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Synthesis and crystal structure of bis{2-((*E*)-((4-((*E*)-1-(methoxyimino)ethyl)phenyl)imino)methyl) phenolato- $\kappa^2 N,O$ }cobalt(II) – ethanol (1/1), $C_{34}H_{36}CoN_4O_5$

Table 1: Data collection and handling.

Crystal:	Yellow
Size:	0.28 × 0.28 × 0.26 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.60 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II CCD, φ and ω
$\theta_{\max}$, completeness:	26.5°, 99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	9989, 6366, 0.031
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 4614
$N(\text{param})_{\text{refined}}$:	424
Programs:	Bruker [1], Olex2 [2], SHELX [3]

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Abstract

$C_{34}H_{36}CoN_4O_5$, triclinic, $P\bar{1}$ (no. 2), $a = 8.7040(5)$ Å, $b = 12.7375(9)$ Å, $c = 14.2626(9)$ Å, $\alpha = 99.054(2)^\circ$, $\beta = 95.727(2)^\circ$, $\gamma = 92.477(2)^\circ$, $V = 1550.96(17)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0554$, $wR_{\text{ref}}(F^2) = 0.1369$, $T = 296(2)$ K.

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The asymmetric unit of the title crystal structure is shown in the figure (The disorder isn't shown for clarity.). Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

All solvents and other reagents were of analytical grade. The ligand 4-amino acetophenone methoxy oxime (HL) was

synthesized in accordance with a similar method reported earlier [4]. To a stirring solution of HL (268.32 mg, 1 mmol) in chloroform (3 mL) was added cobalt acetate tetrahydrate (249.08 mg, 1 mmol) in ethanol (2 mL). Afterwards the mixture was stirred for about 10 min at room temperature. The mixture was filtered and the filtrate was allowed to stand at room temperature for about 1 week. The solvent was partially evaporated and clear light yellow single crystals were obtained. Elemental analysis – Anal. Calcd. for $C_{34}H_{36}CoN_4O_5$: C, 63.85%; H, 5.67%; N, 8.76%; Co, 9.21%. Found: C, 63.96%; H, 5.74%; N, 8.69%; Co, 9.03%.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms. A part of the complex appeared to be disordered (Table 2).

Comment

As we know, oxime-type ligands with interesting properties have been widely studied for many decades [5, 6], and their metal complexes have been playing an important part in the development of modern coordination chemistry, because they could be used as supramolecular tectons [7–10], in the electrochemistry fields [11], as magnetic materials [12, 13], in the area of molecular recognition [14, 15]. Such complexes may have biological activities [16, 17], and optical properties [18, 19], and so on.

The title complex is built up by the $C_{34}H_{36}CoN_4O_5$ and ethanol molecules, in which all bond lengths are within the normal ranges (cf. the figure) [4]. Each Co1 is four-coordinated by two O atoms and two N atoms from two

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

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
Co1	0.85818(5)	0.47804(4)	0.29908(3)	0.02922(14)
O1	0.7061(3)	0.58043(18)	0.31753(15)	0.0393(6)
O2	0.1876(3)	−0.0786(2)	0.1251(2)	0.0546(7)
O3	1.0626(3)	0.52369(19)	0.27987(16)	0.0392(6)
O4	1.3037(3)	−0.04295(19)	0.57759(16)	0.0417(6)
O5 ^a	0.8805(12)	0.7104(6)	0.1958(6)	0.072(4)
H5A ^a	0.844300	0.661072	0.218990	0.108*
O5A ^b	0.6575(7)	0.6943(4)	0.1746(3)	0.078(2)
H5AA ^b	0.679349	0.652336	0.211293	0.117*
N1	0.8463(3)	0.4229(2)	0.42139(17)	0.0271(6)
N2	1.2128(3)	0.0449(2)	0.56962(19)	0.0326(7)
N3	0.8172(3)	0.3771(2)	0.17564(18)	0.0299(6)
N4	0.3205(4)	−0.0102(2)	0.1339(2)	0.0445(8)
C1	0.6527(4)	0.6144(3)	0.4001(2)	0.0312(7)
C2	0.5574(4)	0.7019(3)	0.4060(3)	0.0362(8)
H2	0.535237	0.734208	0.352510	0.043*
C3	0.4970(4)	0.7399(3)	0.4891(3)	0.0384(9)
H3	0.433970	0.797161	0.490964	0.046*
C4	0.5287(4)	0.6943(3)	0.5699(3)	0.0455(10)
H4	0.488514	0.721113	0.626264	0.055*
C5	0.6202(4)	0.6089(3)	0.5664(3)	0.0449(10)
H5	0.640487	0.577739	0.620699	0.054*
C6	0.6842(4)	0.5674(3)	0.4819(2)	0.0326(8)
C7	0.7738(4)	0.4757(3)	0.4881(2)	0.0344(8)
H7	0.781051	0.451299	0.546403	0.041*
C8	0.9267(4)	0.3316(3)	0.4411(2)	0.0290(7)
C9	0.9396(4)	0.2954(3)	0.5275(2)	0.0311(7)
H9	0.890606	0.330036	0.577633	0.037*
C10	1.0239(4)	0.2088(3)	0.5409(2)	0.0345(8)
H10	1.031406	0.186811	0.600282	0.041*
C11	1.0983(4)	0.1532(2)	0.4678(2)	0.0286(7)
C12	1.0849(5)	0.1903(3)	0.3824(2)	0.0546(12)
H12	1.134000	0.155821	0.332262	0.066*
C13	1.0008(5)	0.2771(3)	0.3682(3)	0.0577(13)
H13	0.993885	0.299300	0.308895	0.069*
C14	1.1919(4)	0.0616(3)	0.4834(2)	0.0300(7)
C15	1.2568(5)	−0.0035(3)	0.4010(3)	0.0543(12)
H15A	1.346786	0.033940	0.385871	0.081*
H15B	1.180373	−0.015485	0.346464	0.081*
H15C	1.284760	−0.070700	0.418013	0.081*
C16	1.3231(5)	−0.0554(3)	0.6758(3)	0.0570(12)
H16A	1.376426	−0.118740	0.682209	0.085*
H16B	1.223574	−0.061071	0.698717	0.085*
H16C	1.382461	0.005262	0.712477	0.085*
C17	1.1256(4)	0.5057(2)	0.1994(2)	0.0321(8)
C18	1.2677(4)	0.5598(3)	0.1934(3)	0.0421(9)
H18	1.314275	0.606453	0.246365	0.051*
C19	1.3393(5)	0.5452(3)	0.1110(3)	0.0467(10)
H19	1.432399	0.582969	0.108843	0.056*
C20	1.2746(5)	0.4747(3)	0.0308(3)	0.0485(11)
H20	1.324167	0.464805	−0.024454	0.058*
C21	1.1375(4)	0.4202(3)	0.0344(2)	0.0414(9)
H21	1.095097	0.372634	−0.019057	0.050*
C22	1.0573(4)	0.4337(3)	0.1169(2)	0.0326(8)
C23	0.9133(4)	0.3742(3)	0.1112(2)	0.0326(8)

Table 2 (continued)

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
H23	0.884471	0.327719	0.054433	0.039*
C24	0.6848(4)	0.3044(3)	0.1574(2)	0.0311(8)
C25	0.6911(4)	0.1977(3)	0.1164(2)	0.0353(8)
H25	0.783501	0.172962	0.096538	0.042*
C26	0.5622(4)	0.1290(3)	0.1051(2)	0.0387(9)
H26	0.569066	0.058350	0.077811	0.046*
C27	0.4207(4)	0.1628(3)	0.1336(2)	0.0329(8)
C28	0.4151(4)	0.2704(3)	0.1723(2)	0.0371(8)
H28	0.321789	0.295916	0.189674	0.044*
C29	0.5443(4)	0.3393(3)	0.1852(2)	0.0351(8)
H29	0.537704	0.409929	0.212698	0.042*
C30	0.2862(4)	0.0860(3)	0.1260(2)	0.0381(8)
C31	0.1227(4)	0.1191(3)	0.1121(3)	0.0473(10)
H31A	0.074880	0.085840	0.050407	0.071*
H31B	0.123490	0.195101	0.116321	0.071*
H31C	0.065541	0.097529	0.160733	0.071*
C32	0.2366(6)	−0.1795(3)	0.1460(3)	0.0611(12)
H32A	0.310239	−0.205577	0.103486	0.092*
H32B	0.148699	−0.229506	0.137850	0.092*
H32C	0.283727	−0.170825	0.210792	0.092*
C33	0.7772(7)	0.7827(5)	0.1905(3)	0.0923(19)
H33A ^a	0.736528	0.788514	0.251837	0.111*
H33B ^a	0.840715	0.847928	0.193699	0.111*
H33C ^b	0.770617	0.826982	0.251654	0.111*
H33D ^b	0.879020	0.754603	0.191175	0.111*
C34A ^b	0.7541(10)	0.8458(5)	0.1145(4)	0.054(2)
H34A ^b	0.840043	0.896865	0.119122	0.081*
H34B ^b	0.660486	0.882410	0.120221	0.081*
H34C ^b	0.746385	0.799916	0.053756	0.081*
C34 ^a	0.6452(14)	0.7978(11)	0.1273(9)	0.061(4)
H34D ^a	0.659320	0.864329	0.104721	0.092*
H34E ^a	0.554630	0.798453	0.160555	0.092*
H34F ^a	0.632938	0.740664	0.073944	0.092*

^aOccupancy: 0.354(6), ^bOccupancy: 0.646(6).

deprotonated ligand L-ligands. There are strong intermolecular O5A–H5AA ··· O1, C3–H3 ··· O4, hydrogen bonds involving the ethanol molecule too.

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