Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Aquabis(4-chlorobenzoato)-$\kappa^2O,O';\kappa O$-bis(pyridine-κN)cobalt(II)

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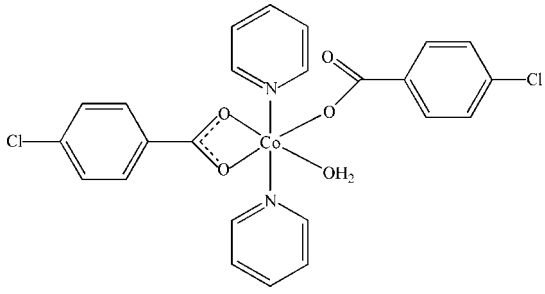
Received 6 March 2013; accepted 10 March 2013

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.039; wR factor = 0.082; data-to-parameter ratio = 13.6.

In the title compound, $[Co(C_7H_4ClO_2)_2(C_5H_5N)_2(H_2O)]$, the Co^{II} atom is six-coordinated by three O atoms from a bidentate and a monodentate 4-chlorobenzoate ligand, two N atoms from two pyridine ligands and a water O atom, giving a distorted octahedral geometry. In the crystal, the complex molecules are connected by O—H···O hydrogen bonds and π–π interactions between the benzene rings [centroid–centroid distance = 3.8924 (17) Å] into a chain along [010]. Between adjacent chains, π–π interactions occur between the pyridine rings [centroid–centroid distance = 3.898 (2) Å], giving an overall two-dimensional architecture.

Related literature

For structures and applications of related compounds, see: Macgillivray *et al.* (1998); Masaoka *et al.* (2001); Qiu *et al.* (2008); Wang & Sun (2012).



Experimental

Crystal data

$[Co(C_7H_4ClO_2)_2(C_5H_5N)_2(H_2O)]$ M_r = 546.25
Monoclinic, $P2_1/c$
a = 15.1157 (8) Å
b = 5.8696 (3) Å
c = 28.5419 (9) Å
β = 109.682 (3)°
V = 2384.4 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.98 mm^{-1}
T = 298 K
0.40 × 0.30 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.695, T_{max} = 0.828
15626 measured reflections
4175 independent reflections
3590 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.082
S = 1.10
4175 reflections
307 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H1W···O4^{i}	0.84	1.81	2.648 (3)	178
O5—H2W···O2^{i}	0.81	1.99	2.737 (3)	154

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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*.

This work was supported by the Natural Science Foundation of China (No. 21174114), the Plan for the Yangtze River Scholar and Innovation Team Development of the Ministry of Education (No. IRT1177), the Scientific and Technical Plan Project of Gansu Province (No. 1204 GKCA006), the Natural Science Foundation of Gansu Province (No. 1010RJZA024) and the Scientific and Technical Innovation Project of Northwest Normal University (nwnu-kjcxgc-03–63).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2620).

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supporting information

Acta Cryst. (2013). E**69**, m210 [doi:10.1107/S1600536813006752]

Aquabis(4-chlorobenzoato)-$\kappa^2O,O';\kappa O$-bis(pyridine-κN)cobalt(II)

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S1. Comment

Metal-organic frameworks (MOFs) of aromatic acid are of great interest not only owing to their various structural motifs, but also due to their potential applications in the areas of material chemistry, medical chemistry, biological chemistry, molecular recognition and molecular device (Macgillivray *et al.*, 1998; Masaoka *et al.*, 2001). Sometimes hydrogen bonds play important roles in MOFs (Qiu *et al.*, 2008; Wang & Sun, 2012). In order to achieve MOFs by self-assembly and to explore their hydrogen bonds, herein we report the synthesis and crystal structure of a cobalt complex with 4-chlorobenzoic acid.

As shown in Fig. 1, the Co^{II} atom is six-coordinated by three O atoms from two 4-chlorobenzoate ligands, two N atoms from two pyridine molecules and a water molecule. The Co^{II} atom adopts a distorted octahedral geometry, in which two N atoms occupy the axial sites. The axial Co—N bond distances are 2.158 (2) and 2.168 (2) Å. The Co1—O3 bond distance [1.9931 (19) Å] for the monodentate 4-chlorobenzoate ligand is slightly shorter than Co1—O1 and Co1—O2 [2.1674 (18) and 2.2196 (18) Å] for the bidentate ligand. The crystal packing shows that the molecules are linked by O—H···O hydrogen bonds and π–π interactions between the benzene rings [centroid–centroid distances = 3.8924 (17) Å] into a polymeric chain along [010], as shown in Fig. 2. Between the adjacent chains, π–π interactions exist between the pyridine rings [centroid–centroid distance is 3.898 (2) Å] to give an overall 2D architecture.

S2. Experimental

A pyridine solution (5 ml) of $Co(NO_3)_2.4H_2O$ (0.1 mmol) was added dropwise to an ethyl acetate solution (15 ml) of 4-chlorobenzoic acid (0.2 mmol). The mixture was sealed in a Teflon-lined autoclave and heated under autogenous pressure to 120°C for 3 days and then allowed to cool to room temperature at a rate of 1°C per minute. Block-shaped purple crystals of the title complex were collected in 43% yield.

S3. Refinement

H atoms on C atoms were place at calculated positions and refined as riding atoms, with C—H = 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C). H atoms of water molecule were located from a difference Fourier map and refined as riding with U_{iso}(H) = 1.5U_{eq}(O).

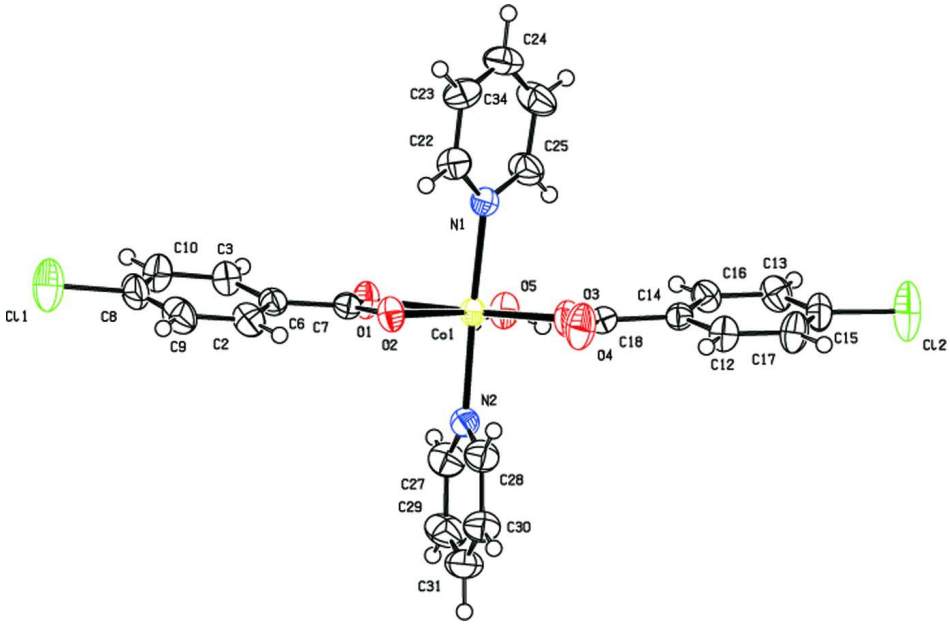

Figure 1

The molecular structure of the title complex. Displacement ellipsoids are drawn at the 30% probability level.

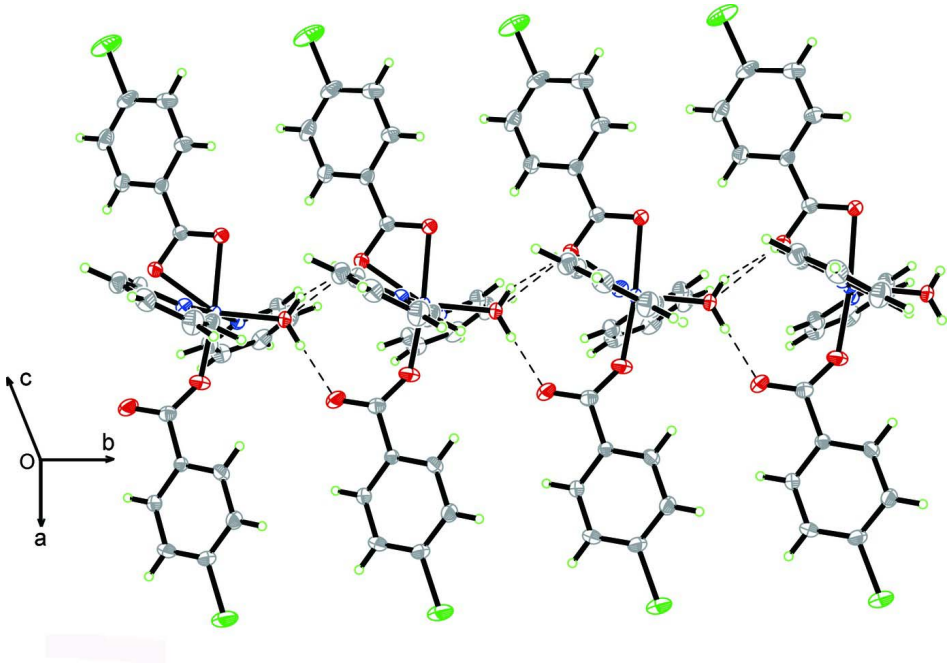

Figure 2

The chain structure of the title complex, constructed by hydrogen bonds (dashed lines).

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Crystal data

$[Co(C_7H_4ClO_2)_2(C_5H_5N)_2(H_2O)]$
M_r = 546.25

Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc

a = 15.1157 (8) Å
b = 5.8696 (3) Å
c = 28.5419 (9) Å
β = 109.682 (3)°
V = 2384.4 (2) Å^3
Z = 4
F(000) = 1116
D_x = 1.522 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6935 reflections
θ = 2.4–28.2°
μ = 0.98 mm^{-1}
T = 298 K
Block, purple
0.40 × 0.30 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.695, T_{max} = 0.828

15626 measured reflections
4175 independent reflections
3590 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 25.0°, θ_{min} = 2.4°
h = −17→17
k = −6→6
l = −33→33

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.082
S = 1.10
4175 reflections
307 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0201P)^2 + 2.9673P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Co1	0.23784 (2)	0.86593 (6)	0.875872 (13)	0.02636 (11)
Cl1	−0.21542 (8)	0.3351 (2)	0.95560 (5)	0.0979 (4)
Cl2	0.71492 (7)	0.92030 (19)	0.78128 (5)	0.0839 (4)
O1	0.10651 (13)	0.9072 (3)	0.88994 (7)	0.0379 (5)
O2	0.17142 (13)	0.5694 (3)	0.89912 (7)	0.0359 (5)
O3	0.35454 (13)	0.7911 (4)	0.86129 (7)	0.0451 (5)
O4	0.40222 (15)	0.4307 (4)	0.86863 (9)	0.0556 (6)
O5	0.24608 (13)	1.2116 (3)	0.86343 (7)	0.0366 (5)
H1W	0.2964	1.2776	0.8651	0.055*

H2W	0.2166	1.2839	0.8774	0.055*
N1	0.16311 (15)	0.8021 (4)	0.79767 (8)	0.0326 (5)
N2	0.31910 (15)	0.9057 (4)	0.95367 (8)	0.0325 (5)
C2	0.0318 (2)	0.3927 (5)	0.93584 (10)	0.0412 (7)
H2	0.0852	0.3037	0.9411	0.049*
C3	−0.0535 (2)	0.7357 (6)	0.90731 (11)	0.0420 (7)
H3	−0.0569	0.8806	0.8936	0.050*
C6	0.02714 (19)	0.6065 (5)	0.91523 (9)	0.0319 (6)
C7	0.10590 (18)	0.7004 (5)	0.90078 (9)	0.0301 (6)
C8	−0.1215 (2)	0.4410 (6)	0.94008 (12)	0.0524 (9)
C9	−0.0427 (2)	0.3096 (6)	0.94881 (12)	0.0496 (8)
H9	−0.0391	0.1663	0.9633	0.060*
C10	−0.1284 (2)	0.6540 (6)	0.91935 (12)	0.0526 (9)
H10	−0.1824	0.7411	0.9136	0.063*
C12	0.55779 (19)	0.5577 (5)	0.84130 (11)	0.0374 (7)
H12	0.5598	0.4156	0.8560	0.045*
C13	0.5506 (2)	0.9779 (5)	0.79653 (11)	0.0420 (7)
H13	0.5482	1.1187	0.7812	0.050*
C14	0.48302 (18)	0.7019 (4)	0.83676 (9)	0.0288 (6)
C15	0.6245 (2)	0.8322 (5)	0.80206 (12)	0.0436 (7)
C16	0.4800 (2)	0.9117 (5)	0.81416 (10)	0.0356 (7)
H16	0.4298	1.0094	0.8108	0.043*
C17	0.6296 (2)	0.6223 (5)	0.82424 (12)	0.0471 (8)
H17	0.6802	0.5258	0.8277	0.056*
C18	0.40645 (18)	0.6316 (5)	0.85674 (10)	0.0343 (6)
C22	0.1111 (2)	0.6170 (5)	0.78027 (11)	0.0402 (7)
H22	0.1064	0.5078	0.8029	0.048*
C23	0.0641 (2)	0.5797 (5)	0.73044 (11)	0.0466 (8)
H23	0.0285	0.4483	0.7200	0.056*
C24	0.0700 (2)	0.7357 (6)	0.69669 (11)	0.0487 (8)
H24	0.0374	0.7157	0.6629	0.058*
C25	0.1706 (2)	0.9504 (6)	0.76401 (11)	0.0468 (8)
H25	0.2081	1.0784	0.7750	0.056*
C27	0.3169 (2)	1.0861 (5)	0.98112 (11)	0.0455 (8)
H27	0.2752	1.2033	0.9667	0.055*
C28	0.3784 (2)	0.7390 (5)	0.97579 (11)	0.0425 (7)
H28	0.3801	0.6097	0.9573	0.051*
C29	0.3737 (3)	1.1083 (6)	1.03022 (12)	0.0572 (9)
H29	0.3704	1.2379	1.0483	0.069*
C30	0.4374 (2)	0.7476 (6)	1.02459 (11)	0.0497 (8)
H30	0.4778	0.6275	1.0386	0.060*
C31	0.4349 (2)	0.9365 (6)	1.05170 (12)	0.0545 (9)
H31	0.4745	0.9486	1.0846	0.065*
C34	0.1252 (2)	0.9234 (6)	0.71350 (11)	0.0541 (9)
H34	0.1321	1.0317	0.6912	0.065*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.02674 (19)	0.02380 (19)	0.02987 (19)	−0.00091 (15)	0.01127 (14)	0.00061 (15)
Cl1	0.0735 (7)	0.1326 (11)	0.1053 (9)	−0.0426 (7)	0.0536 (7)	0.0101 (8)
Cl2	0.0694 (6)	0.0799 (7)	0.1319 (10)	−0.0037 (5)	0.0727 (7)	0.0154 (7)
O1	0.0372 (11)	0.0302 (11)	0.0534 (12)	0.0000 (9)	0.0246 (10)	0.0037 (9)
O2	0.0396 (11)	0.0296 (10)	0.0458 (11)	−0.0011 (9)	0.0240 (9)	−0.0020 (9)
O3	0.0355 (11)	0.0561 (14)	0.0504 (13)	0.0067 (10)	0.0233 (10)	0.0017 (11)
O4	0.0485 (13)	0.0444 (14)	0.0834 (17)	−0.0051 (11)	0.0348 (12)	0.0148 (12)
O5	0.0400 (11)	0.0224 (10)	0.0523 (13)	−0.0030 (8)	0.0220 (10)	−0.0017 (9)
N1	0.0320 (12)	0.0334 (13)	0.0325 (13)	−0.0028 (10)	0.0111 (10)	−0.0001 (10)
N2	0.0337 (12)	0.0308 (13)	0.0336 (12)	−0.0027 (10)	0.0120 (10)	−0.0015 (10)
C2	0.0516 (18)	0.0354 (16)	0.0411 (17)	−0.0053 (14)	0.0215 (14)	−0.0031 (14)
C3	0.0391 (17)	0.0479 (18)	0.0434 (18)	−0.0028 (14)	0.0195 (14)	0.0011 (15)
C6	0.0359 (15)	0.0320 (15)	0.0290 (14)	−0.0078 (12)	0.0127 (12)	−0.0058 (12)
C7	0.0316 (15)	0.0320 (16)	0.0268 (14)	−0.0024 (12)	0.0101 (12)	−0.0047 (12)
C8	0.051 (2)	0.069 (2)	0.0457 (19)	−0.0261 (18)	0.0284 (16)	−0.0083 (17)
C9	0.068 (2)	0.0407 (18)	0.0465 (19)	−0.0185 (17)	0.0278 (17)	−0.0013 (15)
C10	0.0381 (18)	0.069 (2)	0.057 (2)	−0.0014 (17)	0.0235 (16)	−0.0030 (18)
C12	0.0384 (16)	0.0290 (15)	0.0486 (18)	0.0013 (12)	0.0196 (14)	0.0022 (13)
C13	0.0524 (19)	0.0335 (16)	0.0463 (18)	−0.0039 (14)	0.0249 (15)	0.0013 (14)
C14	0.0287 (14)	0.0283 (14)	0.0296 (14)	−0.0035 (11)	0.0102 (11)	−0.0050 (11)
C15	0.0393 (17)	0.0460 (19)	0.0549 (19)	−0.0064 (14)	0.0283 (15)	−0.0045 (15)
C16	0.0383 (16)	0.0343 (16)	0.0375 (15)	0.0082 (13)	0.0169 (13)	0.0028 (13)
C17	0.0364 (17)	0.0445 (18)	0.068 (2)	0.0080 (14)	0.0280 (16)	0.0014 (17)
C18	0.0287 (14)	0.0429 (17)	0.0294 (14)	−0.0012 (13)	0.0075 (12)	−0.0009 (13)
C22	0.0436 (17)	0.0338 (16)	0.0405 (16)	−0.0031 (14)	0.0106 (13)	0.0024 (14)
C23	0.0450 (18)	0.0433 (19)	0.0443 (18)	−0.0075 (15)	0.0055 (15)	−0.0102 (15)
C24	0.054 (2)	0.056 (2)	0.0304 (17)	0.0062 (17)	0.0064 (15)	−0.0060 (15)
C25	0.059 (2)	0.0460 (18)	0.0364 (17)	−0.0149 (16)	0.0173 (15)	0.0008 (14)
C27	0.0542 (19)	0.0370 (18)	0.0449 (18)	−0.0008 (14)	0.0161 (15)	−0.0032 (14)
C28	0.0462 (18)	0.0401 (17)	0.0403 (18)	0.0021 (15)	0.0135 (14)	−0.0021 (14)
C29	0.080 (3)	0.050 (2)	0.0416 (19)	−0.018 (2)	0.0209 (18)	−0.0157 (17)
C30	0.0466 (19)	0.060 (2)	0.0375 (18)	0.0030 (16)	0.0071 (15)	0.0085 (16)
C31	0.056 (2)	0.069 (2)	0.0323 (17)	−0.0182 (19)	0.0068 (15)	0.0001 (17)
C34	0.075 (2)	0.054 (2)	0.0351 (17)	−0.0041 (18)	0.0209 (17)	0.0077 (15)

Geometric parameters (Å, º)

Co1—O3	1.9931 (19)	C12—C14	1.382 (4)
Co1—O5	2.0710 (18)	C12—C17	1.384 (4)
Co1—N2	2.158 (2)	C12—H12	0.9300
Co1—O1	2.1674 (18)	C13—C15	1.373 (4)
Co1—N1	2.168 (2)	C13—C16	1.381 (4)
Co1—O2	2.2196 (18)	C13—H13	0.9300
Cl1—C8	1.738 (3)	C14—C16	1.384 (4)
Cl2—C15	1.741 (3)	C14—C18	1.510 (4)

O1—C7	1.253 (3)	C15—C17	1.376 (4)
O2—C7	1.268 (3)	C16—H16	0.9300
O3—C18	1.256 (3)	C17—H17	0.9300
O4—C18	1.235 (4)	C22—C23	1.377 (4)
O5—H1W	0.8405	C22—H22	0.9300
O5—H2W	0.8101	C23—C24	1.354 (4)
N1—C25	1.329 (4)	C23—H23	0.9300
N1—C22	1.335 (4)	C24—C34	1.368 (5)
N2—C27	1.324 (4)	C24—H24	0.9300
N2—C28	1.334 (4)	C25—C34	1.381 (4)
C2—C6	1.378 (4)	C25—H25	0.9300
C2—C9	1.387 (4)	C27—C29	1.381 (4)
C2—H2	0.9300	C27—H27	0.9300
C3—C10	1.375 (4)	C28—C30	1.379 (4)
C3—C6	1.388 (4)	C28—H28	0.9300
C3—H3	0.9300	C29—C31	1.366 (5)
C6—C7	1.491 (4)	C29—H29	0.9300
C8—C9	1.370 (5)	C30—C31	1.359 (5)
C8—C10	1.372 (5)	C30—H30	0.9300
C9—H9	0.9300	C31—H31	0.9300
C10—H10	0.9300	C34—H34	0.9300

O3—Co1—O5	94.10 (8)	C17—C12—H12	119.6
O3—Co1—N2	90.09 (8)	C15—C13—C16	118.8 (3)
O5—Co1—N2	91.37 (8)	C15—C13—H13	120.6
O3—Co1—O1	173.52 (9)	C16—C13—H13	120.6
O5—Co1—O1	91.95 (7)	C12—C14—C16	119.1 (2)
N2—Co1—O1	92.10 (8)	C12—C14—C18	120.3 (2)
O3—Co1—N1	86.43 (8)	C16—C14—C18	120.7 (2)
O5—Co1—N1	91.91 (8)	C13—C15—C17	121.9 (3)
N2—Co1—N1	175.38 (9)	C13—C15—Cl2	118.5 (2)
O1—Co1—N1	91.03 (8)	C17—C15—Cl2	119.6 (2)
O3—Co1—O2	114.26 (8)	C13—C16—C14	120.8 (3)
O5—Co1—O2	151.53 (7)	C13—C16—H16	119.6
N2—Co1—O2	86.29 (8)	C14—C16—H16	119.6
O1—Co1—O2	59.84 (7)	C15—C17—C12	118.6 (3)
N1—Co1—O2	92.35 (8)	C15—C17—H17	120.7
C7—O1—Co1	91.20 (16)	C12—C17—H17	120.7
C7—O2—Co1	88.45 (16)	O4—C18—O3	126.3 (3)
C18—O3—Co1	144.4 (2)	O4—C18—C14	118.8 (3)
Co1—O5—H1W	123.2	O3—C18—C14	114.9 (3)
Co1—O5—H2W	110.7	N1—C22—C23	123.2 (3)
H1W—O5—H2W	111.6	N1—C22—H22	118.4
C25—N1—C22	116.5 (2)	C23—C22—H22	118.4
C25—N1—Co1	119.32 (19)	C24—C23—C22	119.5 (3)
C22—N1—Co1	124.12 (19)	C24—C23—H23	120.2
C27—N2—C28	117.0 (3)	C22—C23—H23	120.2
C27—N2—Co1	125.2 (2)	C23—C24—C34	118.3 (3)

C28—N2—Co1	117.81 (19)	C23—C24—H24	120.9
C6—C2—C9	120.3 (3)	C34—C24—H24	120.9
C6—C2—H2	119.8	N1—C25—C34	123.1 (3)
C9—C2—H2	119.8	N1—C25—H25	118.4
C10—C3—C6	121.3 (3)	C34—C25—H25	118.4
C10—C3—H3	119.3	N2—C27—C29	123.0 (3)
C6—C3—H3	119.3	N2—C27—H27	118.5
C2—C6—C3	118.9 (3)	C29—C27—H27	118.5
C2—C6—C7	121.6 (3)	N2—C28—C30	123.7 (3)
C3—C6—C7	119.5 (3)	N2—C28—H28	118.2
O1—C7—O2	120.5 (2)	C30—C28—H28	118.2
O1—C7—C6	120.0 (2)	C31—C29—C27	118.8 (3)
O2—C7—C6	119.5 (2)	C31—C29—H29	120.6
C9—C8—C10	121.8 (3)	C27—C29—H29	120.6
C9—C8—Cl1	119.2 (3)	C31—C30—C28	118.2 (3)
C10—C8—Cl1	119.1 (3)	C31—C30—H30	120.9
C8—C9—C2	119.2 (3)	C28—C30—H30	120.9
C8—C9—H9	120.4	C30—C31—C29	119.4 (3)
C2—C9—H9	120.4	C30—C31—H31	120.3
C8—C10—C3	118.4 (3)	C29—C31—H31	120.3
C8—C10—H10	120.8	C24—C34—C25	119.2 (3)
C3—C10—H10	120.8	C24—C34—H34	120.4
C14—C12—C17	120.9 (3)	C25—C34—H34	120.4
C14—C12—H12	119.6		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H1*W*···O4^{i}	0.84	1.81	2.648 (3)	178
O5—H2*W*···O2^{i}	0.81	1.99	2.737 (3)	154

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