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Diaquabis(4-hydroxybenzoato-κO)(1,10-phenanthroline-$\kappa^2 N,N'$)cobalt(II) monohydrate

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The title complex, $[Co(C_7H_5O_3)_2(C_{12}H_8N_2)(H_2O)_2]\cdot H_2O$, displays a distorted octahedral coordination geometry about the Co^{II} atom, involving two 4-hydroxybenzoate anions, one 1,10-phenanthroline (phen) molecule and two water molecules. The face-to-face distance of 3.420 (5) Å between partially overlapped parallel phen rings reflects a π–π stacking interaction between neighboring Co^{II} complex molecules. A network of O—H···O hydrogen bonds helps to stabilize the crystal packing.

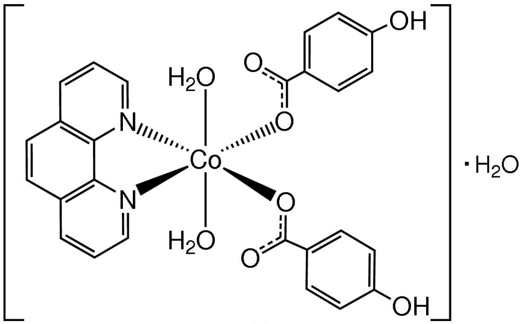
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.030
wR factor = 0.076
Data-to-parameter ratio = 12.4

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

Comment

As part of our ongoing investigations of aromatic π–π stacking interactions in metal complexes (Su *et al.*, 2005), the title Co^{II} complex incorporating 1,10-phenanthroline (phen), (I) (Fig. 1), has been prepared and its crystal structure is presented here.



(I)

The Co^{II} atom in (I) assumes a distorted CoO_4N_2 octahedral coordination geometry formed by two 4-hydroxybenzoate anions, a phen molecule and two coordinated water molecules. The two monodentate 4-hydroxybenzoate anions coordinate to the Co^{II} atom in a *cis* configuration, their benzene rings being nearly perpendicular, with a dihedral angle of 86.84 (5)°. The uncoordinated carboxy O atoms (O22 and O32) accept intramolecular hydrogen bonds from a coordinated water molecule (O1) (Fig. 1 and Table 2).

A partially overlapped disposition between the parallel phen ligands of neighboring Co^{II} complex molecules is observed, as shown in Fig. 2. The face-to-face distance of 3.420 (5) Å between the parallel N2-phen and N2^{v}-phen planes [symmetry code: (v) $-x$, $1-y$, $1-z$] suggests the existence of π–π stacking between adjacent Co^{II} complex molecules.

Extensive intermolecular hydrogen-bonding interactions are observed in the crystal structure of (I). Neighboring Co^{II} complexes are linked *via* O—H···O hydrogen bonds (Table

2). Hydrogen bonding also occurs between uncoordinated water molecules and the Co^{II} complex (Table 2).

Experimental

An aqueous solution (10 ml) containing Co$(CH_3COO)_2\cdot 4H_2O$ (0.25 g, 1 mmol), 4-hydroxybenzoic acid (0.14 g, 1 mmol) and Na_2CO_3 (0.06 g, 1 mmol) was mixed with an ethanol solution (10 ml) of phen (0.20 g, 1 mmol). The mixture was refluxed for 5 h, then cooled to room temperature and filtered. Orange–red single crystals of (I) were obtained from the filtrate after 3 weeks.

Crystal data

$[Co(C_7H_5O_3)_2(C_{12}H_8N_2)(H_2O)_2]\cdot H_2O$
M_r = 567.40
Monoclinic, $P2_1/c$
a = 11.8707 (4) Å
b = 21.2746 (6) Å
c = 11.2385 (4) Å
β = 117.639 (8)°
V = 2514.3 (2) Å^3
Z = 4

D_x = 1.499 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10537 reflections
θ = 2.6–24.8°
μ = 0.74 mm^{-1}
T = 295 (3) K
Block, orange–red
0.28 × 0.25 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.811, T_{max} = 0.892
17650 measured reflections

4241 independent reflections
3635 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 25.0°
$h = -14 \rightarrow 14$
$k = -25 \rightarrow 24$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.076
S = 1.02
4241 reflections
343 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0423P)^2 + 0.8385P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co—O1	2.1453 (14)	Co—O31	2.0604 (13)
Co—O2	2.1361 (13)	Co—N1	2.1497 (16)
Co—O21	2.1349 (13)	Co—N2	2.1226 (16)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1—H1$\cdots$O22	0.87	1.74	2.595 (2)	165
O1—H2$\cdots$O32	0.94	1.77	2.650 (2)	154
O2—H3$\cdots$O31^{i}	0.86	2.07	2.840 (2)	149
O2—H4$\cdots$O21^{i}	0.88	1.96	2.783 (2)	155
O23—H23$\cdots$O32^{ii}	0.92	1.77	2.687 (2)	171
O33—H33$\cdots$O1W	0.93	1.70	2.631 (3)	177
O1W—H1$A\cdots$O1^{iii}	0.88	1.87	2.745 (3)	174
O1W—H1$B\cdots$O22^{iv}	0.89	1.94	2.820 (3)	168

Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $1-x, 1-y, -z$; (iii) $1+x, \frac{3}{2}-y, \frac{1}{2}+z$; (iv) $1-x, \frac{1}{2}+y, \frac{1}{2}-z$.

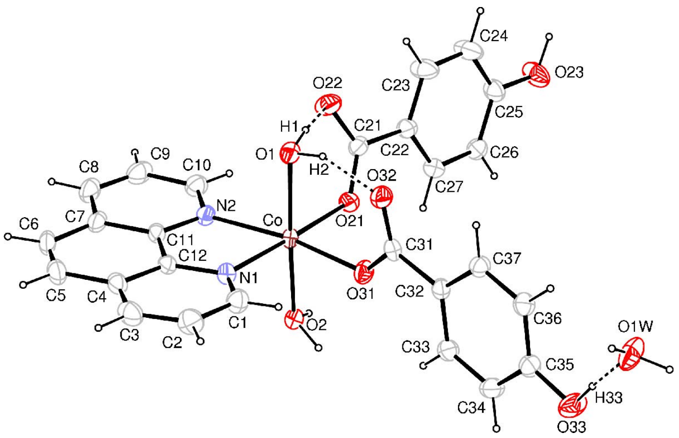


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for the H atoms). The dashed lines indicate hydrogen-bonding interactions.

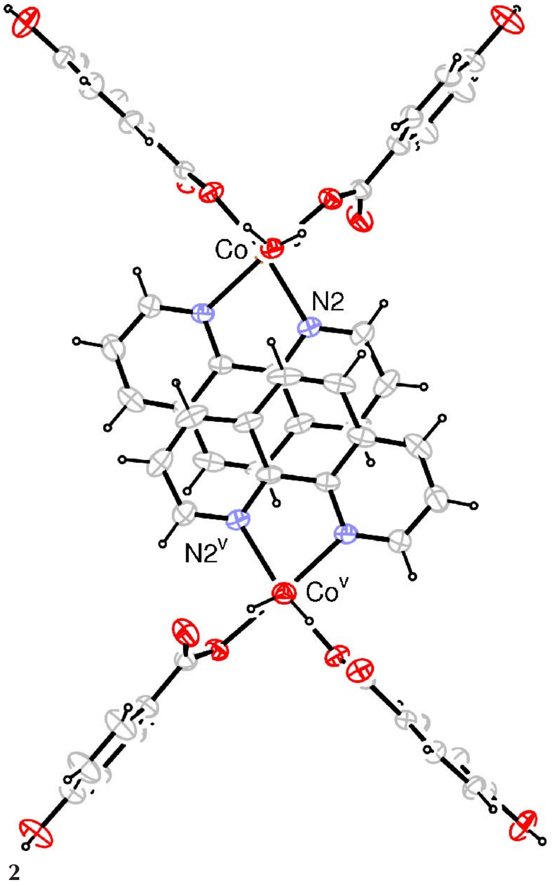


Figure 2
π–π stacking between parallel phen rings of neighboring Co^{II} complex molecules in (I). [Symmetry code: (v) $-x, 1-y, 1-z$.]

Aromatic H atoms were placed in calculated positions, with C—H = 0.93 Å, and refined as riding with the constraint U_{iso}(H) = 1.2U_{eq}(carrier) applied. The other H atoms were located in a difference Fourier map and refined as riding in their as-found relative positions, with a fixed U_{iso} of 0.05 Å^2.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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