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Crystal structure of bis{2-(((4-(1-(hydroxyl-imino)ethyl)phenyl)imino)methyl)phenolato- $\kappa^2 N, O$ } cobalt(II), $C_{30}H_{26}CoN_4O_4$

Table 1: Data collection and handling.

Crystal:	Red block
Size:	0.19 × 0.17 × 0.14 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.71 mm ⁻¹
Diffractometer, scan mode:	Bruker D8 Venture, φ and ω
$\theta_{\max}$, completeness:	25.4°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	27339, 4709, 0.045
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3751
$N(\text{param})_{\text{refined}}$:	358
Programs:	Bruker [1], SHELX [2]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.74731(2)	0.43934(2)	0.37733(2)	0.02373(11)
O1	0.82360(11)	0.48662(9)	0.45013(10)	0.0286(4)
N1	0.69604(12)	0.38128(10)	0.45953(12)	0.0237(4)
C1	0.83809(15)	0.47118(13)	0.52682(15)	0.0263(5)
N2	0.41722(13)	0.14739(12)	0.40231(13)	0.0338(5)
O2	0.34500(12)	0.11064(11)	0.37963(12)	0.0447(5)
H2A	0.3426(11)	0.0684(18)	0.4111(18)	0.067*
C2	0.90436(18)	0.50524(14)	0.56937(17)	0.0350(7)
H2	0.937538	0.537733	0.542337	0.042*
O3	0.67156(11)	0.48823(9)	0.30517(10)	0.0297(4)
N3	0.79967(12)	0.38342(10)	0.29381(12)	0.0253(5)
C3	0.92185(19)	0.49228(16)	0.64930(18)	0.0427(8)
H3	0.967406	0.515582	0.676229	0.051*
N4	1.07329(14)	0.14491(12)	0.35527(13)	0.0358(5)
O4	1.14596(13)	0.10895(11)	0.37776(12)	0.0467(5)
H4A	1.1487(11)	0.0666(19)	0.3468(19)	0.070*
C4	0.87437(18)	0.44583(16)	0.69170(17)	0.0407(7)
H4	0.886542	0.437708	0.747111	0.049*
C5	0.80956(17)	0.41208(14)	0.65142(16)	0.0336(6)
H5	0.776474	0.380674	0.680085	0.040*
C6	0.79016(15)	0.42230(13)	0.56881(15)	0.0261(5)
C7	0.72269(15)	0.38164(12)	0.53407(15)	0.0261(5)
H7	0.694614	0.351927	0.569231	0.031*
C8	0.62912(15)	0.33508(13)	0.43514(14)	0.0252(5)
C9	0.62881(15)	0.26510(13)	0.45680(15)	0.0288(6)
H9	0.673686	0.246452	0.489409	0.035*
C11	0.49572(15)	0.24892(13)	0.38429(15)	0.0253(5)
C10	0.56331(15)	0.22277(13)	0.43094(15)	0.0291(6)
H10	0.564249	0.174841	0.445179	0.035*
C12	0.49805(16)	0.31873(13)	0.36151(16)	0.0299(6)

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Abstract

$C_{30}H_{26}CoN_4O_4$, monoclinic, $C2/c$ (no. 15), $a = 16.0520(5)$ Å, $b = 19.1890(5)$ Å, $c = 16.7292(4)$ Å, $\beta = 93.064(1)^\circ$, $Z = 8$, $V = 5145.6(2)$ Å³, $R_{\text{gt}}(F) = 0.0400$, $wR_{\text{ref}}(F^2) = 0.0932$, $T = 173(2)$ K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
H12	0.453237	0.337502	0.328924	0.036*
C13	0.56450(16)	0.36123(13)	0.38553(16)	0.0300(6)
H13	0.565820	0.408299	0.368023	0.036*
C14	0.42261(16)	0.20464(13)	0.36227(15)	0.0278(6)
C15	0.35862(18)	0.22933(16)	0.30051(18)	0.0426(7)
H15A	0.383966	0.233235	0.248685	0.064*
H15B	0.337534	0.274997	0.316140	0.064*
H15C	0.312400	0.195941	0.296192	0.064*
C16	0.66026(15)	0.47724(13)	0.22702(15)	0.0260(5)
C17	0.59728(17)	0.51499(14)	0.18439(17)	0.0328(6)
H17	0.564443	0.547141	0.212276	0.039*
C18	0.58212(18)	0.50647(15)	0.10338(18)	0.0379(7)
H18	0.539406	0.532960	0.076151	0.045*
C19	0.62876(18)	0.45935(15)	0.06070(17)	0.0382(7)
H19	0.617721	0.453252	0.004779	0.046*
C20	0.69052(17)	0.42210(14)	0.10042(16)	0.0332(6)
H20	0.722803	0.390607	0.071048	0.040*
C21	0.70810(15)	0.42884(13)	0.18410(15)	0.0271(5)
C22	0.77454(16)	0.38646(13)	0.21899(15)	0.0275(6)
H22	0.803045	0.357581	0.183279	0.033*
C23	0.86621(15)	0.33682(13)	0.31798(14)	0.0261(5)
C24	0.86606(16)	0.26708(13)	0.29573(15)	0.0296(6)
H24	0.820763	0.248770	0.263397	0.035*
C25	0.93149(16)	0.22441(13)	0.32047(15)	0.0304(6)
H25	0.930426	0.176725	0.305201	0.036*
C26	0.99954(16)	0.24982(13)	0.36763(15)	0.0274(5)
C27	0.99701(16)	0.31923(14)	0.39149(16)	0.0329(6)
H27	1.041568	0.337521	0.424792	0.039*
C28	0.93112(16)	0.36212(13)	0.36779(17)	0.0323(6)
H28	0.930272	0.409091	0.385675	0.039*
C29	1.07295(16)	0.20528(13)	0.38951(15)	0.0286(6)
C30	1.14302(18)	0.23117(16)	0.44496(17)	0.0414(7)
H30A	1.196566	0.218239	0.423624	0.062*
H30B	1.138546	0.210138	0.497941	0.062*
H30C	1.139629	0.281996	0.449455	0.062*

Source of material

Synthesis of the title complex was prepared by a similar method reported earlier [3, 4] and the ligand was prepared according to the literature reported earlier [5]. A solution of cobalt acetate tetrahydrate (249.08 mg, 1 mmol) in MeOH (2 mL) was added to a stirring solution of the educt 1-(4-((2-hydroxybenzylidene)amino)phenyl)ethan-1-one oxime (254.30 mg, 1 mmol) in CH₂Cl₂ (2 mL). The mixture was continuously stirred for 1 h at room temperature. The product was filtered and the filtrate was allowed to stand at room temperature 20 days in a quiet environment. Several clear light red block crystals were obtained. **Anal. Calcd.** for C₃₀H₂₆CoN₄O₄: C, 63.72%; H, 4.63%; N, 9.91%. Found: C, 63.56%; H, 4.81%; N, 9.33%.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

The transition metal complexes based on Schiff bases ligand have also attracted considerable attention in the past decade [6, 7]. Cobalt complexes show effective applications in various fields of scientific research [8, 9]. For example, the cobalt complex based on Schiff base are widely utilized in magnetic [10, 11], luminescence materials [12, 13] and supramolecular constructing [13, 14] fields and so on.

The crystal structure of the title compound was determined by X-ray crystallography. Co1 is four-coordinated by two O atoms and two N atoms forming a N₂O₂ coordination mode. The bond lengths of Co1–O1 is 1.9096(17) Å and the Co1–O3 is 1.9128(18) Å. And the bond lengths of Co1–N1 is 1.983(2) Å and the Co1–N3 is 1.984(2) Å. On the other hand, the angles of N1–Co1–O1 is 95.76(8)° and O1–Co1–O3 is 122.27(7)°. Compared with other similar structures, all geometric parameters are in the typical ranges [3, 4].

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