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cis-Diaquabis(4-cyanobenzoato)-(1,10-phenanthroline)cobalt(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.046
wR factor = 0.084
Data-to-parameter ratio = 11.6

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

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The coordination polyhedron of Co^{II} in the title structure, $[Co(C_8H_4NO)_2(C_{12}H_8N_2)(H_2O)_2]$, is a slightly distorted octahedron defined by an N_2O_4 donor set. Hydrogen bonds are formed between the coordinated water molecules and O atoms of the carboxylate groups, stabilizing the structure and leading to the formation of a one-dimensional ladder architecture.

Comment

The design and construction of functional molecular blocks or architectures, such as ladders, zigzag chains, crowns, loops and zippers, for example, are of much interest because of their potential use as molecular devices (Alam, 2003; Chen & Liu, 2002; Liddle & Clegg, 2002). In the present paper, we report a one-dimensional hydrogen-bonded ladder of the title compound, (I), in which the 4-cyanobenzoato (cba) ligands form the hydrogen-bonded rungs of the ladder.

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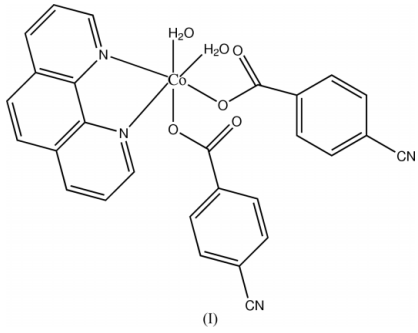

(I)

A mixture of cobalt(II) nitrate, 4-cyanobenzoic acid and 1,10-phenanthroline in dimethylformamide led to the formation of single crystals of the title complex, $[Co(C_8H_4NO_2)_2(C_{12}H_8N_2)_2(H_2O)_2]$, (I). The structure of (I) is a monomeric species (Fig. 1), with the Co atom in a slightly distorted octahedral geometry defined by two O atoms from two water molecules, two O atoms from two monodentate cba ligands and two N atoms of a chelating 1,10-phenanthroline ligand. The Co—O bond (carboxylate) distances in (I) (Table 1) are close to those of $[Co(4,4'\text{-bipy})(cba)_2(H_2O)_2]_n$, (II) (He *et al.*, 2003), and $[Co(apy)_2(cba)_2(H_2O)_2](2H_2O)$, (III) (He & Zhu, 2003*a*). In (I), (II) and (III) the Co—N bond distances are nearly equivalent and range from 2.126 (2) to 2.165 (2) Å.

The monodentate carboxylate binding mode of the two cba ligands in (I) is similar to that observed in (II), (III), $[Cu(4,4'\text{-bipyridine})(cba)_2]_n$ (He & Zhu, 2003*b*) and [Cu(1,10-phenanthroline)(H_2O)Cl(cba)]·H_2O (Zhou *et al.*, 2003). The coordination configurations for the carboxyl groups in (I) are

different. The dihedral angle between the carboxyl group (O1/C13/O2) and benzene ring (C14–C19) is 16.8 (2)°, and the Co/O2/C13/C14 torsion angle is 112.0 (2)°, which indicates that this carboxylate ligand has a non-planar coordination mode. By contrast, the dihedral angle between the O3/C21/O4 plane and the plane of the C22–C27 benzene ring is 4.2 (4)°, and the Co/O4/C21/C22 torsion angle is 171.3 (2)°. The two carboxyl groups are roughly perpendicular to each other, the dihedral angle between them being 70.18 (8)°.

There are significant hydrogen-bonding interactions in the structure. The water molecules form intramolecular hydrogen bonds with the non-coordinated carbonyl O atoms (Table 2). Intermolecular hydrogen bonds involving atoms O1 and O6 from adjacent molecules lead to the formation of a one-dimensional chain. Links between these chains, *via* hydrogen bonds involving the water molecules, hold the chains in a one-dimensional hydrogen-bonded ladder motif, as represented in Fig. 2.

Experimental

An aqueous solution (10 ml) of $Co(NO_3)_2{\cdot}6H_2O$ (0.0879 g, 0.3 mmol) was added to a dimethylformamide solution (10 ml) of 4-cyanobenzoic acd (0.0881 g, 0.6 mmol) and 1,10-phenanthroline (0.0591 g, 0.3 mmol). After the mixture had been allowed to stand for four weeks at room temperature, red crystals of (I) were obtained.

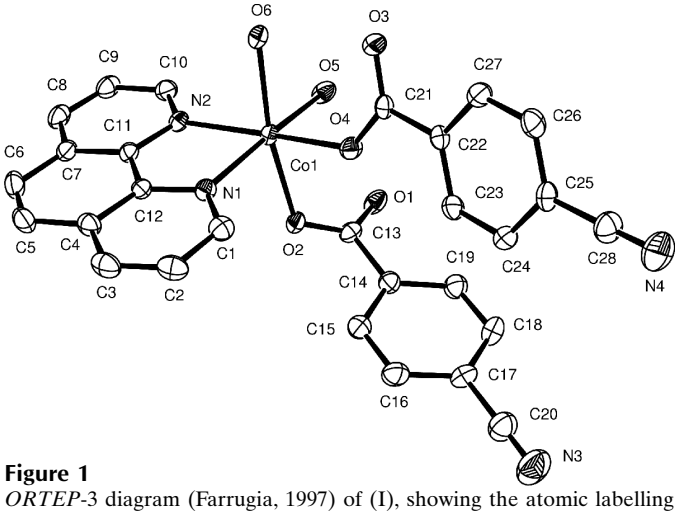

Figure 1
ORTEP-3 diagram (Farrugia, 1997) of (I), showing the atomic labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

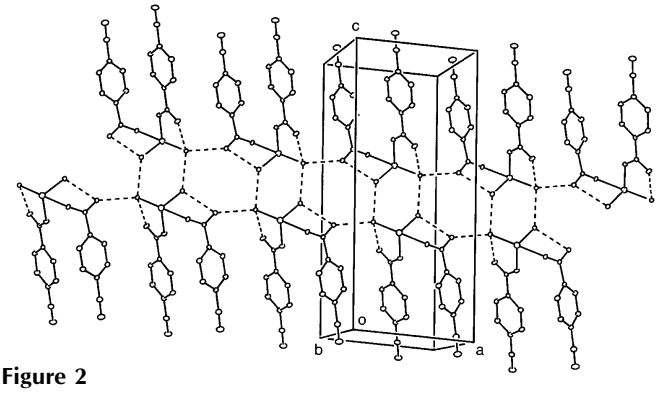

Figure 2
View of the one-dimensional hydrogen-bonded ladder motif. The H atoms and 1,10-phenanthroline ligands have been omitted for clarity.

Crystal data

$[Co(C_8H_4NO)_2(C_{12}H_8N_2)(H_2O)_2]$	$Z = 2$
$M_r = 567.41$	$D_x = 1.532$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 7.6930$ (8) Å	Cell parameters from 1529 reflections
$b = 8.9579$ (10) Å	$\theta = 4.9$–$47.7°$
$c = 18.538$ (2) Å	$\mu = 0.75$ mm^{-1}
$\alpha = 96.987$ (2)°	$T = 293$ (2) K
$\beta = 95.358$ (2)°	Plate, red
$\gamma = 102.126$ (2)°	0.43 × 0.22 × 0.12 mm
$V = 1230.4$ (2) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	4983 independent reflections
φ and ω scans	3285 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)	$R_{int} = 0.046$
$T_{min} = 0.734$, $T_{max} = 0.925$	$\theta_{max} = 26.5°$
7011 measured reflections	$h = -9 \rightarrow 9$
	$k = -11 \rightarrow 11$
	$l = -23 \rightarrow 17$

Refinement

Refinement on F^2	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)] = 0.046$	$w = 1/[\sigma^2(F_o^2) + (0.0232P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.084$	$(\Delta/\sigma)_{max} < 0.001$
$S = 0.83$	$\Delta\rho_{max} = 0.49$ e Å^{-3}
4983 reflections	$\Delta\rho_{min} = -0.39$ e Å^{-3}
431 parameters	

Table 1
Selected geometric parameters (Å, °).

Co1—O2	2.1097 (19)	Co1—O6	2.156 (2)
Co1—O4	2.0710 (18)	Co1—N1	2.126 (2)
Co1—O5	2.114 (2)	Co1—N2	2.132 (2)
O2—Co1—O5	86.55 (9)	O4—Co1—N2	168.76 (8)
O2—Co1—O6	170.69 (8)	O5—Co1—O6	87.05 (9)
O2—Co1—N1	86.77 (8)	O5—Co1—N1	170.89 (9)
O2—Co1—N2	100.25 (8)	O5—Co1—N2	97.40 (9)
O4—Co1—O2	85.13 (8)	O6—Co1—N1	100.28 (9)
O4—Co1—O5	92.75 (9)	O6—Co1—N2	87.27 (9)
O4—Co1—O6	88.44 (8)	N1—Co1—N2	77.72 (9)
O4—Co1—N1	92.85 (8)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O6—H19···O3	0.87 (3)	1.74 (3)	2.591 (3)	169 (3)
O6—H20···O1^{i}	0.860 (17)	1.840 (18)	2.687 (3)	168 (3)
O5—H18···O6^{ii}	0.853 (17)	1.908 (19)	2.753 (3)	171 (3)
O5—H17···O1	0.868 (18)	1.844 (19)	2.702 (3)	169 (3)

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

All H atoms were located in difference Fourier maps and their parameters were refined isotropically. The C—H and O—H bond lengths are in the ranges 0.896 (16)–0.993 (17) and 0.853 (17)–0.87 (3) Å, respectively.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); 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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