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catena-Poly[[diaquabis(isoquinoline- κ N)-cobalt(II)]- μ -succinato- κ^2 O¹:O⁴]

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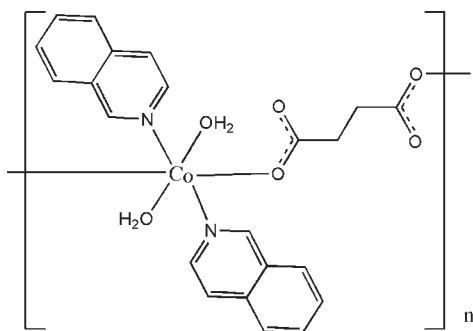
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Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å;
R factor = 0.033; wR factor = 0.057; data-to-parameter ratio = 13.3.

In the title compound, $[\text{Co}(\text{C}_4\text{H}_4\text{O}_4)(\text{C}_9\text{H}_7\text{N})_2(\text{H}_2\text{O})_2]_n$, the Co^{II} cation, located on an inversion center, is coordinated by two succinate anions, two isoquinoline ligands and two water molecules in a distorted octahedral geometry. The succinate anion, located across another inversion center, bridges the Co cations, forming polymeric chains running along the b axis. The partially overlapped arrangement of parallel isoquinoline ring systems of adjacent polymeric chains and the shorter face-to-face distance of 3.402 (6) Å indicates the existence of weak π - π stacking in the crystal structure. Classical intra- and intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonding and weak non-classical intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonding help to stabilize the crystal structure.

Related literature

For general background to π - π stacking, see: Deisenhofer & Michel (1989); Su & Xu (2004); Xu *et al.* (2007). For two related isoquinoline complexes, see: Li *et al.* (2009a,b). For a related polymeric Ni^{II} complex bridged by succinate anions, see: Liu *et al.* (2003).



Experimental

Crystal data

$[\text{Co}(\text{C}_4\text{H}_4\text{O}_4)(\text{C}_9\text{H}_7\text{N})_2(\text{H}_2\text{O})_2]$
 $M_r = 469.35$
Monoclinic, $P2_1/n$
 $a = 11.258$ (4) Å
 $b = 9.023$ (5) Å
 $c = 11.390$ (7) Å
 $\beta = 114.667$ (5)°
 $V = 1051.4$ (9) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 0.86$ mm⁻¹
 $T = 294$ K
 $0.24 \times 0.14 \times 0.12$ mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\text{min}} = 0.788$, $T_{\text{max}} = 0.862$
4907 measured reflections
1891 independent reflections
1165 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.040$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.057$
 $S = 0.82$
1891 reflections
142 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.23$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.23$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1W}-\text{H1A}\cdots\text{O2}^{\text{i}}$	0.90	1.89	2.774 (3)	169
$\text{O1W}-\text{H1B}\cdots\text{O2}$	0.87	1.90	2.689 (3)	150
$\text{C5}-\text{H5}\cdots\text{O2}^{\text{ii}}$	0.93	2.56	3.487 (5)	176

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2211).

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supporting information

Acta Cryst. (2010). E66, m840 [doi:10.1107/S1600536810023895]

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Meng-Jiao Li, Jing-Jing Nie and Duan-Jun Xu

S1. Comment

The $\pi\cdots\pi$ stacking between aromatic rings is an important non-covalent interaction and correlated with the electron transfer process in some biological systems (Deisenhofer & Michel, 1989). As part of our ongoing investigation on the nature of $\pi\cdots\pi$ stacking (Su & Xu, 2004; Xu *et al.*, 2007), the title complex incorporating isoquinoline ligand has recently been prepared in the laboratory and its crystal structure is reported here.

A part of the polymeric molecular structure is shown in Fig. 1. The Co^{II} cation located on an inversion center is coordinated by two succinate anions, two isoquinoline ligands and two water molecules with a distorted octahedral geometry. The succinate anion is located across another inversion center, and bridges Co cations to form the one-dimensional polymeric chains running along the crystallographic *b* axis, similar to that found in a Ni^{II} complex bridged by succinate anions (Liu *et al.*, 2003). The carboxyl group is oriented with respect to the carbon skeleton of succinate anion at a dihedral angle of 28.4 (2)°.

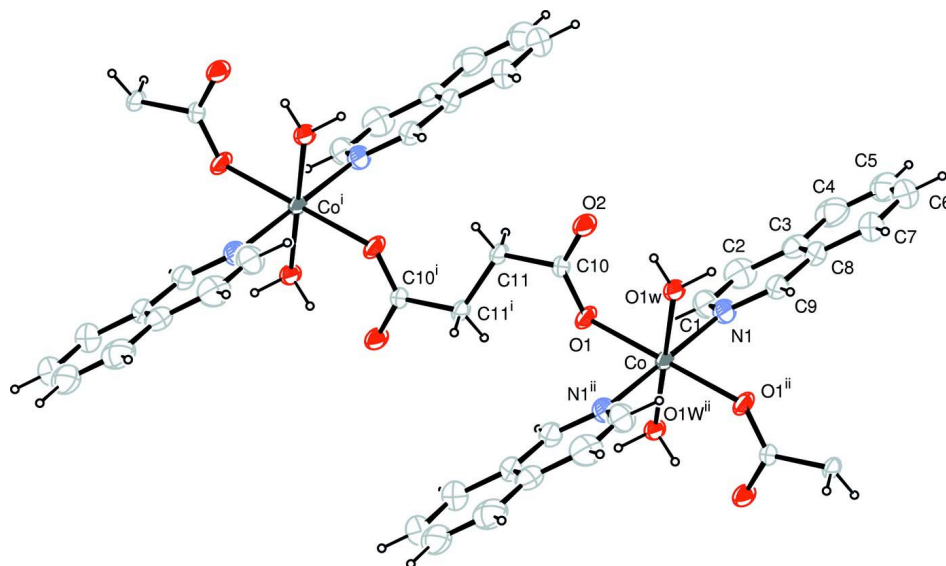
The partially overlapped arrangement of parallel isoquinoline ring systems of adjacent polymeric chains related by a symmetry operation of (1-*x*, 1-*y*, -*z*) and shorter face-to-face distance of 3.402 (6) Å indicate the existence of weak $\pi\cdots\pi$ stacking in the crystal structure. Classical intra- and intermolecular O–H \cdots O hydrogen bonding and weak non-classical intermolecular C–H \cdots O hydrogen bonding help to stabilize the crystal structure (Table 1).

S2. Experimental

The CoCl₂·6H₂O (0.48 g, 2 mmol), succinic acid (0.24 g, 2 mmol), NaOH (0.16 g, 4 mmol) and isoquinoline (0.23 ml, 2 mmol) were dissolved in a water/ethanol solution (20 ml, 1:1). The solution was refluxed for 4 h. The reaction mixture was cooled to room temperature and filtered. The single crystals were obtained from the filtrate after two weeks.

S3. Refinement

Water H atoms were located in a difference Fourier map and refined as-riding in as-found relative positions with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$. Other H atoms were placed in calculated positions with C–H = 0.93 Å (aromatic) and 0.97 Å (methylene), and refined in riding mode with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

**Figure 1**

A part of the polymeric molecular structure of the title compound with atom numbering scheme. Displacement ellipsoids are drawn at 50% probability level. H atoms are presented as a small spheres of arbitrary radius. Symmetry codes: (i) 1-x, -y, 1-z; (ii) 1-x, 1-y, 1-z.

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Crystal data

[Co(C₄H₄O₄)(C₉H₇N)₂(H₂O)₂]

$M_r = 469.35$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 11.258$ (4) Å

$b = 9.023$ (5) Å

$c = 11.390$ (7) Å

$\beta = 114.667$ (5)°

$V = 1051.4$ (9) Å³

$Z = 2$

$F(000) = 486$

$D_x = 1.482$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2408 reflections

$\theta = 3.5$ – 24.6 °

$\mu = 0.86$ mm⁻¹

$T = 294$ K

Prism, pink

$0.24 \times 0.14 \times 0.12$ mm

Data collection

Rigaku R-AXIS RAPID IP

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 10.0 pixels mm⁻¹

ω -scan

Absorption correction: multi-scan

(*ABSCOR*; Higashi, 1995)

$T_{\min} = 0.788$, $T_{\max} = 0.862$

4907 measured reflections

1891 independent reflections

1165 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.040$

$\theta_{\max} = 25.2$ °, $\theta_{\min} = 3.3$ °

$h = -13 \rightarrow 13$

$k = -10 \rightarrow 8$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.033$

$wR(F^2) = 0.057$

$S = 0.82$

1891 reflections

142 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods
Secondary atom site location: difference Fourier
map
Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0207P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.23 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.23 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co	0.5000	0.5000	0.5000	0.03143 (14)
N1	0.5562 (2)	0.5432 (2)	0.34392 (16)	0.0394 (6)
O1	0.50790 (18)	0.27225 (15)	0.47973 (14)	0.0392 (4)
O2	0.31969 (17)	0.21732 (17)	0.31456 (15)	0.0434 (5)
O1W	0.29833 (13)	0.50231 (19)	0.37221 (11)	0.0369 (4)
H1A	0.2673	0.5677	0.3070	0.044*
H1B	0.2846	0.4213	0.3263	0.044*
C1	0.6531 (3)	0.4608 (3)	0.3341 (2)	0.0513 (8)
H1	0.6940	0.3889	0.3965	0.062*
C2	0.6927 (3)	0.4788 (4)	0.2376 (2)	0.0572 (8)
H2	0.7600	0.4205	0.2357	0.069*
C3	0.6326 (3)	0.5844 (3)	0.1411 (2)	0.0462 (7)
C4	0.6658 (3)	0.6069 (4)	0.0350 (3)	0.0647 (9)
H4	0.7314	0.5506	0.0274	0.078*
C5	0.6012 (4)	0.7107 (4)	-0.0549 (3)	0.0698 (10)
H5	0.6228	0.7246	-0.1246	0.084*
C6	0.5030 (4)	0.7973 (4)	-0.0451 (3)	0.0700 (10)
H6	0.4603	0.8681	-0.1080	0.084*
C7	0.4689 (3)	0.7791 (3)	0.0560 (2)	0.0583 (9)
H7	0.4034	0.8372	0.0620	0.070*
C8	0.5334 (3)	0.6720 (3)	0.1506 (2)	0.0410 (7)
C9	0.4999 (3)	0.6448 (3)	0.2554 (2)	0.0399 (6)
H9	0.4343	0.7022	0.2620	0.048*
C10	0.4249 (2)	0.1817 (2)	0.4066 (2)	0.0294 (6)
C11	0.4568 (2)	0.0192 (2)	0.43056 (17)	0.0335 (6)
H11A	0.4999	-0.0128	0.3768	0.040*
H11B	0.3758	-0.0360	0.4039	0.040*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co	0.0357 (3)	0.0151 (2)	0.0285 (2)	-0.0009 (3)	-0.00145 (17)	0.0019 (2)
N1	0.0390 (13)	0.0305 (13)	0.0367 (11)	0.0033 (10)	0.0040 (9)	0.0038 (9)
O1	0.0391 (11)	0.0153 (8)	0.0426 (10)	-0.0025 (9)	-0.0035 (8)	-0.0015 (8)
O2	0.0444 (12)	0.0209 (10)	0.0399 (9)	0.0028 (8)	-0.0073 (8)	-0.0005 (8)
O1W	0.0410 (9)	0.0205 (8)	0.0306 (7)	0.0015 (10)	-0.0034 (6)	0.0011 (8)
C1	0.0472 (19)	0.044 (2)	0.0487 (15)	0.0098 (15)	0.0061 (13)	0.0064 (13)
C2	0.0420 (17)	0.059 (2)	0.0639 (17)	0.0070 (17)	0.0159 (14)	-0.0038 (17)
C3	0.0436 (19)	0.0442 (18)	0.0443 (15)	-0.0146 (15)	0.0119 (13)	-0.0090 (14)
C4	0.061 (2)	0.073 (2)	0.0654 (19)	-0.028 (2)	0.0313 (18)	-0.0158 (19)
C5	0.086 (3)	0.070 (3)	0.056 (2)	-0.041 (2)	0.033 (2)	-0.0074 (19)
C6	0.096 (3)	0.056 (2)	0.0468 (18)	-0.020 (2)	0.0196 (19)	0.0072 (16)
C7	0.072 (2)	0.0434 (19)	0.0503 (18)	-0.0043 (17)	0.0166 (17)	0.0055 (15)
C8	0.0474 (19)	0.0300 (15)	0.0382 (14)	-0.0077 (14)	0.0104 (12)	0.0015 (13)
C9	0.0428 (17)	0.0304 (15)	0.0383 (14)	-0.0012 (13)	0.0087 (12)	0.0010 (13)
C10	0.0384 (16)	0.0185 (13)	0.0264 (11)	0.0001 (13)	0.0087 (11)	0.0025 (11)
C11	0.0413 (14)	0.0142 (13)	0.0323 (11)	0.0007 (12)	0.0030 (9)	0.0003 (11)

Geometric parameters (\AA , $^\circ$)

Co—N1 ⁱ	2.157 (2)	C3—C8	1.409 (4)
Co—N1	2.157 (2)	C3—C4	1.420 (4)
Co—O1	2.0740 (18)	C4—C5	1.354 (4)
Co—O1 ⁱ	2.0740 (18)	C4—H4	0.9300
Co—O1W ⁱ	2.1249 (14)	C5—C6	1.397 (5)
Co—O1W	2.1249 (14)	C5—H5	0.9300
N1—C9	1.314 (3)	C6—C7	1.367 (4)
N1—C1	1.363 (3)	C6—H6	0.9300
O1—C10	1.259 (3)	C7—C8	1.404 (4)
O2—C10	1.253 (3)	C7—H7	0.9300
O1W—H1A	0.8975	C8—C9	1.416 (3)
O1W—H1B	0.8743	C9—H9	0.9300
C1—C2	1.357 (3)	C10—C11	1.507 (3)
C1—H1	0.9300	C11—C11 ⁱⁱ	1.511 (4)
C2—C3	1.398 (4)	C11—H11A	0.9700
C2—H2	0.9300	C11—H11B	0.9700
O1—Co—O1 ⁱ	180.0	C2—C3—C4	123.6 (3)
O1—Co—O1W ⁱ	89.04 (7)	C8—C3—C4	118.9 (3)
O1 ⁱ —Co—O1W ⁱ	90.96 (7)	C5—C4—C3	119.6 (3)
O1—Co—O1W	90.96 (7)	C5—C4—H4	120.2
O1 ⁱ —Co—O1W	89.04 (7)	C3—C4—H4	120.2
O1W ⁱ —Co—O1W	180.0	C4—C5—C6	121.3 (3)
O1—Co—N1 ⁱ	87.33 (7)	C4—C5—H5	119.4
O1 ⁱ —Co—N1 ⁱ	92.67 (7)	C6—C5—H5	119.4
O1W ⁱ —Co—N1 ⁱ	91.76 (7)	C7—C6—C5	120.7 (3)

O1W—Co—N1 ⁱ	88.24 (7)	C7—C6—H6	119.7
O1—Co—N1	92.67 (7)	C5—C6—H6	119.7
O1 ⁱ —Co—N1	87.33 (7)	C6—C7—C8	119.5 (3)
O1W ⁱ —Co—N1	88.24 (7)	C6—C7—H7	120.3
O1W—Co—N1	91.76 (7)	C8—C7—H7	120.3
N1 ⁱ —Co—N1	180.0	C7—C8—C3	120.0 (2)
C9—N1—C1	117.7 (2)	C7—C8—C9	122.1 (3)
C9—N1—Co	123.03 (19)	C3—C8—C9	117.8 (2)
C1—N1—Co	119.26 (16)	N1—C9—C8	123.7 (3)
C10—O1—Co	131.47 (16)	N1—C9—H9	118.2
Co—O1W—H1A	120.6	C8—C9—H9	118.2
Co—O1W—H1B	105.9	O2—C10—O1	124.7 (2)
H1A—O1W—H1B	98.3	O2—C10—C11	118.2 (2)
C2—C1—N1	123.1 (2)	O1—C10—C11	117.2 (2)
C2—C1—H1	118.5	C10—C11—C11 ⁱⁱ	114.4 (2)
N1—C1—H1	118.5	C10—C11—H11A	108.7
C1—C2—C3	120.3 (3)	C11 ⁱⁱ —C11—H11A	108.7
C1—C2—H2	119.9	C10—C11—H11B	108.7
C3—C2—H2	119.9	C11 ⁱⁱ —C11—H11B	108.7
C2—C3—C8	117.4 (2)	H11A—C11—H11B	107.6

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

Hydrogen-bond geometry (\AA , $^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1W—H1A \cdots O2 ⁱⁱⁱ	0.90	1.89	2.774 (3)	169
O1W—H1B \cdots O2	0.87	1.90	2.689 (3)	150
C5—H5 \cdots O2 ^{iv}	0.93	2.56	3.487 (5)	176

Symmetry codes: (iii) $-x+1/2, y+1/2, -z+1/2$; (iv) $-x+1, -y+1, -z$.