catena-Poly[[diaquabis(5-carboxypentanoato-κO)cobalt(II)]-μ-1,2-di-4-pyridylethane-κ²N:N′]

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The title compound, $[Co(C_6H_9O_4)_2(C_{12}H_{12}N_2)(H_2O)_2]_n$, crystallizes in the space group $P\bar{1}$. The Co atom is on a center of symmetry and the 1,2-di-4-pyridylethane (bpe) ligand also sits across a crystallographic inversion center. The Co atom is octahedrally coordinated by two aqua ligands, two carboxylate O atoms and two pyridyl N atoms, and is bridged by the *anti*-bpe ligands to generate one-dimensional $^1_\infty\{[Co(Hadip)_2(H_2O)_2](bpe)_{2/2}\}$ chains (Hadip is 5-carboxypentanoate), which are further interlinked by O—H···O and C—H···O hydrogen bonds into two-dimensional layers.

Comment

Investigation of coordination polymers has attracted increasing interest over the past decade (Moulton & Zaworotko, 2001) because of the intriguing structural motifs and their potential applications in catalysis, host–guest chemistry and magnetism (Leininger et al., 2000; Hagrman et al., 1999; Zhang et al., 2002; Feng & Xu, 2001; Yuan et al., 2002) of these compounds, and the rational design and syntheses of coordination polymers have been focused on the use of benzene di- and polycarboxylates as rigid bridging spacers (Li et al., 1999; Chui et al., 1999). On the other hand, utilization of aliphatic α,ω-dicarboxylates to construct supramolecular aggregates is of growing interest (Rao et al., 2004; Kitagawa et al., 2004). Our recent research has been concentrated on the construction of coordination polymers with specific topologies based on co-bridging of rigid 4,4′-bipyridine and α,ω-dicarboxylates (Zheng et al., 2004; Zheng & Ying, 2005). However, investigation of coordination polymers using 1,2-di-4-pyridylethane (bpe) and dicarboxylate anions to co-bridge metal ions has been very limited (Mukherjee et al., 2003). We report here a novel coordination polymer, $[Co(C_6H_9O_4)_2(anti\text{-}bpe)(H_2O)_2]$, (I), which was obtained by reaction of bpe, adipic acid and $CoCl_2 \cdot 6H_2O$ in CH_3OH–H_2O (1:1 $v:v$).

In (I), the Co atoms sit on crystallographic inversion centers, and each Co atom is octahedrally coordinated by two

N atoms of different *anti*-bpe ligands, four O atoms of two carboxypentanoate (Hadip) ligands and two aqua ligands. The

(1)
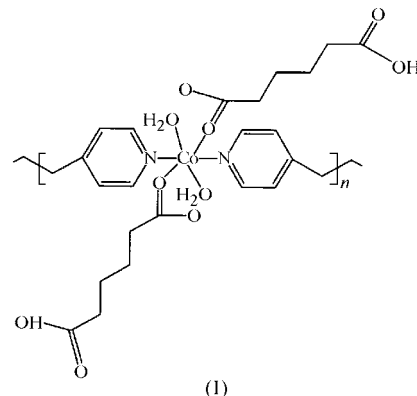
Co—O bond distances are 2.1102 (14) and 2.1223 (14) Å, and the Co—N distance is 2.1576 (13) Å, with the *cis* bond angles in the range 88.51 (6)–91.49 (6)°. The *anti*-bpe ligands bridge the Co atoms along the [110] direction to generate one-dimensional $^1_\infty\{[Co(Hadipa)_2(H_2O)_2](bpe)_{2/2}\}$ chains, as shown in Fig. 1, which exhibit a relatively strong intrachain hydrogen bond between the aqua O atom and uncoordinated carboxylate atom O1 [O···O = 2.624 (2) Å and O—H···O = 163 (3)°]. Additionally (Table 1), aqua ligand O5 and carboxyl atom O3 donate H atoms, respectively, to carboxyl atom O4^i [symmetry code: (i) $-x$, $-y + 1$, $-z + 2$] and the coordinating carboxylate atom O2^{ii} [symmetry code: (ii) x, y, $z + 1$] of neighboring chains, thus forming interchain hydrogen bonds [O···O = 2.753 (2) and 2.658 (2) Å, and O—H···O = 179 (3) and 161 (3)°]. The polymeric chains are linked through these bonds to form two-dimensional layers parallel to (100). The resulting layers are further stabilized by weak interchain hydrogen bonds between atom C12 of one *anti*-bpe ligand and uncoordinated carboxylate atom O1^{iii} [symmetry code: (iii) x, $y + 1$, z]. The twisted carboxypentanoate ligands of one layer protrude into the grooves of the neighboring layers, as shown in Fig. 2. The carboxypentanoate ligands exhibit normal
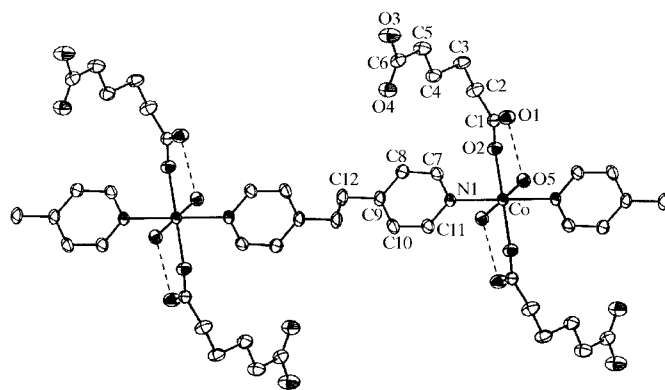
Figure 1
A view of a fragment of the one-dimensional $^1_\infty\{[Co(Hadipa)_2(H_2O)_2](bpe)_{2/2}\}$ polymeric chains in (I). Displacement ellipsoids are drawn at the 45% probability level. Dashed lines indicate hydrogen bonds.
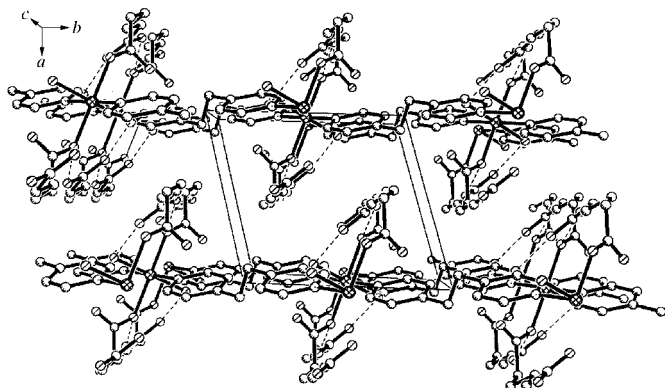
Figure 2
The crystal structure of (I) (dashed lines indicate hydrogen bonds).

Table 1
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O5—H5D···O1	0.82 (3)	1.83 (4)	2.624 (2)	163 (3)
O5—H5C···O4[i]	0.86 (3)	1.89 (3)	2.753 (2)	179 (3)
O3—H3C···O2[ii]	0.82 (3)	1.87 (3)	2.658 (2)	161 (3)

Symmetry codes: (i) $-x, -y+1, -z+2$; (ii) $x, y, z+1$.

Compound (I) is triclinic; space group $P\bar{1}$ was assumed and confirmed by the analysis. H atoms associated with C atoms were positioned geometrically and refined using a riding model [C—H = 0.93 and 0.97 Å, and $U_{iso}(H) = 1.2U_{eq}(C)$], while H atoms of the aqua ligands and carboxyl atom O3 were located from difference Fourier syntheses, and their O—H distances were refined.

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

geometry (Ying *et al.*, 2004), and the C6—O4 distance [1.205 (2) Å] is distinctly shorter than the C6—O3 distance [1.320 (2) Å], indicating C6=O4 double-bond character.

Experimental

In a typical synthesis, bpe (0.0921 g) and adipic acid (0.0731 g) were dissolved in CH_3OH-H_2O (1:1 *v/v*, 50 ml), and $CoCl_2 \cdot 6H_2O$ (0.1190 g) was added to the resulting solution with stirring. The mixture was stirred for a further *ca* 30 min, yielding a red-colored solution, which was then maintained at room temperature; red crystals suitable for X-ray analysis were obtained after two weeks.

Crystal data

[Co(C6H9O4)2(C12H12N2)(H2O)2]
$M_r = 569.46$
Triclinic, $P\bar{1}$
$a = 8.6928 (17)$ Å
$b = 8.8579 (18)$ Å
$c = 9.6059 (19)$ Å
$\alpha = 85.17 (3)°$
$\beta = 65.14 (3)°$
$\gamma = 74.03 (3)°$
$V = 644.8 (2)$ Å^3

$Z = 1$
$D_x = 1.466$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 10-25°$
$\mu = 0.72$ mm^{-1}
$T = 296 (2)$ K
Prism, red
$0.39 \times 0.31 \times 0.22$ mm

Data collection

Bruker *P4* diffractometer
$\theta/2\theta$ scans
Absorption correction: ψ scan (*XSCANS*; Siemens, 1996)
$T_{min} = 0.818$, $T_{max} = 0.853$
3546 measured reflections
2959 independent reflections
2670 reflections with $I > 2\sigma(I)$

$R_{int} = 0.024$
$\theta_{max} = 27.5°$
$h = -1 \rightarrow 11$
$k = -11 \rightarrow 11$
$l = -11 \rightarrow 12$
3 standard reflections
every 97 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.078$
$S = 1.05$
2959 reflections
182 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0298P)^2 + 0.2282P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

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