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Crystal structure of *trans*-bis(*N*-cyclohexyl-3-methoxy-salicylideneiminato)cobalt(II), $Co(C_{14}H_{18}NO_2)_2$

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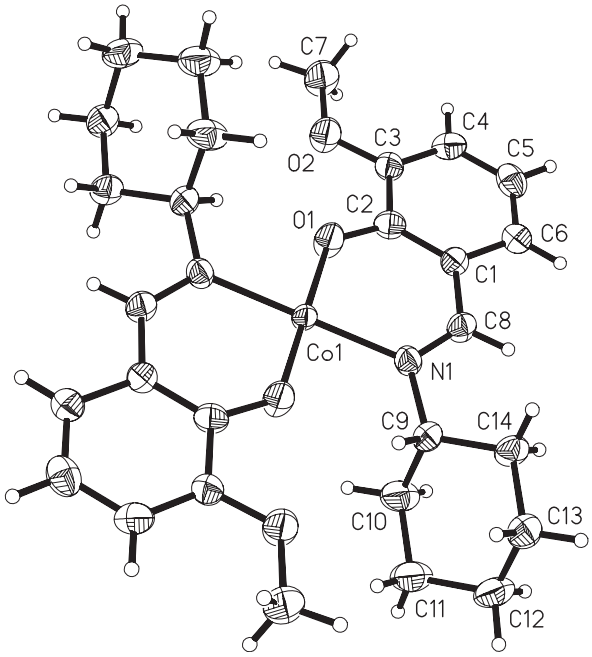

Abstract

$C_{28}H_{36}CoN_2O_4$, monoclinic, $P12_1/c1$ (no. 14), a = 11.054(2) Å, b = 18.062(4) Å, c = 6.474(3) Å, β = 100.02(2)°, V = 1272.9 Å^3, Z = 2, $R_{gt}(F)$ = 0.079, $wR_{ref}(F^2)$ = 0.198, T = 298 K.

Source of material

Reagents and solvents used were of commercially available quality. 3-Methoxy-2-hydroxybenzaldehyde (0.2 mmol, 30.5 mg) and cyclohexylamine (0.2 mmol, 19.8 mg) were dissolved in methanol (10 ml). The mixture was stirred for 30 min at room temperature. To the above solution was added with stirring a methanol solution (5 ml) of cobalt(II) acetate hexahydrate (0.1 mmol, 29.1 mg). The final mixture was stirred at room temperature for another 30 min and filtered. Small block-shaped crystals, suitable for X-ray structural determination were formed by slow evaporation of the filtrate for about a week.
Elemental analysis – found: C, 64.01 %; H, 7.02 %; N, 5.23 %; calc. for $C_{28}H_{36}CoN_2O_4$: C, 64.24 %; H, 6.93 %; N, 5.35 %.

Experimental details

The H atoms were positioned geometrically and constrained as riding atoms, with C—H distances of 0.93 Å – 0.97 Å and U_{iso}(H) set to 1.2 or 1.5U_{eq}(C) of the parent atoms. The value of R_{int} is 0.23, and the ratio of observed to unique reflections is low (38 %), probably due to the poor diffraction quality of the crystal.

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Discussion

The design of multidentate ligands and their metallosupramolecular chemistry are of great interest in the last few years [1-3]. The condensation reaction of an aromatic carbaldehyde with a primary amine has been shown to offer an easy and inexpensive way of forming a variety of polydentate Schiff base ligands. It has previously been shown that such ligands readily lead to the formation of diverse complexes [4,5].
The Co^{II} ion in the mononuclear title complex, lying on the inversion center, is tetra-coordinated by two imine N and two phenol-ate O atoms from two Schiff base ligands, forming a square planar environment. All the bond values subtended at the metal center are typical and comparable to those observed in other similar complexes [4,5]. As expected, the cyclohexyl groups in the complex adopt chair conformations to minimize steric effects. The title crystal structure is isostructural with the copper(II) analogue [6] and similar to other copper(II) complexes reported previously [7].

Table 1. Data collection and handling.

Crystal:	red block, size 0.02 × 0.08 × 0.09 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	7.11 cm^{-1}
Diffractometer, scan mode:	Siemens P4, ω
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	9320, 237
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 911
$N(param)_{refined}$:	162
Program:	SHELXTL [8]

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

Atom	Site	x	y	z	U_{iso}
H(4)	4*e*	0.7248	0.2162	–0.5574	0.073
H(5)	4*e*	0.9043	0.2110	–0.3190	0.077
H(6)	4*e*	0.9180	0.1367	–0.0220	0.068
H(7A)	4*e*	0.5202	0.2395	–0.6983	0.127
H(7B)	4*e*	0.4280	0.1816	–0.8180	0.127
H(7C)	4*e*	0.5693	0.1734	–0.8170	0.127
H(8)	4*e*	0.8347	0.0499	0.1794	0.061
H(9)	4*e*	0.6499	–0.0502	0.4065	0.065
H(10A)	4*e*	0.8159	–0.1178	0.1816	0.092
H(10B)	4*e*	0.6767	–0.1394	0.1601	0.092
H(11A)	4*e*	0.7062	–0.1834	0.5029	0.100
H(11B)	4*e*	0.8049	–0.2215	0.3914	0.100
H(12A)	4*e*	0.8915	–0.1779	0.7313	0.090
H(12B)	4*e*	0.9574	–0.1437	0.5577	0.090
H(13A)	4*e*	0.9202	–0.0487	0.7810	0.076
H(13B)	4*e*	0.7799	–0.0692	0.7486	0.076
H(14A)	4*e*	0.8096	0.0330	0.5315	0.068
H(14B)	4*e*	0.8992	–0.0147	0.4224	0.068

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)	2*b*	½	0	0	0.0376(9)	0.0456(9)	0.0358(9)	–0.0049(9)	0.0012(6)	0.0117(9)
O(1)	4*e*	0.5332(5)	0.0641(3)	–0.2126(8)	0.055(4)	0.101(5)	0.057(4)	–0.022(3)	–0.001(3)	0.044(3)
O(2)	4*e*	0.5202(6)	0.1437(3)	–0.5481(9)	0.065(4)	0.092(4)	0.061(4)	–0.015(4)	0.002(3)	0.027(4)
N(1)	4*e*	0.6759(5)	0.0039(4)	0.1464(8)	0.049(4)	0.050(4)	0.045(4)	–0.010(4)	0.006(3)	0.004(4)
C(1)	4*e*	0.7419(7)	0.0963(4)	–0.088(1)	0.052(6)	0.048(5)	0.035(5)	–0.002(4)	0.006(4)	–0.002(4)
C(2)	4*e*	0.6329(8)	0.0992(4)	–0.231(1)	0.064(7)	0.056(6)	0.047(6)	–0.005(5)	0.009(5)	0.017(5)
C(3)	4*e*	0.6297(8)	0.1443(5)	–0.414(1)	0.057(6)	0.053(5)	0.054(6)	–0.008(5)	0.003(5)	0.010(5)
C(4)	4*e*	0.7297(8)	0.1858(4)	–0.440(1)	0.065(7)	0.057(6)	0.064(7)	0.011(5)	0.018(5)	0.013(5)
C(5)	4*e*	0.8370(8)	0.1831(5)	–0.297(2)	0.063(7)	0.057(6)	0.077(7)	–0.008(5)	0.024(6)	–0.017(5)
C(6)	4*e*	0.8454(8)	0.1386(4)	–0.119(1)	0.059(6)	0.051(5)	0.060(6)	–0.002(5)	0.009(5)	–0.001(5)
C(7)	4*e*	0.5085(8)	0.1883(5)	–0.736(1)	0.092(8)	0.098(8)	0.056(6)	–0.012(6)	–0.007(5)	0.028(6)
C(8)	4*e*	0.7583(8)	0.0488(4)	0.092(1)	0.055(5)	0.059(6)	0.035(5)	–0.002(5)	0.002(4)	0.005(4)
C(9)	4*e*	0.7189(7)	–0.0447(4)	0.331(1)	0.053(5)	0.057(5)	0.048(5)	–0.001(4)	–0.004(4)	0.006(5)
C(10)	4*e*	0.7473(9)	–0.1208(4)	0.256(1)	0.118(9)	0.049(6)	0.054(6)	0.007(5)	–0.010(6)	–0.008(5)
C(11)	4*e*	0.7792(9)	–0.1745(4)	0.442(1)	0.115(9)	0.059(6)	0.068(7)	0.012(6)	–0.005(6)	0.009(6)
C(12)	4*e*	0.8808(8)	–0.1449(5)	0.611(1)	0.090(8)	0.070(7)	0.059(6)	0.020(6)	–0.004(6)	0.013(5)
C(13)	4*e*	0.8516(7)	–0.0676(4)	0.681(1)	0.066(6)	0.069(7)	0.053(6)	0.000(5)	0.003(5)	0.003(5)
C(14)	4*e*	0.8267(7)	–0.0167(4)	0.488(1)	0.066(5)	0.064(6)	0.039(5)	0.002(5)	0.005(4)	0.011(4)

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