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Aqua(oxydiacetato-κ^3O,O',O'')(1,10-phenanthroline-κ^2N,N')cobalt(II) sesquihydrate

Zhi-Yong Wu, Yu-Hong Xue and Duan-Jun Xu*

Department of Chemistry, Zhejiang University, People's Republic of China

Correspondence e-mail: xudj@mail.hz.zj.cn

The title compound, $[Co(C_4H_4O_5)(C_{12}H_8N_2)H_2O]\cdot 1.5H_2O$, consists of the octahedral complex and lattice water. The asymmetric unit contains two molecules of the complex, which form a hydrogen-bonded dimer. The overlapped arrangement and shorter separations of 3.532 (6) and 3.385 (12) Å between neighboring parallel phenanthroline rings suggest the existence of π–π-stacking interactions.

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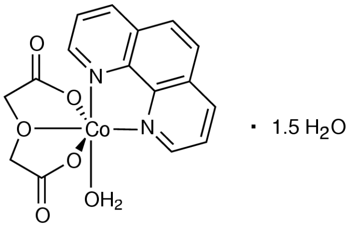
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.038
wR factor = 0.109
Data-to-parameter ratio = 16.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Aromatic π–π stacking interactions are important for some biological systems (Deisenhofer & Michel, 1989). As part of our investigation of π–π stacking in metal complexes (Chen *et al.*, 2003), the title Co^{II} complex, (I), was prepared.



(I)

Co^{II} compound (I) is isomorphous with the Ni^{II} (Baggio *et al.*, 2000) and Zn^{II} analogues (Baggio *et al.*, 1996). The asymmetric unit of (I) contains two molecules of the complex and three molecules of lattice water, as shown in Fig. 1. The two independent complex molecules display a similar octa-

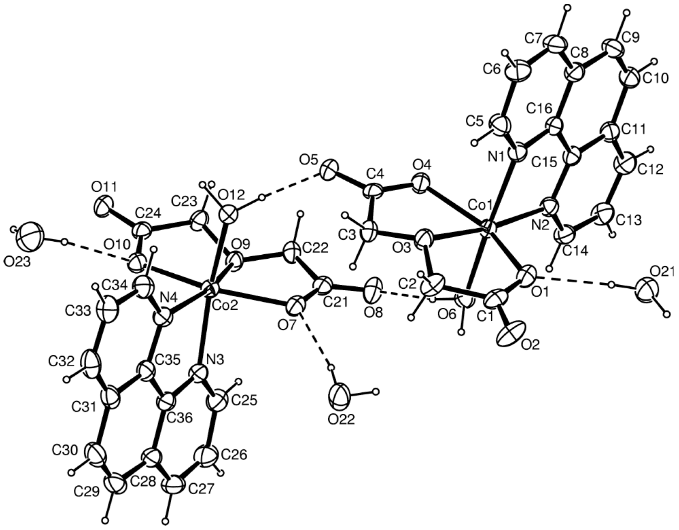


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids. Dashed lines indicate hydrogen bonding.

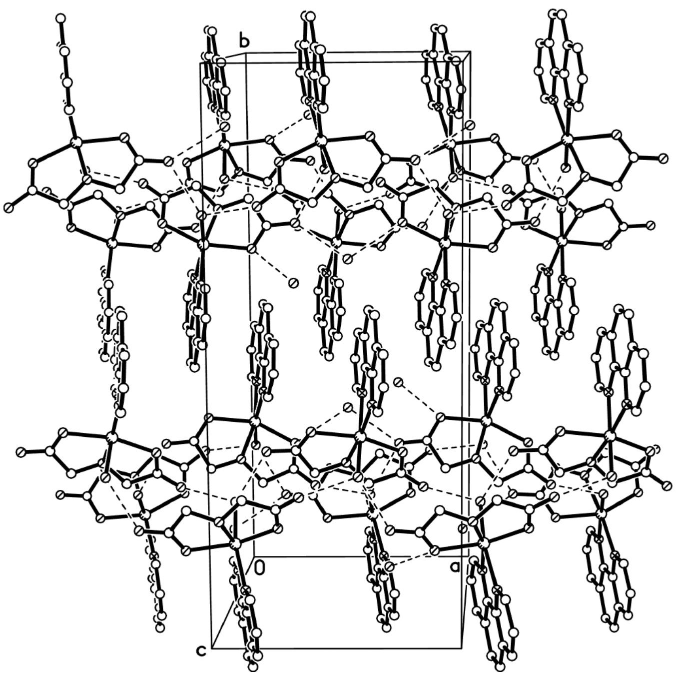
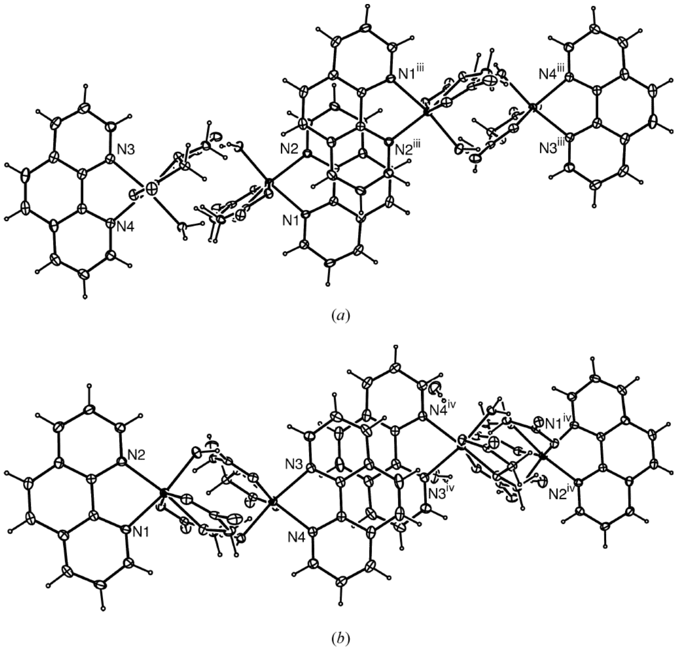


Figure 2
The molecular packing diagram, showing the hydrophilic and hydrophobic layered structure. H atoms have been omitted for clarity.



(*a*)

(*b*)

Figure 3
A diagram showing the π–π stacking between (*a*) N1-phen and N1^{iii}-phen rings, and (*b*) N3-phen and N3^{iv}-phen rings. [Symmetry codes: (iii) $1 - x, -y, 1 - z$; (iv) $-x, 1 - y, 1 - z$.]

hedral coordination geometry (Table 1), formed by a phenanthroline (phen), a meridional oxydiacetate and a coordinated water molecule. The lattice water molecules are hydrogen bonded to the adjacent carboxyl groups (Table 2). Through hydrogen bonding between carboxyl groups and coordinated water molecules, two independent complex molecules link to each other to form a dimer (Fig. 1). All lattice water molecules are ordered in the Co^{II} compound, as is the case in the isomorphous Zn^{II} complex but different from the disorder found in the isomorphous Ni^{II} complex.

The molecular packing in the unit cell is illustrated in Fig. 2. The crystal structure consists of the hydrophilic layers formed by carboxylate and water molecules and hydrophobic layers formed by phen ligands. Parallel disposition of phen ligands is observed in the crystal. Fig. 3 shows the overlapped arrangement of neighboring parallel phen ligands. The separations of 3.532 (6) Å between N1-phen and N1^{iii}-phen and 3.385 (12) Å between the N3-phen and N3^{iv}-phen [symmetry codes: (iii) $1 - x, -y, 1 - z$; (iv) $-x, 1 - y, 1 - z$] suggest the existence of aromatic π–π stacking between phen ligands.

Experimental

An aqueous solution (10 ml) containing $CoCl_2\cdot6H_2O$ (0.24 g, 1 mmol) and 1,10-phenanthroline (0.18 g, 1 mmol) was mixed with an aqueous solution (10 ml) containing oxydiacetic acid hydrate (0.15 g, 1 mmol) and NaOH (0.08 g, 2 mmol) at room temperature. The mixture was refluxed for 3 h. Pink single crystals of the title compound were obtained from the filtrate after 2 weeks.

Crystal data

$[Co(C_4H_4O_5)(C_{12}H_8N_2)(H_2O)]\cdot1.5H_2O$
$M_r = 416.25$
Monoclinic, $P2_1/c$
$a = 10.4722$ (16) Å
$b = 24.3161$ (9) Å
$c = 13.6729$ (14) Å
$\beta = 93.627$ (1)°
$V = 3474.7$ (7) Å^3
$Z = 8$
$D_x = 1.591$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 16878 reflections
$\theta = 2.8$–24.0°
$\mu = 1.03$ mm^{-1}
$T = 293$ (2) K
Prism, pink
0.32 × 0.28 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
$T_{min} = 0.715$, $T_{max} = 0.810$
21949 measured reflections
7932 independent reflections
4856 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 27.5°$
$h = -13 \rightarrow 13$
$k = -31 \rightarrow 30$
$l = -11 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.109$
$S = 0.93$
7932 reflections
479 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0452P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.56$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}

Table 1
Selected geometric parameters (Å).

Co1—O1	2.070 (2)	Co2—O12	2.060 (2)
Co1—O6	2.074 (2)	Co2—O10	2.096 (2)
Co1—O4	2.084 (2)	Co2—O7	2.117 (2)
Co1—N2	2.098 (2)	Co2—N3	2.118 (2)
Co1—N1	2.116 (2)	Co2—O9	2.118 (2)
Co1—O3	2.130 (2)	Co2—N4	2.119 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H61···O8	0.87	1.79	2.647 (3)	169
O6—H62···O11^{i}	0.92	1.77	2.685 (3)	178
O12—H121···O5	0.91	1.77	2.676 (3)	175
O12—H122···O2^{ii}	0.96	1.64	2.596 (3)	171
O21—H211···O1	0.91	2.04	2.933 (3)	166
O21—H212···O5^{i}	0.95	1.95	2.890 (3)	168
O22—H221···O7	0.95	1.94	2.867 (3)	163
O22—H222···O11^{i}	0.88	1.95	2.811 (3)	168
O23—H231···O10	0.87	2.07	2.915 (3)	165
O23—H232···O22^{ii}	0.87	2.24	3.094 (3)	168

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

H atoms of the water molecules were located in a difference Fourier map and were included in the structure-factor calculations with fixed coordinates and isotropic displacement parameters of 0.05 Å^2. Other H atoms were placed in calculated positions, with C—H = 0.93 Å (phen) or 0.97 Å (oxydiacetate) and were included in the final cycles of refinement in a riding model, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$ of the carrier atoms.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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