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Crystal structure of 1,1'-((1*E*,1'*E*)-(((ethane-1,2-diylbis(oxy)))bis(2,1-phenylene)))bis(azanylylidene))bis(methanylylidene))bis(naphthalen-2-olato)cobalt(II), C₃₆H₂₆N₂O₄Co

The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Purple block
Size:	0.21 × 0.20 × 0.19 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.68 mm ⁻¹
Diffractometer, scan mode:	Bruker SMART, φ and ω -scans
$\theta_{\max}$, completeness:	25°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	32111, 7156, 0.050
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 5310
$N(\text{param})_{\text{refined}}$:	582
Programs:	Bruker programs [1], SHELX [2]

Source of material

The organic ligand *N,N'*-bis(naphthaldehyde)-1,4-bis(*o*-aminophenoxy)butane (*H₂L*) was prepared by a standard Schiff base condensation reaction of 2-hydroxy-1-naphthaldehyde (1.722 g, 10 mmol) and 1,4-bis(*o*-aminophenoxy)butane (1.222 g, 5 mmol) according to previously reported procedure [3, 4]. The title compound was prepared by a vapor diffusion method. To a dichloromethane (15 mL) solution of (*H₂L*) (0.554 g, 1 mmol), an ethanol solution (15 mL) of cobalt(II) acetate tetrahydrate (0.2496 mg, 1 mmol) was added slowly under vigorously stirring and then continued stirring for 30 min to afford a clear violet solution. The mixture was filtered and the filtrate was shelved in a closed container filled with diethyl ether atmosphere for two days, and the well shaped purple granulometric crystals were obtained in a yield of 32% (based on Co).

Experimental details

All of the hydrogen atoms were placed in the calculated positions and all the non-hydrogen atoms were refined anisotropically.

Discussion

During the past decades, many chemists have focused their efforts on the synthesis and investigation of Schiff bases and

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Abstract

C₃₆H₂₆N₂O₄Co, monolinic, *C*2/*c* (no. 15), *a* = 43.230(14) Å, *b* = 17.100(6) Å, *c* = 11.275(4) Å, β = 103.112(4)°, *V* = 8118(5) Å³, *Z* = 12, *R*_{gt}(*F*) = 0.0370, *wR*_{ref}(*F*²) = 0.0931, *T* = 100(2) K.

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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	0.174951(7)	0.254278(18)	0.78475(3)	0.02584(10)
Co2	0.0000	0.13815(3)	0.7500	0.03363(14)
N1	0.12734(4)	0.27720(11)	0.70968(17)	0.0257(5)
N2	0.22283(4)	0.22666(11)	0.83678(16)	0.0224(4)
N3	0.04827(4)	0.13234(11)	0.81174(18)	0.0277(5)
O1	0.17368(4)	0.33462(10)	0.91089(15)	0.0355(4)
O2	0.16627(4)	0.20569(9)	0.58732(14)	0.0300(4)
O3	0.19777(4)	0.34027(9)	0.67888(14)	0.0288(4)
O4	0.16510(4)	0.15308(10)	0.85239(17)	0.0404(5)
O5	−0.00271(4)	0.20461(12)	0.8900(2)	0.0614(6)
O6	0.01242(4)	0.03260(10)	0.64867(15)	0.0315(4)
C1	0.15042(6)	0.37834(14)	0.9295(2)	0.0303(6)
C2	0.15810(6)	0.43573(16)	1.0242(2)	0.0388(7)
H2A	0.1796	0.4425	1.0658	0.047*
C3	0.13542(7)	0.48068(16)	1.0559(3)	0.0438(7)
H3A	0.1415	0.5180	1.1194	0.053*
C4	0.10297(7)	0.47348(15)	0.9968(2)	0.0369(7)
C5	0.07942(8)	0.51742(18)	1.0360(3)	0.0536(8)
H5A	0.0857	0.5533	1.1014	0.064*
C6	0.04822(8)	0.5098(2)	0.9829(3)	0.0614(9)
H6A	0.0328	0.5402	1.0101	0.074*
C7	0.03907(7)	0.4570(2)	0.8881(3)	0.0585(9)
H7A	0.0172	0.4513	0.8508	0.070*
C8	0.06124(6)	0.41251(18)	0.8467(3)	0.0452(7)
H8A	0.0542	0.3767	0.7817	0.054*
C9	0.09398(6)	0.41935(15)	0.8991(2)	0.0329(6)
C10	0.11855(6)	0.37258(14)	0.8618(2)	0.0271(6)
C11	0.10938(6)	0.32343(14)	0.7578(2)	0.0274(6)
H11A	0.0875	0.3243	0.7185	0.033*
C12	0.11295(6)	0.23561(13)	0.6014(2)	0.0267(6)
C13	0.08041(6)	0.22450(15)	0.5558(2)	0.0360(6)
H13A	0.0658	0.2460	0.5983	0.043*
C14	0.06921(6)	0.18294(16)	0.4502(3)	0.0432(7)
H14A	0.0470	0.1768	0.4204	0.052*
C15	0.08977(7)	0.15006(16)	0.3872(3)	0.0449(7)
H15A	0.0818	0.1222	0.3137	0.054*
C16	0.12229(6)	0.15801(15)	0.4319(2)	0.0357(6)
H16A	0.1367	0.1346	0.3902	0.043*
C17	0.13356(5)	0.20023(14)	0.5375(2)	0.0279(6)
C18	0.18337(6)	0.24997(15)	0.5130(2)	0.0366(7)
H18A	0.1728	0.2442	0.4258	0.044*
H18B	0.2054	0.2302	0.5252	0.044*
C19	0.18365(6)	0.33407(15)	0.5495(2)	0.0361(6)
H19A	0.1961	0.3651	0.5027	0.043*
H19B	0.1617	0.3548	0.5318	0.043*
C20	0.23107(5)	0.33425(13)	0.7098(2)	0.0250(5)
C21	0.24955(6)	0.38679(14)	0.6628(2)	0.0316(6)
H21A	0.2398	0.4253	0.6058	0.038*
C22	0.28226(6)	0.38273(15)	0.6997(2)	0.0340(6)
H22A	0.2952	0.4184	0.6680	0.041*
C23	0.29606(6)	0.32658(14)	0.7827(2)	0.0307(6)
H23A	0.3185	0.3240	0.8083	0.037*
C24	0.27753(5)	0.27390(13)	0.8293(2)	0.0264(6)
H24A	0.2875	0.2354	0.8861	0.032*
C25	0.24443(5)	0.27665(13)	0.7938(2)	0.0219(5)

Table 2 (continued)

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
C26	0.23420(5)	0.16604(13)	0.9037(2)	0.0235(5)
H26A	0.2567	0.1613	0.9241	0.028*
C27	0.21717(5)	0.10631(13)	0.9497(2)	0.0221(5)
C28	0.23523(5)	0.04686(13)	1.0295(2)	0.0231(5)
C29	0.26875(5)	0.04690(14)	1.0689(2)	0.0270(6)
H29A	0.2805	0.0882	1.0437	0.032*
C30	0.28482(6)	−0.01107(14)	1.1426(2)	0.0329(6)
H30A	0.3073	−0.0091	1.1672	0.039*
C31	0.26843(6)	−0.07272(15)	1.1815(2)	0.0386(7)
H31A	0.2796	−0.1133	1.2308	0.046*
C32	0.23595(6)	−0.07374(15)	1.1474(2)	0.0352(6)
H32A	0.2247	−0.1152	1.1745	0.042*
C33	0.21888(6)	−0.01487(13)	1.0731(2)	0.0261(6)
C34	0.18529(6)	−0.01546(14)	1.0424(2)	0.0317(6)
H34A	0.1743	−0.0559	1.0735	0.038*
C35	0.16850(6)	0.03974(14)	0.9703(2)	0.0327(6)
H35A	0.1460	0.0367	0.9514	0.039*
C36	0.18347(5)	0.10325(14)	0.9207(2)	0.0276(6)
C37	0.01972(6)	0.23758(15)	0.9710(3)	0.0448(8)
C38	0.00989(7)	0.28810(18)	1.0564(3)	0.0589(9)
H38A	−0.0122	0.2952	1.0513	0.071*
C39	0.03087(7)	0.32580(18)	1.1438(3)	0.0575(9)
H39A	0.0232	0.3596	1.1976	0.069*
C40	0.06417(7)	0.31668(16)	1.1582(3)	0.0425(7)
C41	0.08559(7)	0.35791(17)	1.2506(3)	0.0493(8)
H41A	0.0775	0.3913	1.3038	0.059*
C42	0.11762(8)	0.35045(17)	1.2647(3)	0.0514(8)
H42A	0.1319	0.3787	1.3265	0.062*
C43	0.12902(7)	0.30069(16)	1.1871(2)	0.0450(7)
H43A	0.1513	0.2948	1.1970	0.054*
C44	0.10896(6)	0.25986(15)	1.0964(2)	0.0370(7)
H44A	0.1177	0.2262	1.0455	0.044*
C45	0.07560(6)	0.26655(14)	1.0768(2)	0.0325(6)
C46	0.05273(6)	0.22593(14)	0.9800(2)	0.0312(6)
C47	0.06464(6)	0.17570(14)	0.8999(2)	0.0280(6)
H47A	0.0871	0.1734	0.9117	0.034*
C48	0.06418(5)	0.08174(14)	0.7446(2)	0.0259(6)
C49	0.09679(5)	0.08031(15)	0.7516(2)	0.0308(6)
H49A	0.1102	0.1162	0.8038	0.037*
C50	0.10999(6)	0.02797(15)	0.6846(2)	0.0371(7)
H50A	0.1323	0.0275	0.6923	0.045*
C51	0.09101(6)	−0.02412(16)	0.6059(2)	0.0402(7)
H51A	0.1003	−0.0604	0.5602	0.048*
C52	0.05848(6)	−0.02271(16)	0.5947(2)	0.0354(6)
H52A	0.0451	−0.0574	0.5400	0.042*
C53	0.04555(5)	0.02934(14)	0.6633(2)	0.0273(6)
C54	−0.00173(6)	−0.03857(15)	0.6823(2)	0.0384(7)
H54A	0.0091	−0.0848	0.6575	0.046*
H54B	−0.0245	−0.0409	0.6405	0.046*

their transition metal complexes due to its various interesting properties and extensive applications [5, 6]. As we have seen, people widely believed that the coordination ability of ether oxygen is weak, while phenolic *O* and imine *N* donor of salen- or salophen-type schiff base can easily coordinate with

transition metal ions to form some superior complexes [7, 8]. However, in this work we report the synthesis and characterization of a Co(II) complex, which contains the salen-type ligand with phenolic O and ether O donor. The crystallographic analysis certified that the title crystal is a mononuclear structure. There are 1.5 complexes in the asymmetric unit. Co(II) is six-coordinated with two phenolic oxygen atoms (O1 and O4), two aromatic ether oxygen atoms (O2 and O3) and two imine nitrogen atoms (N1 and N2), respectively. The coordination sphere can be described as a slightly distorted-octahedral geometry. The axial positions are occupied by N1, N2 atoms with a N1–Co1–N2 bond angle of $172.42(7)^\circ$, and the bond lengths of Co1–N1, Co1–N2 are $2.078(2)$ Å, $2.074(2)$ Å, respectively. The equatorial plane is completed by O1, O2, O3, O4 atoms with Co–O bond distances ranging from $1.9760(17)$ Å to $2.3254(18)$ Å, and the bond angles around Co(II) atom vary from $73.83(6)^\circ$ to $155.89(7)^\circ$.

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