

Guo-Qing Jiang, Xue-Fang Gu,
Yue-Hua Zhang and Yu-Jun Shi*College of Chemistry and Chemical Engineering,
Nantong University, Nantong 226019, People's
Republic of China

Correspondence e-mail: jgq3518@163.com

Key indicators

Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.031
 wR factor = 0.068
Data-to-parameter ratio = 14.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Bis(phenoxyacetato- κO)bis[2-(2-pyridyl)-
ethanol- $\kappa^2\text{N},\text{O}$]cobalt(II)

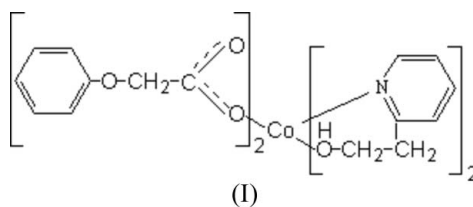
The title compound, $[\text{Co}(\text{C}_7\text{H}_7\text{O}_3)_2(\text{C}_7\text{H}_9\text{NO})_2]$, crystallizes as a centrosymmetric mononuclear Co^{II} complex with two phenoxyacetate and two 2-(2-pyridyl)ethanol molecules acting as ligands. The phenoxyacetate anion binds to the Co^{II} ion through one carboxylate O atom, and the 2-(2-pyridyl)ethanol molecule acts in a chelating mode. The molecular structure of the complex is stabilized by two intramolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds.

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Comment

The rational design, synthesis and characterization of novel supramolecular frameworks are of great current interest. One of the greatest challenges in this area is the construction of porous materials from metal ions and organic ligands as building blocks (Yaghi *et al.*, 1997). As part of our search for new porous metal-organic frameworks, we are studying complexes of transition metals with phenoxyacetate ligands (Jiang *et al.*, 2005, 2006). We report here the crystal structure of the title compound, (I), which is a mononuclear phenoxyacetate Co^{II} complex with 2-(2-pyridyl)ethanol as a co-ligand.



The mononuclear complex molecule of (I) is located on an inversion center (Fig. 1). The Co^{II} atom shows a slightly distorted octahedral geometry and is coordinated by two carboxylate O atoms from the two coordinating phenoxyacetate groups and by two O and two N atoms from the two bidentate 2-(2-pyridyl)ethanol ligands. Bond distances involving the Co^{II} atom are listed in Table 1. There are two intramolecular hydrogen bonds linking the hydroxy and carboxylate groups within the molecule of (I) (Table 2). Interligand $\text{C}-\text{H}\cdots\text{O}$ interactions with $\text{H}\cdots\text{O}$ distances in the range 2.38–2.61 \AA connect molecules of (I) into a three-dimensional framework (Fig. 2).

Experimental

$\text{Co}(\text{O}_2\text{CCH}_2\text{OPh})_2$ was synthesized by mixing solutions of $\text{CoCl}_2\cdot 6\text{H}_2\text{O}$ (10 mmol, 2.38 g) in H_2O (20 ml) and $\text{NaO}_2\text{CCH}_2\text{OPh}$ (20 mmol, 3.48 g) in H_2O (60 ml). The pink powder that precipitated was collected by filtration, washed with water and dried *in vacuo*. Complex (I) was prepared by the reaction of $\text{Co}(\text{O}_2\text{CCH}_2\text{OPh})_2$

(0.2 mmol, 0.072 g) in MeOH (10 ml) and 2-(2-pyridyl)ethanol (0.4 mmol, 0.05 g) under reflux for 30 min. The resulting solution was cooled and filtered. The filtrate was allowed to stand for a few days at room temperature until light-pink crystals were obtained.

Crystal data

$[\text{Co}(\text{C}_7\text{H}_7\text{O}_3)_2(\text{C}_7\text{H}_9\text{NO})_2]$

$M_r = 607.51$

Monoclinic, $P2_1/c$

$a = 8.1938$ (5) Å

$b = 16.0605$ (9) Å

$c = 10.6108$ (6) Å

$\beta = 94.353$ (1)°

$V = 1392.32$ (14) Å³

$Z = 2$

$D_x = 1.449$ Mg m⁻³

Mo $K\alpha$ radiation

$\mu = 0.67$ mm⁻¹

$T = 298$ (2) K

Prism, pink

$0.18 \times 0.13 \times 0.10$ mm

Data collection

Bruker SMART APEX CCD

diffractometer

φ and ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 2000)

$T_{\min} = 0.881$, $T_{\max} = 0.935$

7496 measured reflections

2732 independent reflections

2134 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.047$

$\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.068$

$S = 0.96$

2732 reflections

190 parameters

H atoms treated by a mixture of

independent and constrained

refinement

$w = 1/[\sigma^2(F_o^2) + (0.0276P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\text{max}} = 0.33$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.35$ e Å⁻³

Table 1

Selected bond lengths (Å).

Co1—O2	2.0936 (12)	Co1—N1	2.1548 (14)
Co1—O4	2.1000 (12)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O4—H4A \cdots O3 ⁱ	0.870 (19)	1.71 (2)	2.5643 (18)	166.2 (19)

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

Carbon-bound H atoms were positioned geometrically, with C—H = 0.97 Å for methylene and 0.93 Å for aromatic, and refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$. The hydroxyl H atom was positioned geometrically and freely refined.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics:

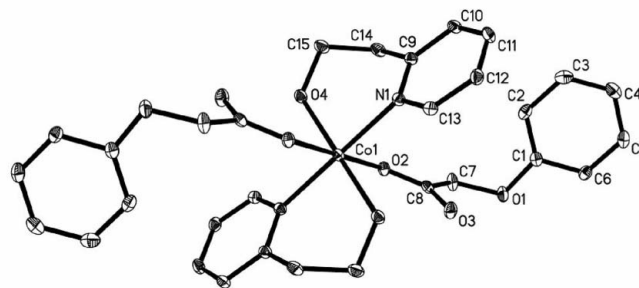


Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity. Unlabelled atoms and those with the suffix i are related to labelled atoms by the symmetry operation $(-x, -y, 1 - z)$.

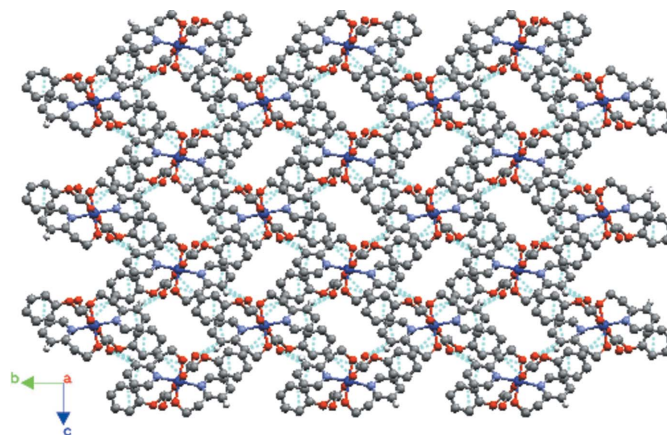


Figure 2

Packing diagram for (I), viewed along [100]. All H atoms have been omitted for clarity. Blue dashed lines indicate O—H \cdots O and C—H \cdots O interactions.

SHELXTL (Bruker, 2000); software used to prepare material for publication: SHELXTL.

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References

- Bruker (2000). SMART, SAINT, SADABS and SHELXTL. Bruker AXS Inc., Madison, Wisconsin, USA.
- Jiang, G.-Q., Li, Y.-Z., Hua, W.-J., Song, Y., Bai, J.-F., Li, S.-H., Scheer, M. & You, X.-Z. (2006). *CrystEngComm*, **8**, 384–387.
- Jiang, G.-Q., Li, Y.-Z., Wang, S.-N., Li, F.-F., Xu, Z.-J. & Bai, J.-F. (2005). *Acta Cryst.* **E61**, m1517–m1519.
- Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.
- Yaghi, O. M., Davis, C. E., Li, G. & Li, H. L. (1997). *J. Am. Chem. Soc.* **119**, 2861–2868.