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(2,9-Dimethyl-1,10-phenanthroline-κ^2N,N')bis(2-hydroxybenzoato)-$\kappa O;\kappa^2O,O'$-cobalt(II)

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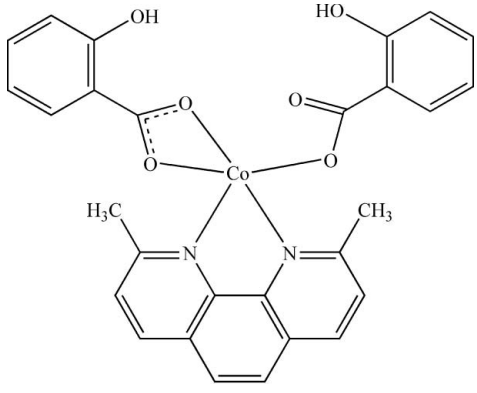
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.040; wR factor = 0.127; data-to-parameter ratio = 17.7.

In the title compound, $[Co(C_7H_5O_3)_2(C_{14}H_{12}N_2)]$, the Co^{II} ion is five-coordinated by two N atoms from one 2,9-dimethyl-1,10-phenanthroline (dmphen) ligand and three O atoms from two 2-hydroxybenzoate anions in a distorted trigonal bipyramidal geometry. The carboxylate group of one of the two 2-hydroxybenzoate anions is monodentate with a normal Co—O distance [1.9804 (18) Å], while the other is bidentate with two longer Co—O bonds [2.1981 (18) and 2.1359 (19) Å]. The crystal structure is stabilized by aromatic π–π stacking interactions [centroid–centroid distances of 4.0380 (3) and 3.8216 (3) Å between dmphen/dmphen and benzene/dmphen rings, respectively] and C—H$\cdots\pi$(benzene) interactions.

Related literature

For related literature, see: Naing *et al.* (1995); Wang *et al.* (1996); Wall *et al.* (1999). For related structures, see: Ding *et al.* (2006); Ren *et al.* (2007); Xuan & Zhao (2007); Zhong *et al.* (2006).



Experimental

Crystal data

$[Co(C_7H_5O_3)_2(C_{14}H_{12}N_2)]$
M_r = 541.41
Monoclinic, $P2_1/n$
a = 11.436 (1) Å
b = 16.528 (2) Å
c = 13.426 (2) Å
β = 105.856 (1)°
V = 2441.1 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.75 mm^{-1}
T = 293 (2) K
0.46 × 0.36 × 0.30 mm

Data collection

Bruker APEX2 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.779, T_{max} = 0.858
(expected range = 0.725–0.799)
20557 measured reflections
5998 independent reflections
4476 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.127
S = 1.04
5998 reflections
338 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.86 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O3—H3$O\cdots$O1	0.82	1.88	2.584 (3)	143
O6—H6$O\cdots$O5	0.82	1.85	2.578 (3)	146
C3—H3$\cdots Cg1^{i}$	0.93	2.59	3.402 (3)	146
C25—H25$\cdots Cg2^{ii}$	0.93	3.06	3.989 (3)	172

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x-1, y, z$. $Cg1$ is the centroid of the C23–C28 benzene ring and $Cg2$ is the centroid of the C16–C21 benzene ring.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2038).

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supplementary materials

Acta Cryst. (2008). E**64**, m740 [**doi:10.1107/S1600536808012002**]

(2,9-Dimethyl-1,10-phenanthroline-κ^2N,N')bis(2-hydroxybenzoato)-$\kappa O;\kappa^2 O,O'$-cobalt(II)

P.-Z. Zhao, X.-P. Xuan and Q.-H. Tang

Comment

Metal-phenanthroline complexes have attracted much attention because of their peculiar features during recent decades (Wang *et al.*, 1996; Wall *et al.*, 1999; Naing *et al.*, 1995). A number of Co(II)-phenanthroline complexes have been synthesized and structures were determined (Ding *et al.*, 2006; Ren *et al.*, 2007; Zhong *et al.*, 2006; Xuan & Zhao, 2007). Herein we report the molecular and crystal structure of the title compound, (I), Bis(2-hydroxybenzoato–$\kappa O,\kappa^2 O,O'$)-(2,9-dimethyl-1, 10-phenanthroline-$\kappa^2 N,N'$)-cobalt (II) (Fig. 1).

The Co atom in (I) is coordinated by a dmphen ligand and two 2-hydroxybenzoato ligands (Fig.1). The values of Co—O1 and Co—O2 distances are larger than the normal Co—O4 bond distance. The Co—O1—C15 and Co—O2—C15 bond angles [89.23 (14)°, 92.28 (15)°] appear to be compressed in order to allow Co and O atoms to approach each other. These imply the existence of genuing bonding interactions bwtween Co and O atoms, *i.e.* the C15-carboxylate group coordinates to the Co atom in chelating mode. The other ligand has a larger Co—O4—C22 angle of 107.71 (16)°. The values of Co···O5 distance is 2.6624 (22) Å, suggesting no bonding between the Co and O5 atoms. Therefore, the CoO_3N_2 unit forms a distorted trigonal-bipyramidal geometry.

A partially overlapped arrangement of neighboring parallel C3-dmphen and C3^{v}-dmphen rings[symmetry code: (v) -*x* + 2, -*y* + 1, -*z* + 1] is observed in the structure of (I) (Fig. 2). The shorter face-to-face separation of 3.3881 (5) Å clearly indicates the existence of π—π stacking between the dmphen ligands. In addition, the distance between the ring centroids *Cg*3 (C2—C5/C13/N1) and *Cg*2^{iii} (C16^{iii}—C21^{iii}) is 3.8216 (3) Å. This value is indentical to van der Waals thickness of the π—π stacking interaction between the nearly parallel dmphen and benzene ligands [dihedral angle 0.208 (68)°], although dmphen and benzene rings are well overlapped with respect to each other (Fig. 2).

The interaction of C—H···π and hydrogen bond intrains in the compound. The crystal structure is further stablilized by C—H···π interactions between the H atom of C3-dmphen ring and C23^{i}-benzene ring, with a C3—H3···*Cg*1^{i} separation of 2.5914 (4) Å (Fig.2 and Table 1; *Cg*1^{i} is the centroid of C23^{i}—C28^{i} benzene ring, symmmetry code as in Fig. 2).

Experimental

2-hydroxybenzoic acid (0.1396 g, 1 mmol) and NaOH (0.0377 g, 1 mmol) were dissolved in distilled water(15 ml) and $Co(NO_3)_2.6H_2O$ (0.1460 g, 0.5 mmol) were added. This solution was added to a solution of 2,9-dimethyl-1,10-phenanthroline hemihydrate ($C_{14}H_{12}N_2.0.5H_2O$, 0.1087 g, 0.5 mmol) in ethanol (10 ml). The mixture was stirred at 323 K and then refluxed for 4 h, cooled to room temperature and filtered. Brown single crystals of (I) were appeared over a period of one day by slow evaporation at room temperature.

Refinement

Methyl H and hydroxy H atoms were placed in calculated positions,with C—H=0.96 and O—H=0.82 Å, and refined with free torsion angles to fit the electron density; U_{iso}(H) = 1.5U_{eq}(carrier). Other H atoms were placed in calculated positions, with C—H=0.93 Å, and refined in the riding-model approximation with U_{iso}(H) = 1.2U_{eq}(C).

Figures

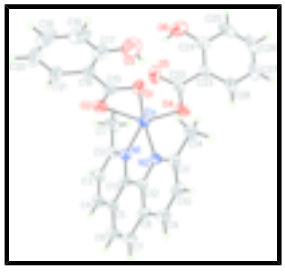


Fig. 1. The molecular structure of the title complex(I), with atom labels and 30% probability displacement ellipsoids.

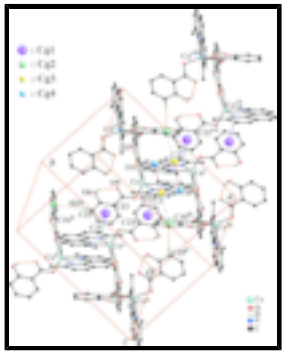


Fig. 2. π—π and C—H···π interactions of neighboring molecules and hydrogen bond intrains in the crystal structure of (I). [symmetry code: (i) -*x* + 1, -*y* + 1, -*z* + 1; (ii) *x* - 1, *y*, *z*; (iii) -*x* + 3/2, *y* - 1/2, -*z* + 1/2; (iv)-*x* + 1/2, *y* - 1/2, -*z* + 1/2; (v) -*x* + 2, -*y* + 1, -*z* + 1; (vi) *x* + 1/2, -*y* + 3/2, *z* + 1/2; (vii) *x* + 1, *y*, *z*; (viii) *x* + 3/2, -*y* + 3/2, *z* + 1/2]

(2,9-Dimethyl-1,10-phenanthroline-κ^2*N*,*N*')bis(2- hydroxybenzoato)-κ*O*;κ^2*O*,*O*'-cobalt(II)

Crystal data

$[Co(C_7H_5O_3)_2(C_{14}H_{12}N_2)]$	F_{000} = 1116
M_r = 541.41	D_x = 1.473 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 6265 reflections
a = 11.4360 (10) Å	θ = 2.4–26.2º
b = 16.528 (2) Å	μ = 0.75 mm^{-1}
c = 13.426 (2) Å	*T* = 293 (2) K
β = 105.8560 (10)º	Block, brown
V = 2441.1 (5) Å^3	0.46 × 0.36 × 0.30 mm
Z = 4	

Data collection

Bruker APEX2 CCD area-detector	5998 independent reflections

diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 10.0 pixels mm^{-1}

T = 293(2) K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 2004)

T_{min} = 0.779, T_{max} = 0.858

20557 measured reflections

4476 reflections with $I > 2\sigma(I)$

R_{int} = 0.023

θ_{max} = 28.4º

θ_{min} = 2.4º

$h = -15 \rightarrow 15$

$k = -21 \rightarrow 22$

$l = -16 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.040

$wR(F^2)$ = 0.127

S = 1.04

5998 reflections

338 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0698P)^2 + 0.571P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max}$ = 0.86 e $Å^{-3}$

$\Delta\rho_{min}$ = −0.39 e $Å^{-3}$

Extinction correction: none

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}
Co	0.66347 (2)	0.522121 (17)	0.26226 (2)	0.04340 (11)
O1	0.65059 (16)	0.59650 (10)	0.12395 (14)	0.0649 (5)
O2	0.77931 (16)	0.62474 (11)	0.27073 (14)	0.0671 (5)
O3	0.6514 (3)	0.67759 (15)	−0.04042 (18)	0.0985 (7)
H3O	0.6371	0.6376	−0.0095	0.148*
O4	0.49377 (15)	0.48299 (12)	0.23285 (17)	0.0713 (5)
O5	0.47135 (18)	0.61052 (14)	0.26953 (17)	0.0841 (6)
O6	0.2585 (2)	0.67472 (13)	0.2052 (2)	0.0926 (7)

H6O	0.3315	0.6732	0.2343	0.139*
N1	0.76714 (15)	0.48305 (10)	0.40730 (13)	0.0422 (4)
N2	0.74922 (14)	0.42206 (10)	0.21681 (13)	0.0397 (4)
C1	0.6828 (2)	0.57760 (19)	0.5073 (2)	0.0727 (8)
H1A	0.6606	0.6079	0.4439	0.109*
H1B	0.7191	0.6132	0.5638	0.109*
H1C	0.6115	0.5532	0.5190	0.109*
C2	0.7717 (2)	0.51308 (14)	0.50009 (18)	0.0492 (5)
C3	0.8578 (2)	0.48496 (15)	0.58982 (18)	0.0546 (6)
H3	0.8597	0.5068	0.6541	0.066*
C4	0.9379 (2)	0.42604 (15)	0.58278 (18)	0.0544 (6)
H4	0.9953	0.4080	0.6419	0.065*
C5	0.93361 (18)	0.39243 (14)	0.48552 (16)	0.0471 (5)
C6	1.0126 (2)	0.32887 (15)	0.4708 (2)	0.0589 (6)
H6	1.0714	0.3087	0.5276	0.071*
C7	1.0031 (2)	0.29808 (15)	0.3768 (2)	0.0588 (6)
H7	1.0553	0.2568	0.3694	0.071*
C8	0.91380 (19)	0.32754 (13)	0.28708 (18)	0.0482 (5)
C9	0.8954 (2)	0.29494 (14)	0.18696 (19)	0.0557 (6)
H9	0.9441	0.2527	0.1757	0.067*
C10	0.8064 (2)	0.32529 (14)	0.10690 (19)	0.0562 (6)
H10	0.7941	0.3038	0.0408	0.067*
C11	0.73282 (19)	0.38898 (13)	0.12356 (17)	0.0468 (5)
C12	0.83719 (17)	0.39055 (12)	0.29830 (15)	0.0397 (4)
C13	0.84636 (16)	0.42332 (12)	0.39942 (15)	0.0402 (4)
C14	0.6317 (2)	0.42116 (17)	0.03642 (19)	0.0638 (6)
H14A	0.5637	0.4351	0.0620	0.096*
H14B	0.6075	0.3806	−0.0163	0.096*
H14C	0.6592	0.4684	0.0078	0.096*
C15	0.7372 (2)	0.63949 (13)	0.17593 (19)	0.0505 (5)
C16	0.7892 (2)	0.70419 (13)	0.12395 (19)	0.0506 (5)
C17	0.7452 (3)	0.71637 (15)	0.0181 (2)	0.0635 (6)
C18	0.7973 (4)	0.7736 (2)	−0.0324 (3)	0.0966 (12)
H18	0.7680	0.7806	−0.1036	0.116*
C19	0.8899 (4)	0.8184 (2)	0.0225 (5)	0.1149 (17)
H19	0.9248	0.8564	−0.0116	0.138*
C20	0.9356 (3)	0.8098 (2)	0.1287 (5)	0.1114 (15)
H20	0.9999	0.8423	0.1643	0.134*
C21	0.8862 (2)	0.75258 (15)	0.1836 (3)	0.0800 (9)
H21	0.9153	0.7468	0.2550	0.096*
C22	0.4271 (2)	0.54319 (17)	0.23779 (18)	0.0539 (6)
C23	0.29299 (19)	0.53232 (13)	0.20118 (16)	0.0454 (5)
C24	0.2156 (2)	0.59876 (17)	0.18600 (19)	0.0593 (6)
C25	0.0897 (3)	0.5876 (2)	0.1481 (2)	0.0805 (9)
H25	0.0374	0.6319	0.1366	0.097*
C26	0.0446 (3)	0.5104 (3)	0.1281 (2)	0.0905 (11)
H26	−0.0390	0.5028	0.1048	0.109*
C27	0.1191 (3)	0.4451 (2)	0.1415 (2)	0.0792 (9)
H27	0.0867	0.3934	0.1265	0.095*

C28	0.2427 (2)	0.45565 (17)	0.17743 (19)	0.0583 (6)
H28	0.2936	0.4108	0.1860	0.070*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co	0.03569 (16)	0.04799 (18)	0.04465 (18)	0.00305 (11)	0.00781 (12)	0.00426 (11)
O1	0.0620 (10)	0.0564 (9)	0.0732 (12)	−0.0129 (8)	0.0131 (9)	0.0073 (8)
O2	0.0662 (11)	0.0710 (11)	0.0597 (11)	0.0084 (9)	0.0098 (9)	0.0131 (9)
O3	0.134 (2)	0.0891 (16)	0.0711 (14)	−0.0045 (15)	0.0268 (14)	−0.0029 (12)
O4	0.0378 (8)	0.0865 (14)	0.0891 (14)	0.0078 (8)	0.0163 (9)	0.0230 (10)
O5	0.0729 (12)	0.0987 (16)	0.0775 (13)	−0.0393 (12)	0.0150 (10)	−0.0125 (11)
O6	0.1171 (18)	0.0672 (13)	0.1017 (18)	0.0126 (12)	0.0439 (16)	−0.0003 (11)
N1	0.0362 (8)	0.0499 (10)	0.0402 (9)	0.0024 (7)	0.0100 (7)	0.0020 (7)
N2	0.0345 (8)	0.0428 (9)	0.0402 (9)	−0.0003 (6)	0.0077 (6)	0.0051 (7)
C1	0.0637 (15)	0.094 (2)	0.0591 (16)	0.0221 (15)	0.0149 (12)	−0.0129 (14)
C2	0.0433 (11)	0.0600 (13)	0.0440 (12)	0.0001 (10)	0.0114 (9)	−0.0001 (10)
C3	0.0538 (13)	0.0711 (15)	0.0383 (12)	−0.0012 (11)	0.0115 (10)	0.0013 (10)
C4	0.0472 (12)	0.0689 (15)	0.0432 (12)	0.0018 (11)	0.0058 (9)	0.0131 (10)
C5	0.0395 (10)	0.0559 (12)	0.0448 (12)	0.0024 (9)	0.0096 (9)	0.0129 (9)
C6	0.0502 (12)	0.0646 (14)	0.0575 (14)	0.0168 (11)	0.0074 (11)	0.0210 (12)
C7	0.0540 (13)	0.0560 (13)	0.0672 (16)	0.0204 (11)	0.0179 (11)	0.0156 (12)
C8	0.0461 (11)	0.0439 (11)	0.0572 (13)	0.0060 (9)	0.0185 (10)	0.0076 (9)
C9	0.0601 (13)	0.0472 (12)	0.0628 (15)	0.0092 (10)	0.0219 (11)	0.0001 (10)
C10	0.0671 (15)	0.0512 (13)	0.0520 (13)	−0.0003 (11)	0.0191 (11)	−0.0069 (10)
C11	0.0478 (11)	0.0475 (11)	0.0448 (12)	−0.0044 (9)	0.0120 (9)	−0.0018 (9)
C12	0.0361 (9)	0.0409 (10)	0.0432 (11)	0.0001 (8)	0.0127 (8)	0.0085 (8)
C13	0.0332 (9)	0.0456 (10)	0.0419 (11)	0.0000 (8)	0.0103 (8)	0.0087 (8)
C14	0.0659 (15)	0.0730 (16)	0.0438 (13)	0.0047 (13)	−0.0001 (11)	−0.0063 (11)
C15	0.0470 (11)	0.0449 (11)	0.0622 (15)	0.0111 (9)	0.0193 (10)	0.0061 (10)
C16	0.0477 (11)	0.0380 (10)	0.0717 (15)	0.0054 (9)	0.0259 (11)	0.0007 (10)
C17	0.0734 (16)	0.0531 (13)	0.0745 (18)	0.0071 (12)	0.0379 (14)	0.0058 (12)
C18	0.112 (3)	0.084 (2)	0.119 (3)	0.022 (2)	0.075 (2)	0.036 (2)
C19	0.104 (3)	0.067 (2)	0.205 (5)	0.007 (2)	0.096 (4)	0.030 (3)
C20	0.068 (2)	0.0577 (18)	0.219 (5)	−0.0157 (15)	0.057 (3)	−0.025 (3)
C21	0.0525 (14)	0.0464 (13)	0.148 (3)	−0.0021 (11)	0.0390 (17)	−0.0123 (16)
C22	0.0408 (11)	0.0775 (16)	0.0422 (12)	−0.0063 (11)	0.0094 (9)	0.0102 (11)
C23	0.0381 (10)	0.0631 (13)	0.0357 (10)	0.0005 (9)	0.0111 (8)	0.0002 (9)
C24	0.0634 (14)	0.0708 (16)	0.0483 (13)	0.0131 (12)	0.0227 (11)	0.0034 (11)
C25	0.0564 (15)	0.130 (3)	0.0573 (16)	0.0379 (18)	0.0187 (13)	0.0141 (17)
C26	0.0416 (14)	0.170 (4)	0.0562 (18)	−0.0097 (19)	0.0079 (12)	−0.012 (2)
C27	0.0581 (16)	0.113 (2)	0.0666 (18)	−0.0316 (17)	0.0173 (13)	−0.0227 (17)
C28	0.0507 (13)	0.0715 (15)	0.0546 (14)	−0.0070 (11)	0.0177 (11)	−0.0093 (11)

Geometric parameters (Å, °)

Co—O4	1.9804 (18)	C8—C9	1.410 (3)
Co—N1	2.0863 (17)	C9—C10	1.359 (3)
Co—N2	2.0967 (17)	C9—H9	0.9300

Co—O2	2.1359 (19)	C10—C11	1.403 (3)
Co—O1	2.1981 (18)	C10—H10	0.9300
O1—C15	1.263 (3)	C11—C14	1.500 (3)
O2—C15	1.256 (3)	C12—C13	1.439 (3)
O3—C17	1.311 (4)	C14—H14A	0.9600
O3—H3O	0.8200	C14—H14B	0.9600
O4—C22	1.266 (3)	C14—H14C	0.9600
O5—C22	1.248 (3)	C15—C16	1.487 (3)
O6—C24	1.347 (3)	C16—C17	1.386 (4)
O6—H6O	0.8200	C16—C21	1.423 (4)
N1—C2	1.329 (3)	C17—C18	1.389 (4)
N1—C13	1.363 (3)	C18—C19	1.337 (6)
N2—C11	1.332 (3)	C18—H18	0.9300
N2—C12	1.371 (2)	C19—C20	1.384 (6)
C1—C2	1.495 (3)	C19—H19	0.9300
C1—H1A	0.9600	C20—C21	1.409 (5)
C1—H1B	0.9600	C20—H20	0.9300
C1—H1C	0.9600	C21—H21	0.9300
C2—C3	1.410 (3)	C22—C23	1.488 (3)
C3—C4	1.358 (3)	C23—C24	1.390 (3)
C3—H3	0.9300	C23—C28	1.392 (3)
C4—C5	1.407 (3)	C24—C25	1.402 (4)
C4—H4	0.9300	C25—C26	1.376 (5)
C5—C13	1.401 (3)	C25—H25	0.9300
C5—C6	1.434 (3)	C26—C27	1.356 (5)
C6—C7	1.337 (4)	C26—H26	0.9300
C6—H6	0.9300	C27—C28	1.375 (4)
C7—C8	1.435 (3)	C27—H27	0.9300
C7—H7	0.9300	C28—H28	0.9300
C8—C12	1.395 (3)		
O4—Co—N1	111.16 (8)	C10—C11—C14	120.6 (2)
O4—Co—N2	101.25 (8)	N2—C12—C8	122.88 (19)
N1—Co—N2	80.55 (7)	N2—C12—C13	117.29 (17)
O4—Co—O2	146.07 (7)	C8—C12—C13	119.79 (18)
N1—Co—O2	90.58 (7)	N1—C13—C5	122.59 (19)
N2—Co—O2	108.01 (7)	N1—C13—C12	117.85 (17)
O4—Co—O1	100.27 (7)	C5—C13—C12	119.56 (18)
N1—Co—O1	148.37 (7)	C11—C14—H14A	109.5
N2—Co—O1	97.12 (7)	C11—C14—H14B	109.5
O2—Co—O1	59.89 (6)	H14A—C14—H14B	109.5
C15—O1—Co	89.23 (14)	C11—C14—H14C	109.5
C15—O2—Co	92.28 (15)	H14A—C14—H14C	109.5
C17—O3—H3O	109.5	H14B—C14—H14C	109.5
C22—O4—Co	107.71 (16)	O2—C15—O1	118.4 (2)
C24—O6—H6O	109.5	O2—C15—C16	121.6 (2)
C2—N1—C13	119.10 (18)	O1—C15—C16	119.9 (2)
C2—N1—Co	128.77 (15)	C17—C16—C21	120.3 (2)
C13—N1—Co	111.84 (13)	C17—C16—C15	120.4 (2)
C11—N2—C12	118.60 (18)	C21—C16—C15	119.4 (2)

C11—N2—Co	129.83 (14)	O3—C17—C16	123.5 (2)
C12—N2—Co	111.53 (13)	O3—C17—C18	115.4 (3)
C2—C1—H1A	109.5	C16—C17—C18	121.0 (3)
C2—C1—H1B	109.5	C19—C18—C17	119.3 (4)
H1A—C1—H1B	109.5	C19—C18—H18	120.4
C2—C1—H1C	109.5	C17—C18—H18	120.4
H1A—C1—H1C	109.5	C18—C19—C20	122.0 (3)
H1B—C1—H1C	109.5	C18—C19—H19	119.0
N1—C2—C3	121.2 (2)	C20—C19—H19	119.0
N1—C2—C1	118.3 (2)	C19—C20—C21	121.0 (4)
C3—C2—C1	120.5 (2)	C19—C20—H20	119.5
C4—C3—C2	120.2 (2)	C21—C20—H20	119.5
C4—C3—H3	119.9	C20—C21—C16	116.5 (4)
C2—C3—H3	119.9	C20—C21—H21	121.8
C3—C4—C5	119.6 (2)	C16—C21—H21	121.8
C3—C4—H4	120.2	O5—C22—O4	121.6 (2)
C5—C4—H4	120.2	O5—C22—C23	120.4 (2)
C13—C5—C4	117.3 (2)	O4—C22—C23	118.0 (2)
C13—C5—C6	119.1 (2)	C24—C23—C28	118.6 (2)
C4—C5—C6	123.6 (2)	C24—C23—C22	120.7 (2)
C7—C6—C5	121.1 (2)	C28—C23—C22	120.6 (2)
C7—C6—H6	119.4	O6—C24—C23	121.6 (2)
C5—C6—H6	119.4	O6—C24—C25	118.4 (3)
C6—C7—C8	121.3 (2)	C23—C24—C25	119.9 (3)
C6—C7—H7	119.4	C26—C25—C24	119.0 (3)
C8—C7—H7	119.4	C26—C25—H25	120.5
C12—C8—C9	117.0 (2)	C24—C25—H25	120.5
C12—C8—C7	119.1 (2)	C27—C26—C25	121.6 (3)
C9—C8—C7	123.9 (2)	C27—C26—H26	119.2
C10—C9—C8	119.9 (2)	C25—C26—H26	119.2
C10—C9—H9	120.1	C26—C27—C28	119.6 (3)
C8—C9—H9	120.1	C26—C27—H27	120.2
C9—C10—C11	120.2 (2)	C28—C27—H27	120.2
C9—C10—H10	119.9	C27—C28—C23	121.2 (3)
C11—C10—H10	119.9	C27—C28—H28	119.4
N2—C11—C10	121.4 (2)	C23—C28—H28	119.4
N2—C11—C14	117.9 (2)		
O4—Co—O1—C15	152.70 (14)	Co—N2—C12—C13	6.9 (2)
N1—Co—O1—C15	−20.9 (2)	C9—C8—C12—N2	−1.6 (3)
N2—Co—O1—C15	−104.45 (14)	C7—C8—C12—N2	−179.73 (19)
O2—Co—O1—C15	2.28 (13)	C9—C8—C12—C13	176.34 (19)
O4—Co—O2—C15	−62.8 (2)	C7—C8—C12—C13	−1.8 (3)
N1—Co—O2—C15	165.78 (14)	C2—N1—C13—C5	−0.5 (3)
N2—Co—O2—C15	85.54 (14)	Co—N1—C13—C5	173.88 (16)
O1—Co—O2—C15	−2.30 (13)	C2—N1—C13—C12	178.44 (18)
N1—Co—O4—C22	108.46 (16)	Co—N1—C13—C12	−7.2 (2)
N2—Co—O4—C22	−167.43 (16)	C4—C5—C13—N1	−0.5 (3)
O2—Co—O4—C22	−18.0 (3)	C6—C5—C13—N1	179.22 (19)
O1—Co—O4—C22	−67.95 (17)	C4—C5—C13—C12	−179.36 (18)

O4—Co—N1—C2	−79.6 (2)	C6—C5—C13—C12	0.3 (3)
N2—Co—N1—C2	−178.06 (19)	N2—C12—C13—N1	0.1 (3)
O2—Co—N1—C2	73.77 (19)	C8—C12—C13—N1	−177.93 (17)
O1—Co—N1—C2	93.7 (2)	N2—C12—C13—C5	179.10 (17)
O4—Co—N1—C13	106.75 (14)	C8—C12—C13—C5	1.0 (3)
N2—Co—N1—C13	8.26 (13)	Co—O2—C15—O1	3.9 (2)
O2—Co—N1—C13	−99.91 (14)	Co—O2—C15—C16	−174.31 (17)
O1—Co—N1—C13	−79.99 (19)	Co—O1—C15—O2	−3.8 (2)
O4—Co—N2—C11	64.42 (19)	Co—O1—C15—C16	174.45 (17)
N1—Co—N2—C11	174.30 (18)	O2—C15—C16—C17	176.6 (2)
O2—Co—N2—C11	−98.18 (18)	O1—C15—C16—C17	−1.6 (3)
O1—Co—N2—C11	−37.59 (18)	O2—C15—C16—C21	−2.3 (3)
O4—Co—N2—C12	−118.05 (13)	O1—C15—C16—C21	179.5 (2)
N1—Co—N2—C12	−8.17 (13)	C21—C16—C17—O3	−175.6 (2)
O2—Co—N2—C12	79.35 (13)	C15—C16—C17—O3	5.6 (4)
O1—Co—N2—C12	139.94 (13)	C21—C16—C17—C18	2.4 (4)
C13—N1—C2—C3	0.8 (3)	C15—C16—C17—C18	−176.4 (2)
Co—N1—C2—C3	−172.49 (16)	O3—C17—C18—C19	177.0 (3)
C13—N1—C2—C1	−179.0 (2)	C16—C17—C18—C19	−1.1 (4)
Co—N1—C2—C1	7.7 (3)	C17—C18—C19—C20	−0.3 (5)
N1—C2—C3—C4	−0.1 (4)	C18—C19—C20—C21	0.4 (6)
C1—C2—C3—C4	179.7 (2)	C19—C20—C21—C16	0.9 (4)
C2—C3—C4—C5	−0.8 (4)	C17—C16—C21—C20	−2.2 (3)
C3—C4—C5—C13	1.1 (3)	C15—C16—C21—C20	176.6 (2)
C3—C4—C5—C6	−178.6 (2)	Co—O4—C22—O5	−8.2 (3)
C13—C5—C6—C7	−0.9 (3)	Co—O4—C22—C23	169.81 (15)
C4—C5—C6—C7	178.7 (2)	O5—C22—C23—C24	10.4 (3)
C5—C6—C7—C8	0.2 (4)	O4—C22—C23—C24	−167.7 (2)
C6—C7—C8—C12	1.2 (4)	O5—C22—C23—C28	−172.3 (2)
C6—C7—C8—C9	−176.8 (2)	O4—C22—C23—C28	9.7 (3)
C12—C8—C9—C10	0.2 (3)	C28—C23—C24—O6	−178.5 (2)
C7—C8—C9—C10	178.2 (2)	C22—C23—C24—O6	−1.0 (3)
C8—C9—C10—C11	0.0 (4)	C28—C23—C24—C25	0.4 (3)
C12—N2—C11—C10	−2.5 (3)	C22—C23—C24—C25	177.8 (2)
Co—N2—C11—C10	174.90 (16)	O6—C24—C25—C26	180.0 (3)
C12—N2—C11—C14	176.70 (19)	C23—C24—C25—C26	1.1 (4)
Co—N2—C11—C14	−5.9 (3)	C24—C25—C26—C27	−1.8 (5)
C9—C10—C11—N2	1.1 (3)	C25—C26—C27—C28	1.0 (5)
C9—C10—C11—C14	−178.0 (2)	C26—C27—C28—C23	0.5 (4)
C11—N2—C12—C8	2.8 (3)	C24—C23—C28—C27	−1.2 (4)
Co—N2—C12—C8	−175.06 (15)	C22—C23—C28—C27	−178.6 (2)
C11—N2—C12—C13	−175.23 (17)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3O···O1	0.82	1.88	2.584 (3)	143
O6—H6O···O5	0.82	1.86	2.578 (3)	146
C3—H3···Cg1^{i}	0.93	2.59	3.402 (3)	146

C25—H25···Cg2^{ii}	0.93	3.07	3.989 (3)	172

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

Fig. 1

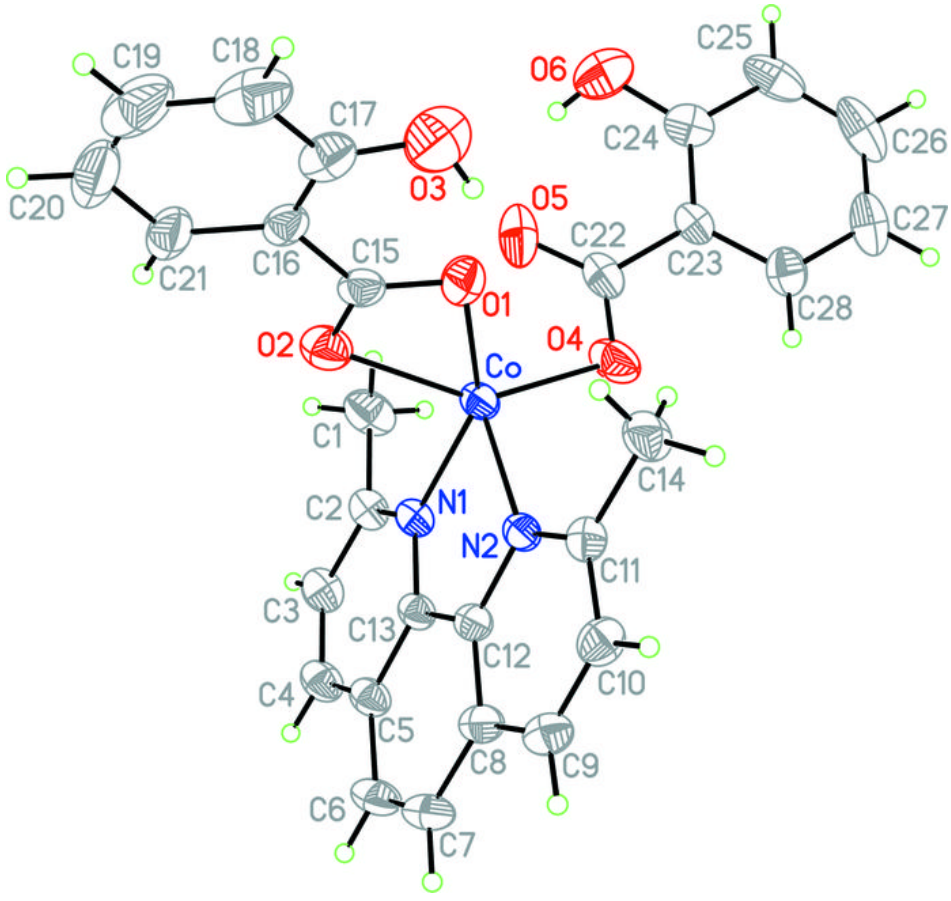
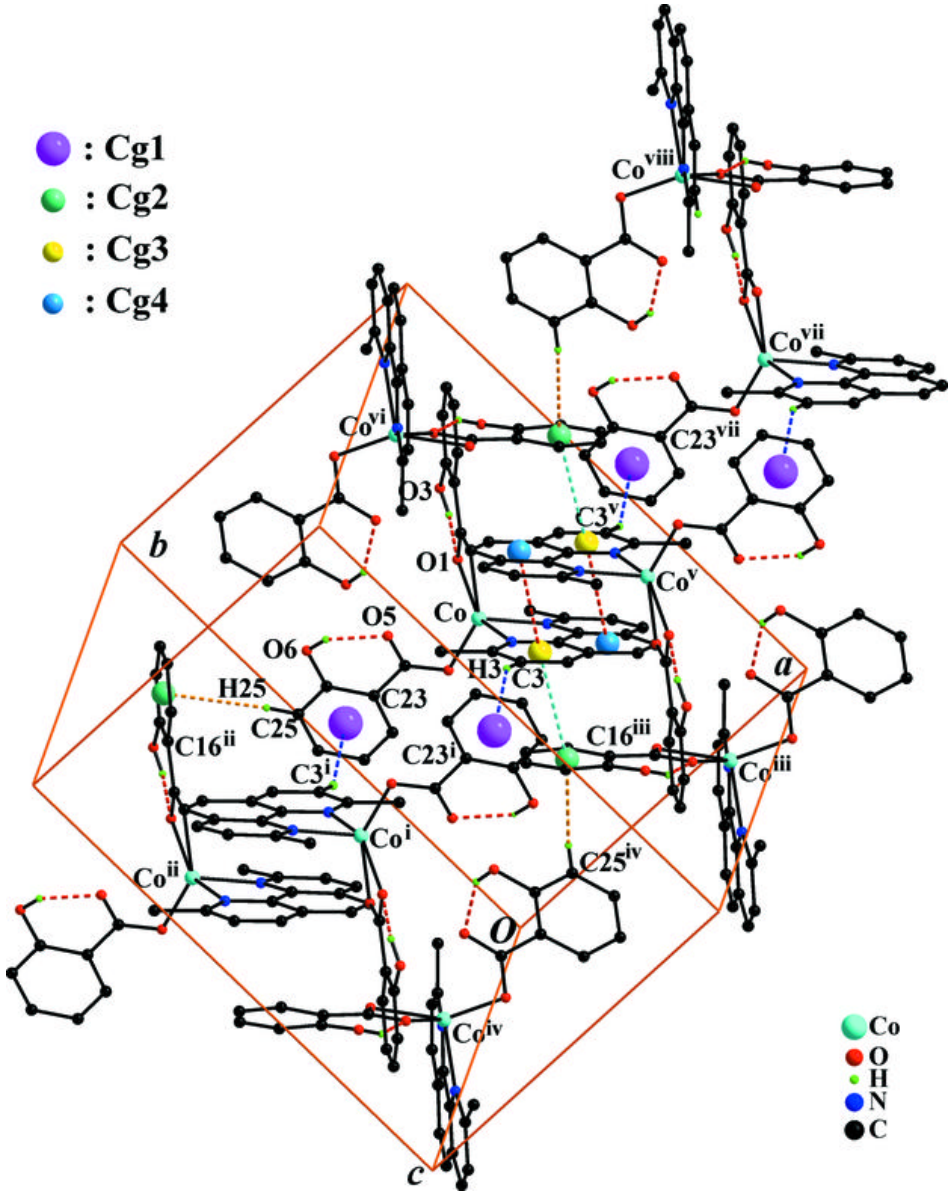


Fig. 2


: Cg1
: Cg2
: Cg3
: Cg4
Co^{viii}
Co^{vii}
C23^{vii}
Co^{vi}
O3
C3^{v}
O1
Co^{v}
Co
O5
O6
H3
C3
H25
C23
C25
C16^{ii}
C23^{i}
C16^{iii}
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