99 (3)
C8—C13—C12	112.49 (15)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O5—H25 \cdots O2	0.90 (4)	2.11 (4)	2.916 (3)	149 (3)
O5—H25 \cdots O1	0.90 (4)	2.45 (4)	3.103 (2)	129 (3)
O5—H26 \cdots O4	0.89 (4)	2.05 (4)	2.895 (3)	159 (4)
O5—H26 \cdots O3	0.89 (4)	2.59 (4)	3.248 (2)	131 (3)

Fig. 1

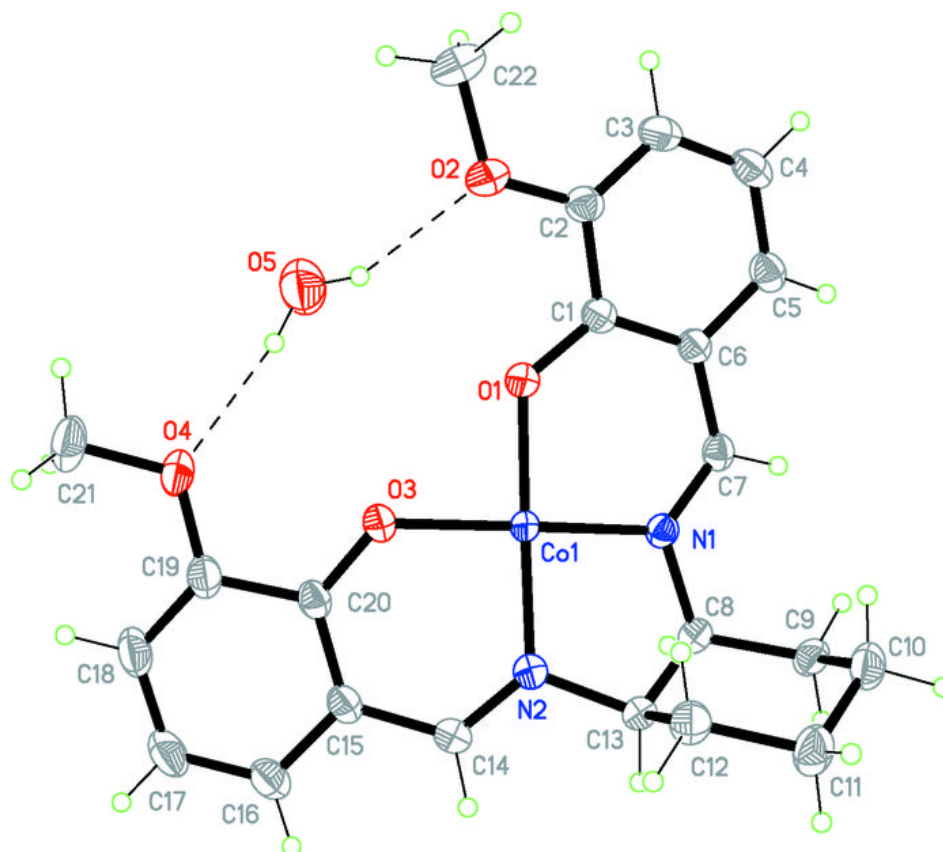


Fig. 2

