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Key indicators

Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.036
 wR factor = 0.098
Data-to-parameter ratio = 17.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>. μ -Aqua- $\kappa^2\text{O}:\text{O}$ -di- μ -phenylacetato- $\kappa^4\text{O}:\text{O}'$ -bis[(1,10-phenanthroline- $\kappa^2\text{N},\text{N}'$)(phenylacetato- κO)cobalt(II)]

The title molecule, $[\text{Co}_2(\text{C}_8\text{H}_7\text{O}_2)_4(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})]$, is a dinuclear Co^{II} complex which is located on a twofold symmetry axis. Each Co^{II} ion is six-coordinated by three O atoms of different phenylacetate ligands, two N atoms of the 1,10-phenanthroline ligands and one O atom of a water molecule, giving a distorted octahedral geometry. The two Co^{II} atoms are bridged by two phenylacetate groups and the water molecule lying on the twofold axis. The $\text{Co}\cdots\text{Co}$ distance is $3.553(2)$ Å. A one-dimensional supramolecular chain is constructed by π - π stacking interactions between adjacent 1,10-phenanthroline molecules.

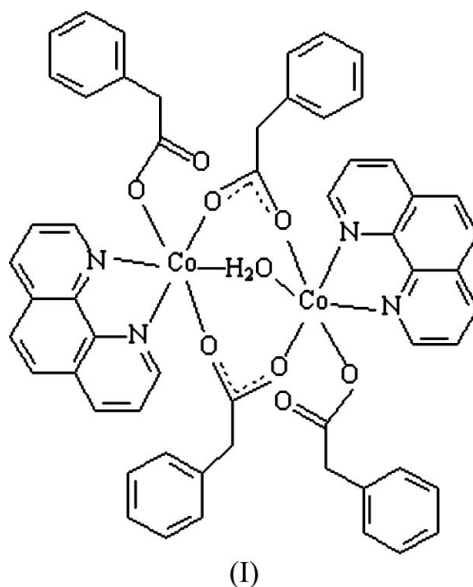
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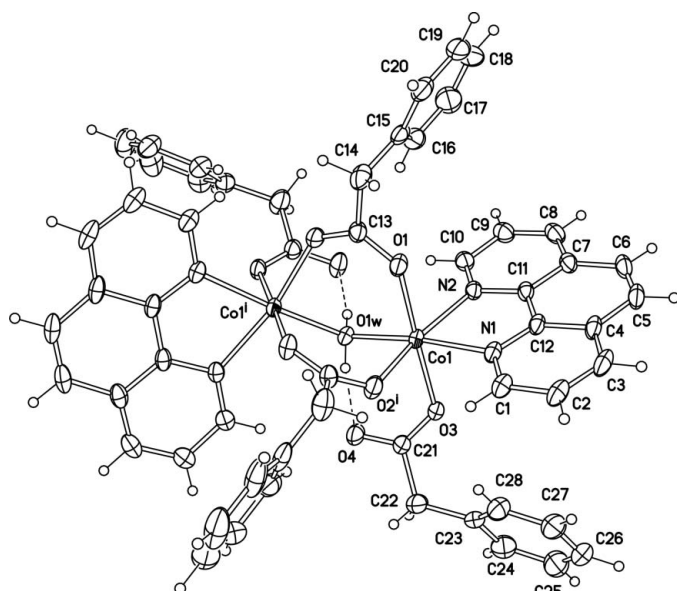
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Comment

The coordination chemistry of dinuclear Co^{II} complexes bridged by phenylacetate has not been much reported. To date, we have found only one report of a dinuclear Co^{II} complex, namely tetrakis(phenylacetato)bis[(quinoline- N)-cobalt(II)] (Cui *et al.*, 1999), and we have recently reported a dinuclear Cu^{II} complex, namely tetrakis(phenylacetato)bis[(N,N -dimethylformamide)copper(II)] (Kong *et al.*, 2005), in which all phenylacetate groups are in bidentate bridging modes. In order to explore further the coordination behaviour of the Co^{II} atom with phenylacetic acid, we used $\text{Co}(\text{acetate})_2\cdot 4\text{H}_2\text{O}$ instead of copper salts in the reaction and synthesized the title dinuclear cobalt complex $[\text{Co}_2(\text{C}_8\text{H}_7\text{O}_2)_4(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})]$, (I), and report its crystal structure here.




Figure 1

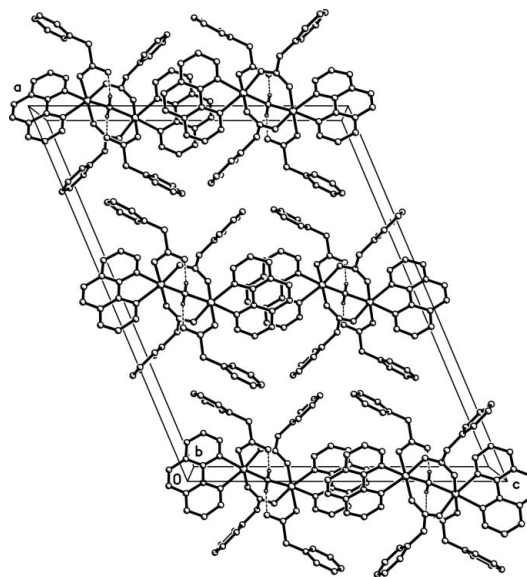
A plot of compound (I), with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) $-x + 1, y, -z + \frac{3}{2}$.]

The dimeric structure of (I) is illustrated in Fig. 1. The two Co^{II} atoms are bridged by two different phenylacetate groups and one water molecule, with a $\text{Co} \cdots \text{Co}$ separation of 3.553 (2) Å. This dimer is arranged around a twofold axis which passes through the bridging water molecule. The $\text{Co1}-\text{O1W}$ distance of 2.1248 (11) Å and $\text{Co1}-\text{O1W}-\text{Co1}^i$ angle of 113.47 (9)° [symmetry code: (i) $-x + 1, y, -z + \frac{3}{2}$] are within the expected ranges for related structures (Turpeinen *et al.*, 1987; Corkery & Hockless, 1997; Lee *et al.*, 2002; Miao *et al.*, 2004). Each Co^{II} atom shows an approximate octahedral geometry, with three carboxylate O atoms from different phenylacetate ligands, two N atoms from 1,10-phenanthroline ligands and one water molecule. Among the four phenylacetate groups, two of them are coordinated in a bidentate bridging mode and the others are monodentate.

The dimeric structure of (I) appears to be stabilized by hydrogen bonding between the uncoordinated carboxyl O4 atom and the bridging water molecule (Table 1). Furthermore, discrete dimers are extended into a one-dimensional supramolecular array through slipped $\pi-\pi$ stacking interactions between the 1,10-phenanthroline molecules of symmetry-related dinuclear units along the *c* axis (Fig. 2). The shortest centroid-centroid separation is 3.546 (1) Å with an interplanar distance of 3.380 (2) Å, resulting in an angle between the ring normal of the pyridine plane and the centroid vector of 17.6°.

Experimental

$\text{Co}(\text{acetate})_2 \cdot 4\text{H}_2\text{O}$ (2 mmol) and 1,10-phenanthroline (2 mmol) were dissolved in an aqueous solution (40 ml) of phenylacetic acid (6 mmol), and the pH of the solution was then raised to 6 with 0.1 M sodium hydroxide. The mixed solution was filtered off and allowed to evaporate at room temperature. Red block crystals of (I) were obtained after several weeks. Analysis calculated for $\text{C}_{56}\text{H}_{46}\text{N}_4\text{O}_9\text{Co}_2$: C 64.87, H 4.47, N 5.40%; found: C 64.89, H 4.48, N 5.37%.


Figure 2

The packing of compound (I), with the $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds denoted by dashed lines. H atoms not involved in hydrogen bonding have been omitted.

Crystal data

$[\text{Co}_2(\text{C}_8\text{H}_7\text{O}_2)_4(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})]$
 $M_r = 1036.83$
 Monoclinic, $C2/c$
 $a = 28.035$ (2) Å
 $b = 8.7132$ (17) Å
 $c = 21.920$ (2) Å
 $\beta = 112.92$ (3)°
 $V = 4931.8$ (16) Å³
 $Z = 4$

$D_x = 1.396$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 21804 reflections
 $\theta = 3.0-27.5^\circ$
 $\mu = 0.74$ mm⁻¹
 $T = 295$ (2) K
 Block, red
 $0.38 \times 0.26 \times 0.21$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer
 ω scans
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\text{min}} = 0.767, T_{\text{max}} = 0.861$
 23060 measured reflections

5633 independent reflections
 4429 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$
 $\theta_{\text{max}} = 27.5^\circ$
 $h = -36 \rightarrow 36$
 $k = -11 \rightarrow 11$
 $l = -28 \rightarrow 28$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.098$
 $S = 1.05$
 5633 reflections
 324 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0517P)^2 + 1.6797P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.002$
 $\Delta\rho_{\text{max}} = 0.37$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.18$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{O1W}-\text{H1W} \cdots \text{O4}^i$	0.86 (2)	1.71 (2)	2.5592 (19)	168 (2)

Symmetry code: (i) $-x + 1, y, -z + \frac{3}{2}$.

H atoms on C atoms were placed in calculated positions and included in the refinement using the riding-model approximation, with C–H = 0.93 Å (aromatic) or 0.97 Å (methylene), and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The H atom of the water molecule was located in a difference map and refined with an O–H distance restraint of 0.85 (1) and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

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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