

## Polymeric bis(glycolato)cobalt(II)

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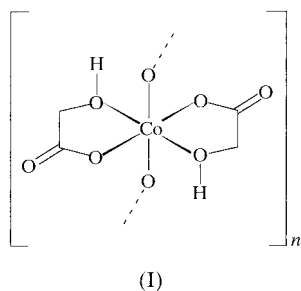
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In the title compound, poly[cobalt(II)-bis( $\mu$ -hydroxyacetato- $O^1, O^2:O^1'$ )],  $[\text{Co}(\text{C}_2\text{H}_3\text{O}_3)_2]_n$ , units of  $[\text{Co}(\text{C}_2\text{H}_3\text{O}_3)_2]$  constitute a bidimensional sheet coordination polymer in which each  $\text{Co}^{\text{II}}$  atom lies on an inversion centre and is octahedrally coordinated to glycolate ligands in a *trans* configuration. Carbonyl O atoms from adjacent units complete the octahedral environment.

## Comment

Previous structure determinations involving coordination compounds of divalent transition metals with the glycolate ligand have been limited to those of copper (Prout *et al.*, 1968, 1993), manganese (Lis, 1980) and zinc (Fischinger & Webb, 1969). The  $\text{Cu}^{\text{II}}$  compound constitutes a coordination sheet polymer, although monomeric units of bis(glycolato)copper have been obtained by means of adduct formation with  $\text{NH}_3$  and pyridine. In both compounds, the Cu atom is in an elongated tetragonally distorted octahedral environment with the N-donor ligands in *trans* positions. Both the  $\text{Mn}^{\text{II}}$  and  $\text{Zn}^{\text{II}}$  compounds (for which the structures has been determined) form discrete units in which two water molecules are coordinated to the metal ion in *cis* positions (Lis, 1980; Fischinger & Webb, 1969). The structure of the title compound, (I), has been elucidated in order to extend the range of metal atoms coordinated by this ligand.



In compound (I), the Co atom is coordinated to two glycolate ligands which form five-membered *trans* chelate

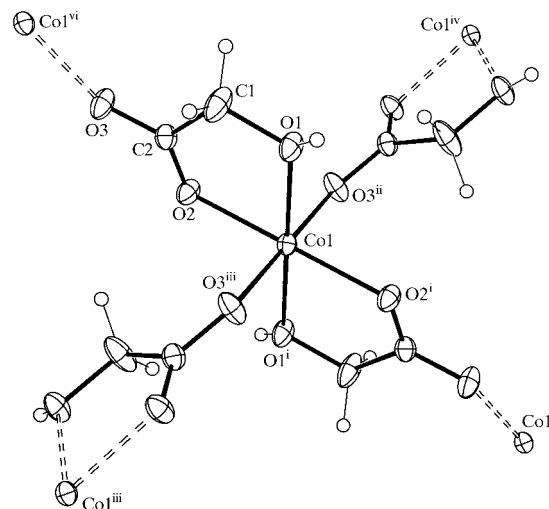


Figure 1

The coordination sphere for the  $\text{Co}^{\text{II}}$  ions in (I) (solid bonds). Dashed bonds indicate Co atoms connected to this unit and belonging to the same layer in the polymer. Displacement ellipsoids are shown at the 50% probability level [symmetry codes: (i)  $-x, -y, 1 - z$ ; (ii)  $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$ ; (iii)  $-\frac{1}{2} - x, -\frac{1}{2} + y, \frac{1}{2} - z$ ; (iv)  $\frac{1}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z$ ; (v)  $\frac{1}{2} - x, -\frac{1}{2} + y, \frac{3}{2} - z$ ; (vi)  $-\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$ ].

rings which constitute the plane of the coordination octahedron. The Co—O distances for both the carboxy-O and the  $\alpha$ -hydroxy-O atoms are similar, with values of 2.0534 (10) Å for the Co—O2 bond and 2.0910 (10) Å for the Co—O1 bond. The coordination octahedron is completed by carbonyl O atoms from adjacent units of the compound in the same layer. The polymeric sheet is thus made up of alternating units of (I) in which the planes of the five-membered chelate rings lie roughly perpendicular to each other, thus accounting for the axial coordination of  $\text{O}3(\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z)$  to Co1. At 2.1180 (10) Å, these bonds are slightly longer than those observed for the Co—O bonds in the chelate ring. The Co $\cdots$ Co distances within the coordination sheet are 5.926 (1) Å, while the Co $\cdots$ Co distances between adjacent coordination sheets in the polymeric compound are 5.189 (1) Å.

A highly ordered array of hydrogen bonds keeps the coordination sheets together. An H atom from an  $\alpha$ -OH group in one glycolate ligand binds to the carbonyl-O atom of the lower sheet, while the other binds to the upper sheet. Intermolecular  $\text{O}1-\text{H}1\cdots\text{O}3$  hydrogen bonds have an H $\cdots$ O distance of 1.804 Å. The coordination environment around the Co atom is closer to octahedral than that observed for the compound with Cu, where tetragonal distortion is significant and results in four short and two long bonds. Metal—oxygen distances for the Cu compound are approximately 0.14 Å shorter than those observed for the Co complex. However, static Jahn–Teller distortions around the Cu atom make the distance between axially coordinated carbonyl-O atoms 0.42 Å longer than those observed in the Co compound. In the Cu and Co compounds, the longest bond present is that occurring with the carbonyl-O atom, whereas the longest bond

present in octahedral monomeric *cis*-MG<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub> compounds (G = glycolato, M = Mn and Zn) is at least one of the α-OH M—O bonds, one Mn—OH bond being 2.225 (3) Å and one Zn—OH bond being 2.1530 (10) Å.

The coordination environment around the Co<sup>II</sup> atom in polymeric (I) resembles that of the *trans*-diaquabis-(hydrogenmalato)cobalt(II) dihydrate (Karipides, 1981). This earlier structure consists of discrete units in which the hydrogenmalate ligands coordinate to the Co<sup>II</sup> atom forming five-membered rings in a *trans* configuration. The ligands bind to the Co<sup>II</sup> atom through the carboxy and α-OH O atoms at distances of 2.066 (1) and 2.076 (1) Å, respectively, while the β-carboxylic acid group remains uncoordinated to the metal ion. Two water molecules coordinate axially at a distance of 2.112 (1) Å. The Co—O bond distances do not differ significantly between the polymeric glycolate compound and the monomeric hydrogenmalate compound.

## Experimental

All chemicals used were *ex* Aldrich Chemical Co. and used with no further purification. Compound (I) was prepared by dissolving Co(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O (1 mmol) and glycolic acid (2 mmol) in methanol. The solution was neutralized with aqueous NH<sub>3</sub> and was left standing overnight, over which time a pink precipitate formed. To this mixture, potassium glycolate (1 mmol) in methanol was added. The pink solid redissolved after the addition of a small amount of water. The pink solution was then concentrated over a steam bath and the resulting pink solid was dissolved in the minimum amount of water necessary. Methanol was added to the solution, which was left standing until small crystals formed. These were filtered and vacuum dried and crystals suitable for X-ray analysis were obtained by slow growth from a water/methanol solution.

### Crystal data

[Co(C<sub>2</sub>H<sub>3</sub>O<sub>3</sub>)<sub>2</sub>]  
*M<sub>r</sub>* = 209.02  
 Monoclinic, *P*<sub>2</sub><sub>1</sub>/*n*  
*a* = 5.1886 (6) Å  
*b* = 7.8583 (10) Å  
*c* = 8.6621 (10) Å  
 $\beta$  = 104.977 (8)°  
*V* = 341.19 (7) Å<sup>3</sup>  
*Z* = 2

*D<sub>x</sub>* = 2.035 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 48 reflections  
 $\theta$  = 4.8–12.4°  
 $\mu$  = 2.494 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Prism, purple  
 0.3 × 0.2 × 0.2 mm

**Table 1**

Selected geometric parameters (Å, °).

Co1—O2	2.0534 (10)	Co1—O3 <sup>i</sup>	2.1180 (10)
Co1—O1	2.0910 (10)		
O2—Co1—O1	78.52 (4)	O1—Co1—O3 <sup>i</sup>	88.00 (4)
O2—Co1—O3 <sup>i</sup>	91.63 (4)		

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

### Data collection

Siemens <i>P4</i> diffractometer	<i>R</i> <sub>int</sub> = 0.018
2θ/ω scans	$\theta$ <sub>max</sub> = 30°
Absorption correction: Gaussian ( <i>XSCANS</i> ; Siemens, 1991)	<i>h</i> = -7 → 7
<i>T</i> <sub>min</sub> = 0.760, <i>T</i> <sub>max</sub> = 0.811	<i>k</i> = -11 → 11
2180 measured reflections	<i>l</i> = -12 → 12
999 independent reflections	3 standard reflections every 97 reflections
886 reflections with <i>I</i> > 2σ( <i>I</i> )	intensity decay: 1.29%

### Refinement

Refinement on <i>F</i> <sup>2</sup>	$w = 1/[\sigma^2(F_o^2) + (0.0203P)^2 + 0.116P]$
<i>R</i> ( <i>F</i> ) = 0.020	where $P = (F_o^2 + 2F_c^2)/3$
<i>wR</i> ( <i>F</i> <sup>2</sup> ) = 0.053	(Δ/σ) <sub>max</sub> < 0.001
<i>S</i> = 1.096	Δρ <sub>max</sub> = 0.34 e Å <sup>-3</sup>
999 reflections	Δρ <sub>min</sub> = -0.24 e Å <sup>-3</sup>
52 parameters	
H-atom parameters constrained	

Data collection, cell refinement and data reduction: *XSCANS* (Siemens, 1991); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1995); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXL97*.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: DA1106). Services for accessing these data are described at the back of the journal.

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