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(OC-6-32)-Diaquabis(glycolato)cobalt(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.023
wR factor = 0.052
Data-to-parameter ratio = 13.8

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

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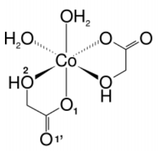
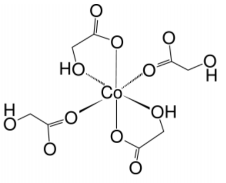
The title neutral complex, [Co(HG)$_2$(H$_2$O)$_2$] or [Co(C$_2$H$_3$O$_3$)$_2$(H$_2$O)$_2$], contains monoanionic O,O'-bidentate glycolate ligands that chelate the cobalt(II) ion through the carboxylate and hydroxyl O atoms to form five-membered chelate rings. The configuration around the cobalt ion can be described as all-*cis*. The nature of the ligands permits the formation of a supramolecular architecture based on hydrogen bonding.

Comment

Hydrogen bonds play a key role in many molecular recognition and self-assembly processes in solution and in the solid state, and can change the properties of many materials that are of importance in biology, crystal engineering and materials science (Beatty, 2001; Braga *et al.*, 1998). As part of our studies of the supramolecular organization of cobalt(II) carboxylate complexes (Carballo *et al.*, 2001, 2002, 2003), in this work we report the three-dimensional hydrogen-bonded structure of the mononuclear complex [Co(HG)$_2$(H$_2$O)$_2$], (1) (H$_2$G is glycolic acid). The structure of another glycolate–cobalt(II) complex was previously reported by Medina *et al.* (2000) and, like the copper(II)–glycolate complex (Prout *et al.*, 1968), it is a bidimensional coordination polymer, [Co(HG)$_2$]$_n$ (2). The glycolate group forms the same chelate ring as in (1), by coordination of O^1 and O^2 atoms, but two Co atoms are bridged by the carboxylate group (O^1 and O$^{1\prime}$). However, (1) is isostructural with the manganese(II) (Lis, 1979; Melikyan *et al.*, 2000) and zinc(II) (Fischinger & Webb, 1969) complexes.



(1)



(2)

In (1), the Co atom is attached to two chelating glycolate ligands and two water molecules; the coordination polyhedron is a distorted octahedron with the main deviations from regularity affecting the bite angles O$_{\rm hydroxyl}$—Co—O$_{\rm carboxy}$ [77.61 (5) and 76.46 (5)°], which are similar to those observed in other α-hydroxycarboxylate–cobalt(II) complexes (Carballo *et al.*, 2002; Karipides, 1981; Matzapetakis *et al.*, 2000; Medina *et al.*, 2000). The configuration around the cobalt center is all-*cis* [OC-6-32 in the CPI system (von Zelewsky, 1996) with the priority order O^1(1) > O^2(2) > O$_{\rm water}$(3)], which is the same as that in the lactate–cobalt(II) complex (Carballo *et al.*, 2002), whereas (2) is all-*trans* [OC-6-12, priority order O^1(1) > O$^{1\prime}$(2) > O^2(3); Medina *et al.*, 2000].

The α-hydroxycarboxylate ligands usually form five-membered chelate rings in which the metal–O$_{\rm carboxy}$ distances are shorter than the metal–O$_{\rm hydroxy}$ distances (see, for example, Karipides, 1981; Matzapetakis *et al.*, 2000; Medina *et al.*, 2000). However, as we previously observed in the lactate–cobalt(II) complex (Carballo *et al.*, 2002), one of the HG$^-$ ligands shows a different behavior [Co—O23 = 2.0877 (13) Å and Co—O21 = 2.1051 (13) Å].

In the carboxylate groups the C—O lengths for the coordinated O atoms [1.256 (2) and 1.261 (2) Å] are only slightly longer than those for the uncoordinated O atoms [1.252 (2) and 1.247 (2) Å], which suggests that there is significant electron delocalization in the carboxylate groups, although the effect of the strong hydrogen bond established by non-coordinating carboxylate oxygen (see below) cannot be ruled out.

In (1), the molecules are linked by hydrogen bonds (Table 2), giving a supramolecular architecture; the hydrogen bonds between the O atoms of the carboxylate group and the hydroxyl groups of an adjacent molecule (O13—H13···O12$^{\rm iii}$ and O23—H23···O11$^{\rm iii}$; symmetry code as in Table 2) form polymeric chains along the crystallographic *b* axis (Fig. 2). These chains are linked by additional hydrogen bonds involving the coordinated water molecules and carboxylate O atoms, resulting in an infinite three-dimensional network (Fig. 3).

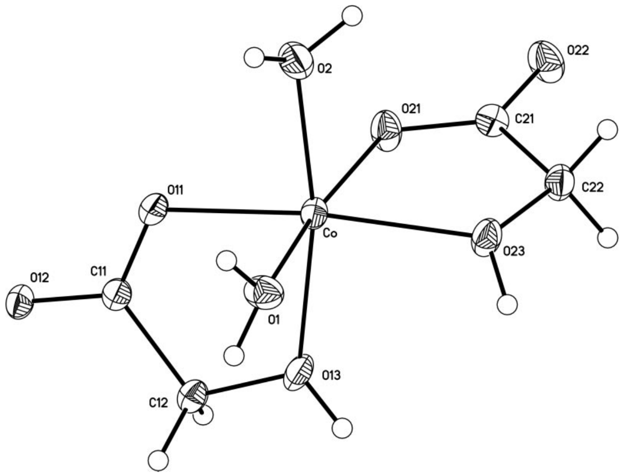


Figure 1
SHELXTL (Bruker, 2000) diagram of [Co(HG)$_2$(H$_2$O)$_2$], showing the atom-numbering system. Non-H atoms are represented as displacement ellipsoids drawn at the 30% probability level.

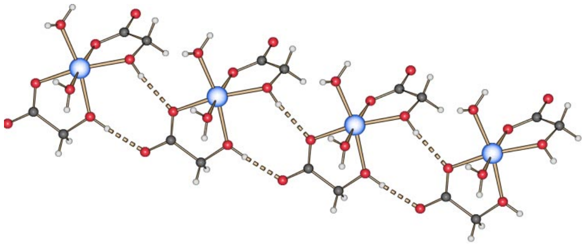


Figure 2
SCHAKAL (Keller, 1999) diagram showing the polymeric chain along the crystallographic *b* axis.

Experimental

Compound (1) was obtained by the reaction of cobalt(II) acetate (1.0 mmol) and glycolic acid (2.0 mmol) in water. The resulting pink solution was heated for 10 min and stirred at room temperature for several days. A pink crystalline product was obtained (95% yield) by slow concentration of the solution (m.p. > 523 K). Analysis found: C 19.6, H 4.1%; $C_4H_{10}CoO_8$ requires: C 19.6, H 4.1%. $\mu_{\rm eff}$ at 298 K: 4.78 M. B. IR (KBr, cm^{-1}): 3244 (*s*, br) ν(OH), 1593 (*vs*) $\nu_{\rm asym}$(COO), 1428 (*s*) $\nu_{\rm sym}$(COO) [$\Delta\nu = \nu_{\rm asym}({\rm COO}) - \nu_{\rm asym}({\rm COO}) = 165$].

Crystal data

[Co(C$_2$H$_3$O$_3$)$_2$(H$_2$O)$_2$]
$M_r = 245.05$
Monoclinic, $P2_1/c$
$a = 11.5388$ (9) Å
$b = 5.8330$ (4) Å
$c = 12.4477$ (9) Å
$\beta = 91.4537$ (14)°
$V = 837.53$ (11) Å^3
$Z = 4$
$D_x = 1.943$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2202 reflections
$\theta = 1.8$–28.0°
$\mu = 2.06$ mm^{-1}
$T = 293$ (2) K
Prism, pink
0.36 × 0.13 × 0.11 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\rm min} = 0.611$, $T_{\rm max} = 0.797$
5031 measured reflections
1964 independent reflections
1602 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.023$
$\theta_{\rm max} = 28.0°$
$h = -13 \rightarrow 14$
$k = -7 \rightarrow 7$
$l = -16 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.053$
$S = 0.94$
1964 reflections
142 parameters
H atoms: see below
$w = 1/[\sigma^2(F_o^2) + (0.0247P)^2 + 0.4285P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.28$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.25$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co—O1	2.0439 (15)	Co—O2	2.0891 (14)
Co—O21	2.0696 (12)	Co—O11	2.1050 (12)
Co—O13	2.0870 (13)	Co—O23	2.1213 (14)
O1—Co—O21	93.32 (6)	O13—Co—O11	77.60 (5)
O1—Co—O13	99.04 (6)	O2—Co—O11	172.23 (5)
O21—Co—O13	164.37 (5)	O1—Co—O23	168.92 (6)
O1—Co—O2	89.40 (6)	O21—Co—O23	76.45 (5)
O21—Co—O2	94.53 (5)	O13—Co—O23	91.78 (6)
O13—Co—O2	95.14 (5)	O2—Co—O23	87.21 (6)
O1—Co—O11	89.04 (6)	O11—Co—O23	95.68 (5)
O21—Co—O11	93.16 (5)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H11···O12$^{\rm i}$	0.86 (3)	1.84 (3)	2.686 (2)	167 (2)
O1—H12···O12$^{\rm ii}$	0.81 (2)	1.92 (3)	2.716 (2)	166 (2)
O23—H23···O22$^{\rm iii}$	0.88 (2)	1.77 (2)	2.6517 (18)	175 (2)
O13—H13···O21$^{\rm iii}$	0.840 (17)	1.964 (19)	2.7547 (19)	156 (3)
O2—H21···O22$^{\rm iv}$	0.86 (2)	1.86 (2)	2.7180 (19)	174 (2)
O2—H22···O11$^{\rm ii}$	0.822 (16)	1.991 (17)	2.8016 (18)	169 (2)

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

Acta Cryst. (2003). E**59**, m588–m590 Rosa Carballo *et al.* • [Co(C$_2$H$_3$O$_3$)$_2$(H$_2$O)$_2$] **m589**

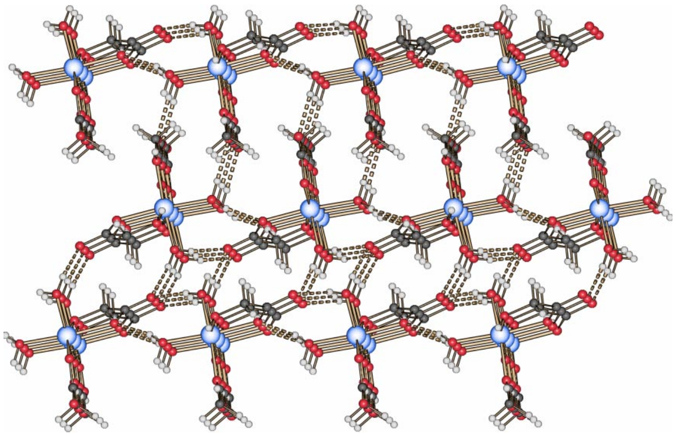


Figure 3
SCHAKAL (Keller, 1999) diagram showing the three-dimensional network, projected on to the *ac* plane.

Hydroxyl and water H atoms were located and refined, subject to the following restraints: O—H = 0.90 (2) Å for the O1—H12 and O23—H23 bonds. All other H atoms were placed geometrically and were allowed to ride on their parent C atoms [C—H = 0.97 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C)].

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000) and *SCHAKAL* (Keller, 1999); software used to prepare material for publication: *SHELXTL*.

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