Crystal structure of (aqua)(benzimidazole-*N*)bis(2,4-pentanedionato-*O*,*O'*)cobalt(II), $C_{17}H_{22}CoN_2O_5$

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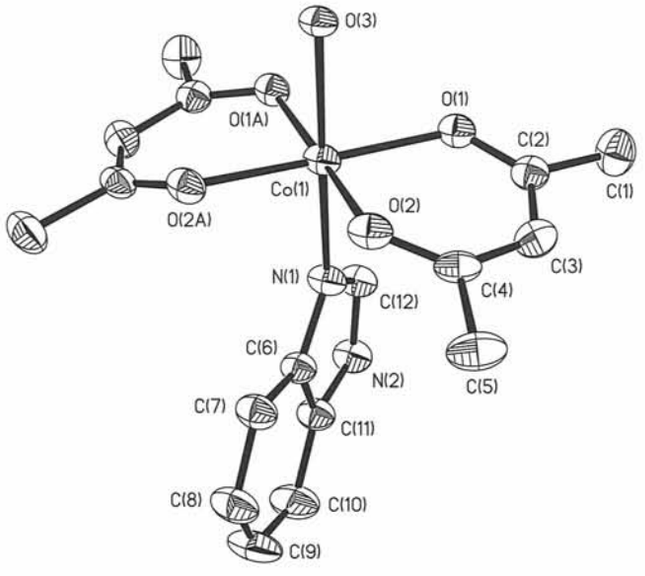

Abstract

$C_{17}H_{22}CoN_2O_5$, orthorhombic, *Pnma* (No. 62), a = 7.944(2) Å, b = 14.346(3) Å, c = 16.544(3) Å, V = 1885.5 Å^3, Z = 4, $R_{gt}(F)$ = 0.044, $wR_{ref}(F^2)$ = 0.123, T = 293 K.

Source of material

To a solution of 0.2 mmol bis(2,4-pentanedionato)cobalt(II) [1] in 10 mL 95% ethanol was added a solution of 0.2 mmol benzimidazole in 10 mL 95% ethanol dropwise with stirring. After stirring for 10 mim, the mixture was filtered to remove any insoluble material. The filtrate was allowed to stand for slow evaporation to provide the red prismatic crystals for the X-ray structure determination.

Discussion

The cobalt(II) complex of β-diketone has been found to catalyze the oxidation of olefins to ketones [2]. Two linear Co(II) complexes of $[Co(acac)_2pz]_n$ and $[Co(acac)_2(4,4'\text{-bipy})]_n$ were described in [3]. Previously, we reported two Co(II) complexes of β-diketones [4]. Here we report on a cobalt(II) complex with 2,4-pentanedione ligand.

The geometry around Co(II) is a distorted octahedral configuration. Four oxygen atoms from the 2,4-pentanediones are coordinated to Co(II), forming a *trans* CoO_4 equatorial plane. The axial positions are occupied by a nitrogen atom from the benzimidazole molecule and a oxygen atom from the water molecule, respectively. The bond lengths of Co1—O1 and Co1–O2 are 2.051(2) Å and 2.034(2) Å, respectively. The bond lengths are similar to those of 2.026(2) Å and 2.051(2) Å in $[Co(acac)2pz]_n$ [3], 2.022(5) Å and 2.029(5) Å in $[Co(acac)2(4,4'\text{-bipy})]_n$ [3], but longer than those of 1.917(3) Å and 1.921(3) Å in $Co(acac)_2$ [1]. The bond length of Co1—O3 is 2.211(3) Å. d(Co—O_{aqua}) is longer than for Co—$O_{carbonyl}$. The molecules pack as a one-dimensional infinite chain along the a axis because the complex molecules are connected to each orther through strong the intermolecular hydrogen bonds with d(O3-H···O1^a) = 2.765 Å and ∠O3–H···O1^a = 154.2°, d(N2–H···O3^b) = 2.890 Å and ∠N2–H···O3^b = 130.2°, respectively (a: x+1/2, y, –z+1/2, b: x–1, y, z).

Table 1. Data collection and handling.

Crystal:	red prism, size 0.25 × 0.30 × 0.40 mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ:	9.38 cm^{-1}
Diffractometer, scan mode:	Rigaku R-AXIS-RAPID, ω
$2\theta_{max}$:	54.96°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	2178, 2178
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1607
$N(param)_{refined}$:	131
Programs:	SHELXS-97 [5], SHELXL-97 [6]

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

Atom	Site	x	y	z	U_{iso}
H(0)	8*d*	0.4720	0.2946	0.2144	0.090
H(2)	4*c*	–0.4381	1/4	0.0667	0.087
H(1A)	8*d*	–0.0178	0.4647	0.2879	0.141
H(1B)	8*d*	0.0868	0.5502	0.2569	0.141
H(1C)	8*d*	–0.0875	0.5268	0.2174	0.141
H(3)	8*d*	0.1281	0.5429	0.0999	0.087
H(5A)	8*d*	0.3430	0.4464	–0.0661	0.142
H(5B)	8*d*	0.1836	0.5094	–0.0543	0.142
H(5C)	8*d*	0.3552	0.5379	–0.0146	0.142
H(7)	4*c*	0.1323	1/4	–0.0772	0.086
H(8)	4*c*	0.0029	1/4	–0.2045	0.111
H(9)	4*c*	–0.2843	1/4	–0.2175	0.139
H(10)	4*c*	–0.4606	1/4	–0.1057	0.121
H(12)	4*c*	–0.2093	1/4	0.1616	0.082

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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(1)	4*c*	0.19214(5)	1/4	0.12457(3)	0.0418(3)	0.0797(4)	0.0434(3)	0	0.0053(2)	0
O(1)	8*d*	0.1146(2)	0.3543(1)	0.20082(9)	0.0547(8)	0.077(1)	0.0520(8)	–0.0003(8)	0.0072(7)	0.0018(8)
O(2)	8*d*	0.2866(2)	0.3480(1)	0.0483(1)	0.0541(8)	0.094(1)	0.0515(9)	–0.0037(8)	0.0081(7)	0.0084(9)
O(3)	4*c*	0.4374(3)	1/4	0.1873(1)	0.048(1)	0.075(1)	0.050(1)	0	–0.007(1)	0
N(1)	4*c*	–0.0512(3)	1/4	0.0666(2)	0.042(1)	0.095(2)	0.046(1)	0	0.004(1)	0
N(2)	4*c*	–0.3281(3)	1/4	0.0537(2)	0.041(1)	0.104(2)	0.071(2)	0	0.003(1)	0
C(1)	8*d*	0.0123(4)	0.5008(2)	0.2412(2)	0.095(2)	0.089(2)	0.097(2)	0.010(2)	0.026(2)	–0.005(2)
C(2)	8*d*	0.0982(3)	0.4394(2)	0.1805(2)	0.046(1)	0.076(2)	0.067(2)	0.002(1)	–0.001(1)	0.001(1)
C(3)	8*d*	0.1530(3)	0.4781(2)	0.1080(2)	0.061(1)	0.079(2)	0.077(2)	0.001(1)	0.001(1)	0.014(1)
C(4)	8*d*	0.2405(3)	0.4322(2)	0.0463(2)	0.045(1)	0.094(2)	0.056(1)	–0.010(1)	–0.008(1)	0.018(1)
C(5)	8*d*	0.2842(4)	0.4864(3)	–0.0291(2)	0.077(2)	0.133(3)	0.074(2)	–0.011(2)	–0.002(2)	0.040(2)
C(6)	4*c*	–0.0905(4)	1/4	–0.0149(2)	0.047(2)	0.074(2)	0.055(2)	0	–0.002(1)	0
C(7)	4*c*	0.0119(5)	1/4	–0.0822(2)	0.062(2)	0.098(3)	0.054(2)	0	0.007(2)	0
C(8)	4*c*	–0.0656(7)	1/4	–0.1567(3)	0.094(3)	0.133(4)	0.052(2)	0	0.007(2)	0
C(9)	4*c*	–0.2360(8)	1/4	–0.1643(3)	0.104(4)	0.181(6)	0.061(3)	0	–0.030(3)	0
C(10)	4*c*	–0.3405(6)	1/4	–0.0995(3)	0.065(2)	0.155(5)	0.083(3)	0	–0.025(2)	0
C(11)	4*c*	–0.2655(5)	1/4	–0.0235(2)	0.052(2)	0.091(3)	0.062(2)	0	–0.003(2)	0
C(12)	4*c*	–0.1972(4)	1/4	0.1038(2)	0.047(2)	0.100(3)	0.057(2)	0	0.004(2)	0

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