Crystal structure of monoaqua(1,10-phenanthroline-*N*,*N*′)-succinatocobalt(II), $Co(H_2O)(C_{12}H_8N_2)(C_4H_4O_4)$

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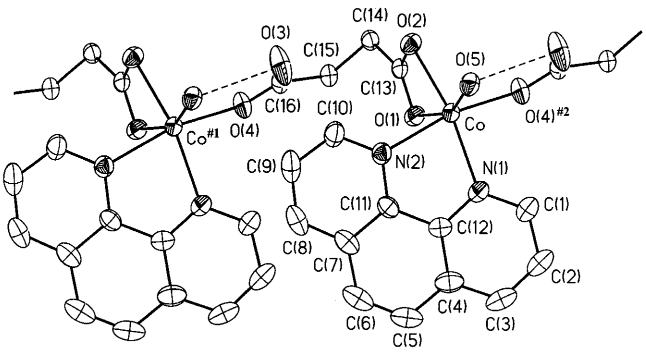

Abstract

$C_{16}H_{14}CoN_2O_5$, triclinic, $P\bar{1}$ (No. 2), $a = 7.499(1)$ Å, $b = 10.270(1)$ Å, $c = 10.490(1)$ Å, $\alpha = 97.65(1)°$, $\beta = 106.80(1)°$, $\gamma = 100.57(1)°$, $V = 745.3$ Å^3, $Z = 2$, $R_{gt}(F) = 0.058$, $wR_{ref}(F^2) = 0.151$, $T = 293$ K.

Source of material

Addition of 3.0 ml (1 M) Na_2CO_3 to a stirred aqueous solution of $Co(NO_3)_2 \cdot 6H_2O$ (0.734 g, 2.50 mmol) yielded red precipitate, which turned rapidly violet on standing. After centrifugation, the violet precipitate was added to a stirred mathanolic aqueous solution of phenanthroline monohydrate (0.50 g, 2.50 mmol) and succinic acid (0.30 g, 2.50 mmol) in 40 ml CH_3OH-H_2O (1:1 v/v). The resulting orange solution (pH = 6.29) was maintained at room temperature and slow evaporation affored rose-colored crystals (yield: over 85% based on the initial $Co(NO_3)_2 \cdot 6H_2O$ input).

Discussion

The crystal structure of the title compound consists of polymeric chains formulated as $_\infty^1[Co(H_2O)(phen)(C_4H_4O_4)_{2/2}]$ resulting from $[Co(H_2O)(phen)]^{2+}$ moieties bridged by succinate anions. Within the chains, the Co atoms are in the severely distorted octahedral sites defined by two N atoms of one phenanthroline ligand and three O atoms of one aqua ligand and two succinate anions. The Co—O bond distances vary from 2.037 Å to 2.190 Å and two Co—N bond lengths are equal to 2.125 Å and 2.147 Å, respectively. The cisoid bond angles around the Co atom fall in the region 60.6° – 105.0° and the transoid ones in the region 159.1° – 165.8°. Both terminal carboxylate groups of the gauche succinate anion function in different coordination modes, one monodentately bonded to one Co atom and the other chelating one Co atom. The succinato ligands are twisted with the torsion angle of 77.2(3)° due to weak intra-chain π-π stacking interactions between phenanthroline ligands (mean interplanar distance: 3.53 Å). The aqua ligand forms an intrachain hydrogen bond to the uncoordinationg carboxylate O atoms with $d(O5\cdots O3^{\#2}) = 2.628$ Å and $\angle O5–H\cdots O3^{\#2} = 158°$ (#2 = x+1, y, z) and a nearly linear interchain hydrogen bond to one chelating carboxylate O atom with $d(O5\cdots O2^{\#3}) = 2.695$ Å and $\angle O5–H\cdots O2^{\#3}) = 176°$ (#3 = $-x$+1, $-y$+1, $-z$+1). The interchain hydrogen bonds and interchain π-π stacking interactions between phenanthroline ligands (mean interplanar distances of 3.30 Å and 3.40 Å) are found to be responsible for supramolecular assembly of the polymeric chains, which extend along the [100] direction.

Table 1. Data collection and handling.

Crystal:	rose-colored block, size 0.29 × 0.38 × 0.56 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	11.82 cm^{-1}
Diffractometer, scan mode:	Bruker P4, $\theta/2\theta$
$2\theta_{max}$:	54.98°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4197, 3418
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3234
$N(param)_{refined}$:	228
Programs:	SHELXS-97 [1], SHELXL-97 [2]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1)	2*i*	1.1424	0.8652	0.8609	0.059
H(2)	2*i*	1.2968	1.0891	0.9517	0.059
H(3)	2*i*	1.1237	1.2524	0.9303	0.059
H(5)	2*i*	0.8048	1.3126	0.8268	0.059
H(6)	2*i*	0.4909	1.2440	0.7029	0.059
H(8)	2*i*	0.1994	1.0503	0.5688	0.059
H(9)	2*i*	0.0797	0.8222	0.4891	0.059
H(10)	2*i*	0.2790	0.6755	0.5366	0.059
H(14A)	2*i*	0.3975	0.4116	0.8982	0.037
H(14B)	2*i*	0.2467	0.3881	0.7532	0.037
H(15A)	2*i*	0.1494	0.4785	0.9431	0.037
H(15B)	2*i*	0.2887	0.6157	0.9518	0.037
HA	2*i*	0.696(7)	0.610(5)	0.465(5)	0.06(1)
HB	2*i*	0.856(7)	0.622(5)	0.550(5)	0.07(2)

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Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Co	2*i*	0.71530(4)	0.69178(3)	0.71243(3)	0.0225(2)	0.0266(3)	0.0301(3)	0.0054(2)	0.0061(2)	0.0054(1)
N(1)	2*i*	0.8862(3)	0.8925(2)	0.7818(2)	0.030(1)	0.032(1)	0.030(1)	0.0013(8)	0.0054(8)	0.0056(8)
N(2)	2*i*	0.5133(3)	0.8100(2)	0.6388(2)	0.029(1)	0.033(1)	0.035(1)	0.0074(9)	0.0080(9)	0.0105(9)
C(1)	2*i*	1.0718(4)	0.9309(3)	0.8498(3)	0.033(1)	0.043(2)	0.040(1)	0.000(1)	0.008(1)	0.008(1)
C(2)	2*i*	1.1658(5)	1.0657(4)	0.9053(3)	0.040(2)	0.050(2)	0.041(2)	–0.012(1)	0.005(1)	0.007(1)
C(3)	2*i*	1.0637(5)	1.1624(3)	0.8908(3)	0.060(2)	0.036(1)	0.037(1)	–0.012(1)	0.012(1)	0.001(1)
C(4)	2*i*	0.8674(5)	1.1262(3)	0.8161(3)	0.061(2)	0.032(1)	0.033(1)	0.004(1)	0.019(1)	0.005(1)
C(5)	2*i*	0.7509(6)	1.2211(3)	0.7917(4)	0.080(3)	0.029(1)	0.053(2)	0.012(2)	0.027(2)	0.003(1)
C(6)	2*i*	0.5636(6)	1.1799(3)	0.7183(4)	0.082(3)	0.042(2)	0.061(2)	0.033(2)	0.036(2)	0.016(2)
C(7)	2*i*	0.4734(5)	1.0401(3)	0.6636(3)	0.055(2)	0.043(2)	0.043(1)	0.026(1)	0.023(1)	0.017(1)
C(8)	2*i*	0.2791(5)	0.9909(4)	0.5871(4)	0.049(2)	0.064(2)	0.061(2)	0.035(2)	0.024(2)	0.027(2)
C(9)	2*i*	0.2083(5)	0.8559(4)	0.5400(4)	0.033(2)	0.073(2)	0.063(2)	0.021(2)	0.015(1)	0.030(2)
C(10)	2*i*	0.3299(4)	0.7678(3)	0.5685(3)	0.031(1)	0.045(2)	0.048(2)	0.007(1)	0.006(1)	0.016(1)
C(11)	2*i*	0.5854(4)	0.9440(3)	0.6868(3)	0.039(1)	0.032(1)	0.032(1)	0.014(1)	0.015(1)	0.0113(9)
C(12)	2*i*	0.7853(4)	0.9883(3)	0.7627(2)	0.041(1)	0.029(1)	0.027(1)	0.005(1)	0.013(1)	0.0062(9)
O(1)	2*i*	0.5653(3)	0.6604(2)	0.8607(2)	0.0297(9)	0.0306(9)	0.0330(9)	0.0031(7)	0.0081(7)	0.0015(7)
O(2)	2*i*	0.5034(3)	0.5087(2)	0.6771(2)	0.0302(9)	0.0345(9)	0.0317(9)	0.0020(7)	0.0118(7)	0.0022(7)
C(13)	2*i*	0.4726(3)	0.5483(2)	0.7869(2)	0.021(1)	0.028(1)	0.029(1)	0.0076(8)	0.0037(8)	0.0067(9)
C(14)	2*i*	0.3295(3)	0.4569(2)	0.8309(3)	0.025(1)	0.029(1)	0.032(1)	0.0086(9)	0.0086(9)	0.0086(9)
C(15)	2*i*	0.2071(3)	0.5334(3)	0.8905(2)	0.024(1)	0.034(1)	0.029(1)	0.0096(9)	0.0081(9)	0.0084(9)
C(16)	2*i*	0.0501(4)	0.5692(3)	0.7828(3)	0.025(1)	0.036(1)	0.035(1)	0.0093(9)	0.0078(9)	0.012(1)
O(3)	2*i*	0.0517(4)	0.5530(4)	0.6642(2)	0.057(2)	0.121(2)	0.037(1)	0.059(2)	0.019(1)	0.027(1)
O(4)	2*i*	–0.0708(3)	0.6167(2)	0.8241(2)	0.032(1)	0.049(1)	0.037(1)	0.0211(9)	0.0109(8)	0.0131(8)
O(5)	2*i*	0.7792(3)	0.6602(2)	0.5319(2)	0.0290(9)	0.040(1)	0.0293(9)	0.0065(8)	0.0056(7)	0.0049(8)

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