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Bis[3-(4-carboxyphenoxy)propionato-κO]bis[3-(4-carboxyphenoxy)propionic acid-κO]bis(pyridine-κN)cobalt(II)

Li-Li Kong, Shan Gao* and Li-Hua Huo

School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China
Correspondence e-mail: shangao67@yahoo.com

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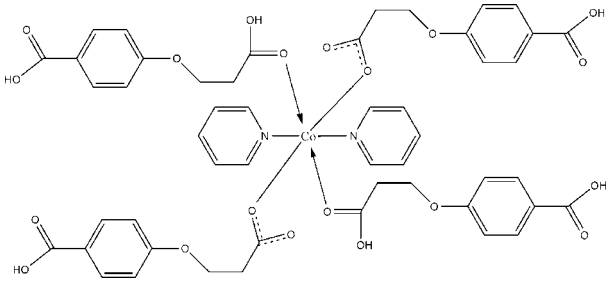
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.006 Å; R factor = 0.056; wR factor = 0.215; data-to-parameter ratio = 15.7.

The title complex, $[Co(C_{10}H_9O_5)_2(C_{10}H_{10}O_5)_2(C_5H_5N)_2]$, is a neutral mononuclear complex. The Co^{II} atom, which lies on a centre of symmetry, has a distorted octahedral geometry involving two O atoms of the 3-(4-carboxyphenoxy)propionate groups, two O atoms of the 3-(4-carboxyphenoxy)propionic acid groups and two N atoms of two pyridine ligands. A two-dimensional supramolecular structure is constructed *via* π–π interactions [centroid-to-centroid distance 3.589 (3) Å] and hydrogen-bonding interactions.

Related literature

3-(4-Carboxyphenoxy)propionic acid [3-(*p*-CPOPH$_2$)] has been reported previously (Gao & Ng, 2006). In our previous work, the cobalt(II) complex of 3-(*p*-CPOPH$_2$) has been characterized by X-ray crystallography (Xiao *et al.*, 2006).



Experimental

Crystal data

$[Co(C_{10}H_9O_5)_2(C_{10}H_{10}O_5)_2(C_5H_5N)_2]$
M_r = 1055.83
Triclinic, $P\overline{1}$
a = 8.2621 (17) Å
b = 8.7358 (17) Å
c = 17.502 (4) Å
α = 76.58 (3)°
β = 76.53 (3)°
γ = 78.94 (3)°
V = 1182.2 (5) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.45 mm^{-1}
T = 295 (2) K
0.38 × 0.25 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.848, T_{max} = 0.920
11688 measured reflections
5356 independent reflections
2748 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.215
S = 1.07
5356 reflections
341 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.98 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O2	2.062 (3)	Co1—N1	2.133 (3)
Co1—O6	2.125 (3)		
O2—Co1—O6	82.86 (12)	O6—Co1—N1	88.11 (11)
O2—Co1—N1	91.23 (11)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H30···O1^{i}	0.86 (3)	1.58 (4)	2.436 (4)	178 (7)
O4—H20···O10^{ii}	0.86 (5)	1.79 (5)	2.637 (4)	173 (6)
O9—H10···O5^{ii}	0.85 (5)	1.79 (5)	2.633 (4)	172 (6)

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $-x-1, -y, -z+1$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2101).

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supplementary materials

Acta Cryst. (2007). E**63**, m2554 [**doi:10.1107/S1600536807045229**]

Bis[3-(4-carboxyphenoxy)propionato-*κO*]bis[3-(4-carboxyphenoxy)propionic acid-*κO*]bis(pyridine-*κN*)cobalt(II)

L.-L. Kong, S. Gao and L.-H. Huo

Comment

Our studies have addressed the metal derivatives of carboxyphenoxypropionic acids. 3-(4-carboxylatophenoxy)propionic acid [3-(*p*-CPOPH$_2$)] is a potential flexible multidentated ligand which could be used as a terminal ligand or a bridging ligand with different coordination modes when coordinated to various metal ions. In addition to its versatile coordination modes, 3-(4-carboxylatophenoxy)propionic acid may take part in hydrogen-bonding interactions by functioning as either a hydrogen-bond donor or acceptor (Gao & Ng, 2006). Recently, we have reported the structure of a dinuclear cobalt(II) complex incorporating 3-(4-carboxylatophenoxy)propionate groups, namely [$Co_2(C_{10}H_8O_5)_2(H_2O)_8$]·4$H_2O$, (I) (Xiao *et al.*, 2006).

In contrast to (I), the title compound is a mononuclear complex (Fig. 1), in which the Co atom lies on a centre of symmetry and displays a distorted octahedral geometry involving two O atoms of the 3-(4-carboxylatophenoxy)propionate groups, two O atoms of the 3-(4-carboxyphenoxy)propionic acid groups and two N atoms of two pyridine ligands. The average Co—*O*(carbonyl) bond length is 2.094 (2) Å, which is somewhat longer than the corresponding value in (I), 2.038 (3) Å. Furthermore, a two-dimensional supramolecular layer is constructed *via* π–π stacking interactions between the pyridine rings [centroid-centroid distance: 3.589 (3) Å] and hydrogen-bonding interactions (Table 2). There is, in additiom, a strong intramolecular H-bond (first entry in Table 2 and Fig. 1), linking the two independent, coordinated carboxylate groups.

Experimental

The title complex was prepared by the addition of cobalt(II) acetate trihydrate (10 mmol), pyridine (1 ml) and 3-(*p*-CPOPH$_2$) (15 mmol) to a H_2O/MeOH (*v*/*v* = 1:1) solution. Red crystals were obtained from the filtered solution at room temperature over several days. CH&N analysis. Calc. for $C_{50}H_{48}N_2O_{20}Co$: C 56.88, H 4.58, N 2.65%. Found: C 56.89, H 4.56, N 2.66%.

Refinement

The H atoms were placed in calculated positions with C—H = 0.93 or 0.97 Å and U_{iso}(H) = 1.2U_{eq} (C) and were included in the refinement in the riding model approximation. The H atoms of hydroxyl groups were located in difference Fourier maps and refined with the O—H distance restrained to 0.85 (1) Å and U_{iso}(H) = 1.5U_{eq}(O).

Figures

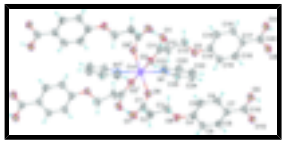


Fig. 1. Molecular structure of the title compound with 30% probability ellipsoid for the non-H atoms. Dashed lines indicate O—H···O hydrogen bonds. [Symmetry code: (i) −*x* + 1,-*y* + 1,-*z*]

Bis[3-(4-carboxyphenoxy)propionato-κ*O*]bis[3- (4-carboxyphenoxy)propionic acid-κ*O*]bis(pyridine-κ*N*)cobalt(II)

Crystal data

$[Co(C_{10}H_9O_5)_2(C_{10}H_{10}O_5)_2(C_5H_5N)_2]$	$Z = 1$
$M_r = 1055.83$	$F_{000} = 549$
Triclinic, $P\overline{1}$	$D_x = 1.483$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.2621$ (17) Å	Cell parameters from 7199 reflections
$b = 8.7358$ (17) Å	$\theta = 3.1$–27.4º
$c = 17.502$ (4) Å	$\mu = 0.45$ mm^{-1}
$\alpha = 76.58$ (3)º	$T = 295$ (2) K
$\beta = 76.53$ (3)º	Block, red
$\gamma = 78.94$ (3)º	0.38 × 0.25 × 0.19 mm
$V = 1182.2$ (5) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	5356 independent reflections
Radiation source: fine-focus sealed tube	2748 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.038$
Detector resolution: 10 pixels mm^{-1}	$\theta_{max} = 27.5$º
$T = 295(2)$ K	$\theta_{min} = 3.1$º
ω scans	$h = -10 \rightarrow 10$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -11 \rightarrow 11$
$T_{min} = 0.848$, $T_{max} = 0.920$	$l = -22 \rightarrow 22$
11688 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
$R[F^2 > 2\sigma(F^2)] = 0.056$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.215$	$w = 1/[\sigma^2(F_o^2) + (0.116P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} < 0.001$
5356 reflections	$\Delta\rho_{max} = 0.52$ e Å^{-3}
341 parameters	$\Delta\rho_{min} = -0.98$ e Å^{-3}
3 restraints	Extinction correction: SHELXL (Sheldrick, 1997), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Primary atom site location: structure-invariant direct methods

Extinction coefficient: 0.010 (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}
Co1	0.5000	0.5000	0.0000	0.0479 (3)
O1	0.5675 (4)	0.1351 (3)	0.13958 (16)	0.0678 (8)
O2	0.5516 (4)	0.3988 (3)	0.11210 (15)	0.0602 (7)
O3	0.2880 (3)	0.1751 (3)	0.29858 (16)	0.0637 (7)
O4	−0.1451 (4)	−0.3393 (4)	0.52659 (19)	0.0735 (9)
H20	−0.224 (5)	−0.394 (6)	0.551 (3)	0.110*
O5	−0.3392 (4)	−0.1726 (4)	0.46859 (19)	0.0738 (8)
O6	0.3566 (4)	0.6826 (3)	0.05983 (17)	0.0659 (8)
O7	0.3480 (5)	0.9294 (4)	−0.00646 (19)	0.0822 (10)
H30	0.380 (8)	0.906 (7)	−0.0533 (16)	0.123*
O8	0.0279 (3)	0.8049 (3)	0.19057 (16)	0.0630 (7)
O9	−0.4260 (4)	0.3466 (4)	0.45047 (19)	0.0741 (9)
H10	−0.509 (5)	0.297 (6)	0.474 (3)	0.111*
O10	−0.6187 (4)	0.5077 (3)	0.38703 (18)	0.0680 (8)
N1	0.2787 (4)	0.3899 (3)	0.02698 (19)	0.0514 (7)
C1	0.3358 (5)	0.8248 (5)	0.0582 (2)	0.0536 (9)
C2	0.2917 (5)	0.8889 (5)	0.1345 (2)	0.0619 (11)
H1	0.3946	0.9019	0.1484	0.074*
H2	0.2248	0.9931	0.1252	0.074*
C3	0.1959 (5)	0.7840 (5)	0.2039 (2)	0.0606 (10)
H3	0.2468	0.6736	0.2066	0.073*
H4	0.1957	0.8142	0.2539	0.073*
C4	−0.0854 (5)	0.7190 (5)	0.2447 (2)	0.0553 (9)
C5	−0.0460 (5)	0.5970 (5)	0.3068 (2)	0.0616 (10)
H5	0.0641	0.5694	0.3147	0.074*
C6	−0.1713 (5)	0.5166 (5)	0.3568 (2)	0.0611 (10)
H6	−0.1447	0.4352	0.3987	0.073*
C7	−0.3353 (5)	0.5547 (4)	0.3459 (2)	0.0546 (9)
C8	−0.3740 (5)	0.6792 (5)	0.2833 (2)	0.0612 (10)
H8	−0.4843	0.7080	0.2756	0.073*
C9	−0.2496 (5)	0.7586 (5)	0.2333 (2)	0.0613 (10)

H9	−0.2757	0.8399	0.1913	0.074*
C10	−0.4689 (5)	0.4657 (5)	0.3978 (2)	0.0576 (10)
C11	0.5552 (4)	0.2669 (5)	0.1590 (2)	0.0516 (9)
C12	0.5483 (6)	0.2669 (5)	0.2461 (2)	0.0660 (11)
H11	0.6623	0.2550	0.2546	0.079*
H12	0.4909	0.3692	0.2576	0.079*
C13	0.4605 (5)	0.1377 (5)	0.3044 (2)	0.0625 (11)
H13	0.5077	0.0348	0.2906	0.075*
H14	0.4729	0.1349	0.3585	0.075*
C14	0.1814 (5)	0.0733 (4)	0.3434 (2)	0.0531 (9)
C15	0.2274 (5)	−0.0672 (5)	0.3948 (2)	0.0572 (10)
H15	0.3389	−0.0980	0.4003	0.069*
C16	0.1063 (5)	−0.1611 (5)	0.4377 (2)	0.0568 (10)
H16	0.1377	−0.2556	0.4717	0.068*
C17	−0.0601 (5)	−0.1172 (4)	0.4310 (2)	0.0536 (9)
C18	−0.1041 (5)	0.0249 (5)	0.3791 (3)	0.0658 (11)
H18	−0.2156	0.0566	0.3736	0.079*
C19	0.0148 (5)	0.1173 (5)	0.3365 (3)	0.0658 (11)
H19	−0.0166	0.2115	0.3022	0.079*
C20	−0.1901 (5)	−0.2154 (5)	0.4776 (2)	0.0549 (9)
C21	0.2354 (5)	0.3318 (5)	−0.0281 (3)	0.0614 (10)
H21	0.3072	0.3351	−0.0778	0.074*
C22	0.0891 (6)	0.2669 (5)	−0.0151 (3)	0.0723 (12)
H22	0.0641	0.2259	−0.0548	0.087*
C23	−0.0170 (6)	0.2644 (6)	0.0567 (3)	0.0810 (14)
H23	−0.1169	0.2223	0.0671	0.097*
C24	0.0248 (6)	0.3247 (7)	0.1140 (3)	0.0831 (14)
H24	−0.0473	0.3250	0.1635	0.100*
C25	0.1731 (5)	0.3845 (5)	0.0981 (2)	0.0662 (11)
H25	0.2014	0.4227	0.1379	0.079*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0527 (5)	0.0506 (4)	0.0412 (4)	−0.0108 (3)	−0.0115 (3)	−0.0058 (3)
O1	0.095 (2)	0.0616 (16)	0.0466 (16)	−0.0208 (15)	−0.0101 (15)	−0.0057 (13)
O2	0.0734 (19)	0.0650 (16)	0.0448 (15)	−0.0213 (14)	−0.0214 (13)	0.0030 (12)
O3	0.0584 (17)	0.0690 (17)	0.0536 (17)	−0.0136 (13)	−0.0069 (13)	0.0071 (13)
O4	0.074 (2)	0.079 (2)	0.0613 (19)	−0.0216 (16)	−0.0135 (16)	0.0065 (16)
O5	0.063 (2)	0.083 (2)	0.072 (2)	−0.0164 (15)	−0.0152 (16)	−0.0020 (16)
O6	0.077 (2)	0.0581 (16)	0.0602 (18)	−0.0128 (14)	−0.0041 (15)	−0.0130 (13)
O7	0.122 (3)	0.0633 (18)	0.0555 (19)	−0.0167 (18)	−0.0097 (19)	−0.0052 (15)
O8	0.0549 (17)	0.0801 (18)	0.0533 (17)	−0.0182 (14)	−0.0148 (13)	−0.0007 (13)
O9	0.070 (2)	0.081 (2)	0.066 (2)	−0.0215 (16)	−0.0178 (16)	0.0090 (16)
O10	0.0594 (19)	0.0753 (18)	0.0654 (19)	−0.0128 (14)	−0.0149 (15)	−0.0013 (14)
N1	0.0548 (19)	0.0526 (17)	0.0468 (18)	−0.0099 (14)	−0.0149 (14)	−0.0030 (13)
C1	0.047 (2)	0.058 (2)	0.057 (2)	−0.0130 (17)	−0.0123 (17)	−0.0068 (18)
C2	0.069 (3)	0.064 (2)	0.060 (3)	−0.022 (2)	−0.011 (2)	−0.018 (2)

C3	0.061 (3)	0.076 (3)	0.051 (2)	−0.014 (2)	−0.0150 (19)	−0.018 (2)
C4	0.057 (2)	0.066 (2)	0.047 (2)	−0.0130 (19)	−0.0110 (18)	−0.0137 (18)
C5	0.054 (2)	0.077 (3)	0.055 (2)	−0.008 (2)	−0.0215 (19)	−0.004 (2)
C6	0.067 (3)	0.069 (2)	0.050 (2)	−0.014 (2)	−0.021 (2)	−0.0037 (19)
C7	0.062 (3)	0.058 (2)	0.048 (2)	−0.0097 (18)	−0.0177 (18)	−0.0104 (17)
C8	0.057 (2)	0.069 (2)	0.059 (3)	−0.0116 (19)	−0.020 (2)	−0.006 (2)
C9	0.060 (3)	0.069 (2)	0.052 (2)	−0.012 (2)	−0.0165 (19)	0.0013 (19)
C10	0.062 (3)	0.069 (2)	0.047 (2)	−0.014 (2)	−0.0146 (19)	−0.0124 (19)
C11	0.044 (2)	0.069 (2)	0.043 (2)	−0.0153 (17)	−0.0109 (16)	−0.0061 (18)
C12	0.075 (3)	0.086 (3)	0.042 (2)	−0.029 (2)	−0.017 (2)	−0.0023 (19)
C13	0.064 (3)	0.084 (3)	0.038 (2)	−0.017 (2)	−0.0119 (18)	−0.0014 (18)
C14	0.057 (2)	0.061 (2)	0.040 (2)	−0.0092 (18)	−0.0070 (17)	−0.0078 (16)
C15	0.055 (2)	0.070 (2)	0.042 (2)	−0.0090 (19)	−0.0146 (17)	0.0022 (17)
C16	0.064 (3)	0.061 (2)	0.042 (2)	−0.0092 (19)	−0.0149 (18)	0.0023 (17)
C17	0.060 (2)	0.062 (2)	0.038 (2)	−0.0124 (18)	−0.0089 (17)	−0.0068 (16)
C18	0.054 (2)	0.079 (3)	0.061 (3)	−0.006 (2)	−0.018 (2)	−0.001 (2)
C19	0.062 (3)	0.067 (2)	0.059 (3)	−0.005 (2)	−0.014 (2)	0.0053 (19)
C20	0.052 (2)	0.066 (2)	0.047 (2)	−0.0067 (19)	−0.0114 (18)	−0.0107 (18)
C21	0.061 (3)	0.068 (2)	0.060 (3)	−0.017 (2)	−0.013 (2)	−0.013 (2)
C22	0.062 (3)	0.088 (3)	0.075 (3)	−0.019 (2)	−0.021 (2)	−0.020 (2)
C23	0.058 (3)	0.104 (4)	0.087 (4)	−0.032 (3)	−0.023 (3)	−0.003 (3)
C24	0.053 (3)	0.123 (4)	0.068 (3)	−0.026 (3)	−0.004 (2)	−0.005 (3)
C25	0.060 (3)	0.092 (3)	0.046 (2)	−0.017 (2)	−0.010 (2)	−0.009 (2)

Geometric parameters (Å, °)

Co1—O2	2.062 (3)	C6—C7	1.379 (5)
Co1—O6	2.125 (3)	C6—H6	0.9300
Co1—N1	2.133 (3)	C7—C8	1.401 (5)
Co1—O2^{i}	2.062 (3)	C7—C10	1.477 (5)
Co1—O6^{i}	2.125 (3)	C8—C9	1.369 (5)
Co1—N1^{i}	2.133 (3)	C8—H8	0.9300
O1—C11	1.254 (5)	C9—H9	0.9300
O2—C11	1.250 (4)	C11—C12	1.512 (5)
O3—C14	1.355 (4)	C12—C13	1.508 (5)
O3—C13	1.422 (5)	C12—H11	0.9700
O4—C20	1.268 (5)	C12—H12	0.9700
O4—H20	0.86 (5)	C13—H13	0.9700
O5—C20	1.253 (5)	C13—H14	0.9700
O6—C1	1.215 (4)	C14—C19	1.382 (6)
O7—C1	1.276 (5)	C14—C15	1.388 (5)
O7—H30	0.86 (3)	C15—C16	1.384 (5)
O8—C4	1.365 (4)	C15—H15	0.9300
O8—C3	1.432 (5)	C16—C17	1.379 (5)
O9—C10	1.274 (5)	C16—H16	0.9300
O9—H10	0.85 (5)	C17—C18	1.398 (5)
O10—C10	1.266 (5)	C17—C20	1.475 (5)
N1—C21	1.331 (5)	C18—C19	1.363 (6)

N1—C25	1.340 (5)	C18—H18	0.9300
C1—C2	1.507 (6)	C19—H19	0.9300
C2—C3	1.502 (5)	C21—C22	1.382 (6)
C2—H1	0.9700	C21—H21	0.9300
C2—H2	0.9700	C22—C23	1.352 (7)
C3—H3	0.9700	C22—H22	0.9300
C3—H4	0.9700	C23—C24	1.371 (7)
C4—C9	1.383 (6)	C23—H23	0.9300
C4—C5	1.384 (5)	C24—C25	1.367 (6)
C5—C6	1.379 (5)	C24—H24	0.9300
C5—H5	0.9300	C25—H25	0.9300
O2—Co1—O2^{i}	180.00 (16)	C8—C9—H9	119.7
O2—Co1—O6	82.86 (12)	C4—C9—H9	119.7
O2—Co1—O6^{i}	97.14 (12)	O10—C10—O9	123.0 (4)
O6—Co1—O6^{i}	180.00 (14)	O10—C10—C7	119.3 (4)
O2—Co1—N1^{i}	88.77 (11)	O9—C10—C7	117.7 (4)
O6—Co1—N1^{i}	91.89 (11)	O2—C11—O1	125.5 (4)
O2—Co1—N1	91.23 (11)	O2—C11—C12	116.9 (4)
O6—Co1—N1	88.11 (11)	O1—C11—C12	117.6 (3)
N1^{i}—Co1—N1	180.00 (17)	C13—C12—C11	114.3 (3)
O2^{i}—Co1—O6^{i}	82.86 (12)	C13—C12—H11	108.7
O2^{i}—Co1—N1^{i}	91.23 (11)	C11—C12—H11	108.7
O6^{i}—Co1—N1^{i}	88.11 (11)	C13—C12—H12	108.7
O6^{i}—Co1—N1	91.89 (11)	C11—C12—H12	108.7
O2^{i}—Co1—N1	88.77 (11)	H11—C12—H12	107.6
O2^{i}—Co1—O6	97.14 (12)	O3—C13—C12	106.5 (3)
C11—O2—Co1	139.0 (2)	O3—C13—H13	110.4
C14—O3—C13	118.3 (3)	C12—C13—H13	110.4
C20—O4—H20	114 (4)	O3—C13—H14	110.4
C1—O6—Co1	143.5 (3)	C12—C13—H14	110.4
C1—O7—H30	123 (4)	H13—C13—H14	108.6
C4—O8—C3	118.5 (3)	O3—C14—C19	115.7 (3)
C10—O9—H10	111 (4)	O3—C14—C15	125.1 (4)
C21—N1—C25	117.3 (3)	C19—C14—C15	119.2 (3)
C21—N1—Co1	121.0 (3)	C16—C15—C14	119.6 (4)
C25—N1—Co1	121.6 (3)	C16—C15—H15	120.2
O6—C1—O7	123.6 (4)	C14—C15—H15	120.2
O6—C1—C2	121.0 (4)	C17—C16—C15	121.3 (3)
O7—C1—C2	115.4 (4)	C17—C16—H16	119.4
C3—C2—C1	113.5 (3)	C15—C16—H16	119.4
C3—C2—H1	108.9	C16—C17—C18	118.3 (3)
C1—C2—H1	108.9	C16—C17—C20	121.5 (3)
C3—C2—H2	108.9	C18—C17—C20	120.2 (4)
C1—C2—H2	108.9	C19—C18—C17	120.6 (4)
H1—C2—H2	107.7	C19—C18—H18	119.7
O8—C3—C2	106.6 (3)	C17—C18—H18	119.7

O8—C3—H3	110.4	C18—C19—C14	121.0 (4)
C2—C3—H3	110.4	C18—C19—H19	119.5
O8—C3—H4	110.4	C14—C19—H19	119.5
C2—C3—H4	110.4	O5—C20—O4	122.9 (4)
H3—C3—H4	108.6	O5—C20—C17	119.3 (4)
O8—C4—C9	115.4 (3)	O4—C20—C17	117.8 (4)
O8—C4—C5	124.9 (4)	N1—C21—C22	123.3 (4)
C9—C4—C5	119.7 (4)	N1—C21—H21	118.4
C6—C5—C4	119.5 (4)	C22—C21—H21	118.4
C6—C5—H5	120.2	C23—C22—C21	118.5 (4)
C4—C5—H5	120.2	C23—C22—H22	120.7
C7—C6—C5	121.3 (4)	C21—C22—H22	120.7
C7—C6—H6	119.4	C22—C23—C24	119.0 (4)
C5—C6—H6	119.4	C22—C23—H23	120.5
C6—C7—C8	118.7 (4)	C24—C23—H23	120.5
C6—C7—C10	121.4 (4)	C25—C24—C23	119.8 (4)
C8—C7—C10	119.8 (4)	C25—C24—H24	120.1
C9—C8—C7	120.1 (4)	C23—C24—H24	120.1
C9—C8—H8	120.0	N1—C25—C24	122.1 (4)
C7—C8—H8	120.0	N1—C25—H25	119.0
C8—C9—C4	120.7 (4)	C24—C25—H25	119.0
O6—Co1—O2—C11	133.4 (4)	C6—C7—C10—O10	178.0 (4)
O6^{i}—Co1—O2—C11	−46.6 (4)	C8—C7—C10—O10	−2.9 (6)
N1^{i}—Co1—O2—C11	−134.6 (4)	C6—C7—C10—O9	−3.8 (6)
N1—Co1—O2—C11	45.4 (4)	C8—C7—C10—O9	175.3 (4)
O2—Co1—O6—C1	125.5 (5)	Co1—O2—C11—O1	20.6 (6)
O2^{i}—Co1—O6—C1	−54.5 (5)	Co1—O2—C11—C12	−160.9 (3)
N1^{i}—Co1—O6—C1	37.0 (5)	O2—C11—C12—C13	148.0 (4)
N1—Co1—O6—C1	−143.0 (5)	O1—C11—C12—C13	−33.4 (6)
O2—Co1—N1—C21	−141.4 (3)	C14—O3—C13—C12	177.7 (3)
O2^{i}—Co1—N1—C21	38.6 (3)	C11—C12—C13—O3	−67.6 (5)
O6—Co1—N1—C21	135.8 (3)	C13—O3—C14—C19	178.8 (4)
O6^{i}—Co1—N1—C21	−44.2 (3)	C13—O3—C14—C15	−0.5 (6)
O2—Co1—N1—C25	42.5 (3)	O3—C14—C15—C16	179.7 (4)
O2^{i}—Co1—N1—C25	−137.5 (3)	C19—C14—C15—C16	0.5 (6)
O6—Co1—N1—C25	−40.3 (3)	C14—C15—C16—C17	−0.6 (6)
O6^{i}—Co1—N1—C25	139.7 (3)	C15—C16—C17—C18	0.4 (6)
Co1—O6—C1—O7	35.9 (7)	C15—C16—C17—C20	−178.9 (4)
Co1—O6—C1—C2	−144.6 (4)	C16—C17—C18—C19	−0.1 (6)
O6—C1—C2—C3	−28.8 (6)	C20—C17—C18—C19	179.3 (4)
O7—C1—C2—C3	150.8 (4)	C17—C18—C19—C14	0.0 (7)
C4—O8—C3—C2	178.5 (3)	O3—C14—C19—C18	−179.5 (4)
C1—C2—C3—O8	−74.8 (4)	C15—C14—C19—C18	−0.2 (6)
C3—O8—C4—C9	172.7 (3)	C16—C17—C20—O5	−178.7 (4)
C3—O8—C4—C5	−8.8 (6)	C18—C17—C20—O5	2.0 (6)
O8—C4—C5—C6	−178.7 (4)	C16—C17—C20—O4	2.6 (6)
C9—C4—C5—C6	−0.2 (6)	C18—C17—C20—O4	−176.8 (4)

C4—C5—C6—C7	0.5 (6)	C25—N1—C21—C22	−0.3 (6)
C5—C6—C7—C8	−1.0 (6)	Co1—N1—C21—C22	−176.5 (3)
C5—C6—C7—C10	178.1 (4)	N1—C21—C22—C23	1.1 (7)
C6—C7—C8—C9	1.3 (6)	C21—C22—C23—C24	−0.5 (8)
C10—C7—C8—C9	−177.8 (4)	C22—C23—C24—C25	−0.8 (8)
C7—C8—C9—C4	−1.1 (6)	C21—N1—C25—C24	−1.1 (6)
O8—C4—C9—C8	179.2 (4)	Co1—N1—C25—C24	175.1 (4)
C5—C4—C9—C8	0.6 (6)	C23—C24—C25—N1	1.6 (8)

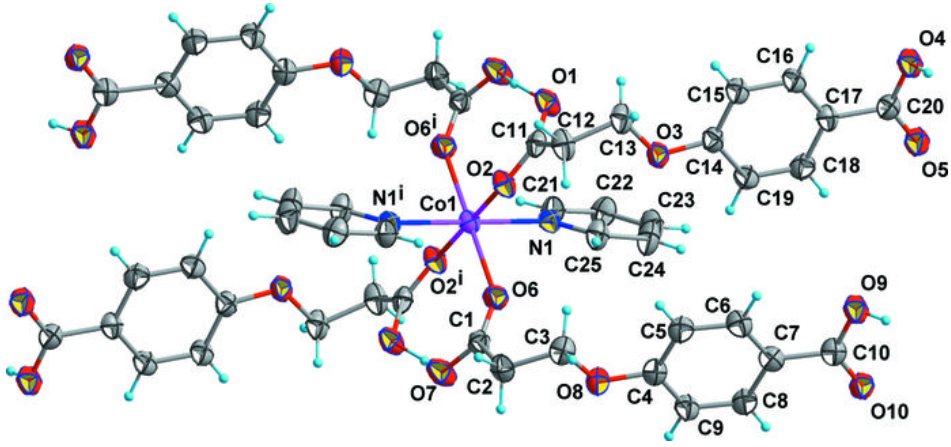
Symmetry codes: (i) −*x*+1, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H30···O1^{i}	0.86 (3)	1.58 (4)	2.436 (4)	178 (7)
O4—H20···O10^{ii}	0.86 (5)	1.79 (5)	2.637 (4)	173 (6)
O9—H10···O5^{ii}	0.85 (5)	1.79 (5)	2.633 (4)	172 (6)

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

Fig. 1


O4
C16
O1
C15
C17
C20
O6i
C11
C12
O3
C13
C14
C18
O5
O2
C21
C22
N1i
Co1
C23
C19
N1
C25
C24
O2i
O6
O9
C1
C6
C5
C7
C10
C3
O7
C2
O8
C4
C8
O10
C9