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Bis{2-[(*E*)-benzyliminomethyl]-4-methylphenolato-κ^2N,O}nickel(II)

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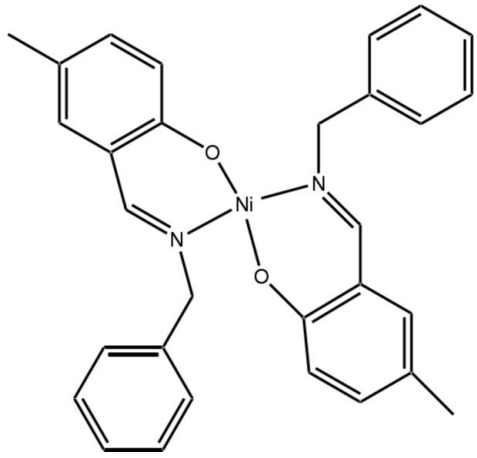
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.030; wR factor = 0.081; data-to-parameter ratio = 17.2.

In the title complex, $[Ni(C_{15}H_{14}NO)_2]$, the Ni^{II} atom is located on an inversion centre and is coordinated by two O and two N atoms from two symmetry-related bidentate Schiff base ligands in a slightly distorted square-planar geometry. The phenyl and benzene rings in the ligand molecule form a dihedral angle of 72.79 (8)°.

Related literature

For the synthesis of 2-[(*E*)-(benzylimino)methyl]-4-methylphenol, see: Cohen *et al.* (1964). For the structure of a related Zn complex, see: Rodriguez de Barbarin *et al.* (1994).



Experimental

Crystal data

$[Ni(C_{15}H_{14}NO)_2]$
M_r = 507.26
Monoclinic, $P2_1/c$
a = 13.7182 (15) Å
b = 10.5842 (11) Å
c = 8.6716 (9) Å
β = 107.593 (1)°
V = 1200.2 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.84 mm^{-1}
T = 296 K
0.37 × 0.29 × 0.24 mm

Data collection

Bruker SMART APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
T_{min} = 0.751, T_{max} = 0.819
10296 measured reflections
2765 independent reflections
2303 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.081
S = 1.04
2765 reflections
161 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.8294 (12)	Ni1—N1	1.9242 (14)
O1^{i}—Ni1—N1	87.01 (6)	O1—Ni1—N1	92.99 (6)

Symmetry code: (i) $-x+2, -y+1, -z$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2434).

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supplementary materials

Acta Cryst. (2009). E**65**, m923 [**doi:10.1107/S1600536809026658**]

Bis{2-[(*E*)-benzyliminomethyl]-4-methylphenolato-κ^2N,O}nickel(II)

S.-Z. Chen and D.-G. Xia

Comment

Schiff bases have played an important role in the development of coordination chemistry as they readily form stable complexes with most of the transition metals (Rodriguez de Barbarin *et al.*, 1994). Salicylaldehyde and its derivatives are useful carbonyl precursors for the synthesis of a large variety of Schiff bases. Here we report on a new Ni(II) complex, (I).

The molecular structure of (I) as illustrated in Fig. 1 has the Ni^{2+} center in a square geometry as it its coordinated by two O atoms and two N atoms from two 2-[(*E*)-(benzylimino)methyl]-4-methylphenol bidentate chelating ligands. The bond lengths and bond angles in (I) are within normal ranges. The Ni1—O1 distance of 1.8294 (12) Å is shorter than the distance of Ni1—N1 [1.9242 (14) Å] (Table 1). The dihedral angle between the plane of O1/N1/Ni1 and the adjacent phenol ring is 10.91 (9)°.

Experimental

1 mmol of $NiCl_2.6H_2O$ (0.240 g) were added to a 15 ml ethanol solution containing 2 mmol (0.450 g) 2-[(*E*)-(benzylimino)methyl]-4-methylphenol. The resulting mixture was stirred for about 0.5 h. The slow vaporization of the solvent yielded after about 6 d dark green single crystals. Yield: 70.2%. Calcd. for $C_{30}H_{28}NiN_2O_2$: C 71.03, H 5.56, N 5.52; Found: C 71.34, H 5.60, N 5.46%.

Synthesis of the ligand 2-[(*E*)-(benzylimino)methyl]-4-methylphenol: Phenylmethanamine and 5-methylsalicylaldehyde (1:1) were dissolved in ethanol and the solution was refluxed for 3 h. After evaporation, a crude product was recrystallized twice from ethanol to give a pure yellow product (Cohen *et al.*, 1964).

Refinement

All H atoms were located in a difference Fourier map. H atoms of the C—H groups were then placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H = 0.93, 0.96 or 0.97 Å, and with U_{iso}(H) = 1.2U_{eq}(C).

Figures

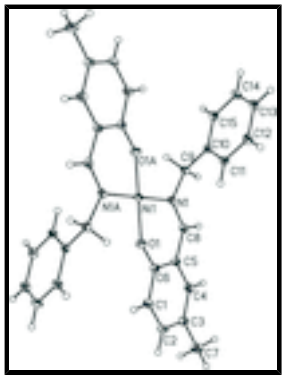

Fig. 1. The structure of (I), showing displacement ellipsoids drawn at the 30% probability level [symmetry code: (A) -*x* + 2, -*y* + 1, -*z*].

Bis{2-[(*E*)-benzyliminomethyl]-4-methylphenolato- κ^2*N*,*O*}nickel(II)

Crystal data

$[Ni(C_{15}H_{14}NO)_2]$	F_{000} = 532.0
M_r = 507.26	D_x = 1.404 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3741 reflections
a = 13.7182 (15) Å	θ = 3.1–27.5º
b = 10.5842 (11) Å	μ = 0.84 mm^{-1}
c = 8.6716 (9) Å	T = 296 K
β = 107.593 (1)º	Block, dark green
V = 1200.2 (2) Å^3	0.37 × 0.29 × 0.24 mm
Z = 2	

Data collection

Bruker SMART APEXII diffractometer	2765 independent reflections
Radiation source: fine-focus sealed tube	2303 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.029
T = 296 K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 2.5º
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)	h = −16→17
T_{min} = 0.751, T_{max} = 0.819	k = −13→12
10296 measured reflections	l = −11→11

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.030$	H-atom parameters constrained
$wR(F^2) = 0.081$	$w = 1/[\sigma^2(F_o^2) + (0.0383P)^2 + 0.6191P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
2765 reflections	$\Delta\rho_{max} = 0.35$ e Å^{-3}
161 parameters	$\Delta\rho_{min} = -0.24$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	1.0000	0.5000	0.0000	0.01763 (10)
O1	1.13609 (9)	0.46366 (12)	0.08566 (15)	0.0256 (3)
N1	1.01028 (10)	0.65072 (13)	0.12801 (16)	0.0188 (3)
C1	1.31316 (14)	0.49471 (18)	0.1963 (2)	0.0264 (4)
H1A	1.3255	0.4178	0.1538	0.032*
C2	1.39446 (14)	0.56674 (19)	0.2854 (2)	0.0283 (4)
H2A	1.4606	0.5370	0.3017	0.034*
C3	1.38044 (13)	0.68377 (19)	0.3525 (2)	0.0282 (4)
C4	1.28159 (13)	0.72439 (18)	0.3268 (2)	0.0257 (4)
H4A	1.2704	0.8009	0.3714	0.031*
C5	1.19653 (12)	0.65377 (16)	0.23490 (19)	0.0205 (3)
C6	1.21133 (13)	0.53616 (17)	0.16842 (19)	0.0215 (3)
C7	1.47135 (16)	0.7606 (2)	0.4500 (3)	0.0432 (5)
H7A	1.4488	0.8236	0.5112	0.065*
H7B	1.5029	0.8009	0.3781	0.065*
H7C	1.5199	0.7058	0.5225	0.065*
C8	1.09560 (13)	0.70026 (16)	0.21563 (19)	0.0207 (3)
H8A	1.0906	0.7736	0.2718	0.025*
C9	0.91662 (12)	0.71815 (15)	0.13304 (19)	0.0200 (3)
H9A	0.8749	0.7359	0.0232	0.024*
H9B	0.9361	0.7984	0.1878	0.024*
C10	0.85332 (12)	0.64504 (15)	0.21800 (18)	0.0184 (3)
C11	0.89270 (13)	0.54673 (16)	0.3250 (2)	0.0211 (3)
H11A	0.9600	0.5209	0.3427	0.025*

C12	0.83210 (14)	0.48676 (17)	0.4056 (2)	0.0257 (4)
H12A	0.8592	0.4209	0.4766	0.031*
C13	0.73212 (15)	0.52398 (18)	0.3814 (2)	0.0288 (4)
H13A	0.6919	0.4838	0.4359	0.035*
C14	0.69245 (14)	0.6218 (2)	0.2752 (2)	0.0314 (4)
H14A	0.6252	0.6477	0.2584	0.038*
C15	0.75229 (13)	0.68172 (18)	0.1936 (2)	0.0258 (4)
H15A	0.7246	0.7470	0.1219	0.031*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.01551 (16)	0.01832 (17)	0.01976 (15)	−0.00024 (12)	0.00637 (11)	−0.00090 (11)
O1	0.0169 (6)	0.0255 (7)	0.0320 (7)	0.0001 (5)	0.0037 (5)	−0.0069 (5)
N1	0.0184 (7)	0.0189 (7)	0.0210 (6)	0.0005 (5)	0.0087 (5)	0.0025 (5)
C1	0.0206 (9)	0.0296 (10)	0.0299 (9)	0.0024 (7)	0.0089 (7)	−0.0021 (7)
C2	0.0169 (8)	0.0387 (11)	0.0307 (9)	−0.0013 (8)	0.0092 (7)	0.0004 (8)
C3	0.0205 (9)	0.0366 (11)	0.0276 (9)	−0.0085 (8)	0.0073 (7)	−0.0024 (8)
C4	0.0247 (9)	0.0262 (10)	0.0278 (8)	−0.0048 (7)	0.0103 (7)	−0.0020 (7)
C5	0.0182 (8)	0.0229 (9)	0.0211 (7)	−0.0031 (6)	0.0072 (6)	0.0012 (6)
C6	0.0194 (8)	0.0247 (9)	0.0208 (8)	−0.0026 (6)	0.0066 (6)	0.0005 (6)
C7	0.0231 (10)	0.0525 (14)	0.0527 (12)	−0.0122 (10)	0.0094 (9)	−0.0174 (11)
C8	0.0239 (9)	0.0184 (8)	0.0222 (8)	−0.0025 (6)	0.0103 (7)	0.0003 (6)
C9	0.0195 (8)	0.0176 (8)	0.0240 (8)	0.0026 (6)	0.0082 (6)	0.0013 (6)
C10	0.0197 (8)	0.0184 (8)	0.0181 (7)	0.0005 (6)	0.0074 (6)	−0.0023 (6)
C11	0.0194 (8)	0.0215 (8)	0.0231 (8)	0.0034 (7)	0.0073 (6)	0.0012 (6)
C12	0.0301 (10)	0.0238 (9)	0.0247 (8)	0.0023 (7)	0.0105 (7)	0.0043 (7)
C13	0.0286 (10)	0.0333 (11)	0.0289 (9)	−0.0050 (8)	0.0153 (8)	0.0008 (7)
C14	0.0191 (9)	0.0446 (12)	0.0334 (9)	0.0053 (8)	0.0123 (7)	0.0035 (8)
C15	0.0230 (9)	0.0303 (10)	0.0248 (8)	0.0068 (7)	0.0084 (7)	0.0055 (7)

Geometric parameters (Å, °)

Ni1—O1^{i}	1.8294 (12)	C7—H7A	0.9600
Ni1—O1	1.8294 (12)	C7—H7B	0.9600
Ni1—N1^{i}	1.9242 (14)	C7—H7C	0.9600
Ni1—N1	1.9242 (14)	C8—H8A	0.9300
O1—C6	1.312 (2)	C9—C10	1.511 (2)
N1—C8	1.298 (2)	C9—H9A	0.9700
N1—C9	1.482 (2)	C9—H9B	0.9700
C1—C2	1.379 (3)	C10—C11	1.390 (2)
C1—C6	1.414 (2)	C10—C15	1.392 (2)
C1—H1A	0.9300	C11—C12	1.391 (2)
C2—C3	1.406 (3)	C11—H11A	0.9300
C2—H2A	0.9300	C12—C13	1.381 (3)
C3—C4	1.375 (3)	C12—H12A	0.9300
C3—C7	1.514 (3)	C13—C14	1.383 (3)
C4—C5	1.412 (2)	C13—H13A	0.9300

C4—H4A	0.9300	C14—C15	1.389 (2)
C5—C6	1.412 (2)	C14—H14A	0.9300
C5—C8	1.431 (2)	C15—H15A	0.9300
$O1^{i}$—Ni1—O1	180.00 (8)	C3—C7—H7C	109.5
$O1^{i}$—Ni1—$N1^{i}$	92.99 (6)	H7A—C7—H7C	109.5
O1—Ni1—$N1^{i}$	87.01 (6)	H7B—C7—H7C	109.5
$O1^{i}$—Ni1—N1	87.01 (6)	N1—C8—C5	126.80 (16)
O1—Ni1—N1	92.99 (6)	N1—C8—H8A	116.6
$N1^{i}$—Ni1—N1	180.00 (7)	C5—C8—H8A	116.6
C6—O1—Ni1	129.55 (12)	N1—C9—C10	113.51 (13)
C8—N1—C9	115.13 (14)	N1—C9—H9A	108.9
C8—N1—Ni1	124.64 (12)	C10—C9—H9A	108.9
C9—N1—Ni1	120.22 (10)	N1—C9—H9B	108.9
C2—C1—C6	120.95 (17)	C10—C9—H9B	108.9
C2—C1—H1A	119.5	H9A—C9—H9B	107.7
C6—C1—H1A	119.5	C11—C10—C15	118.58 (15)
C1—C2—C3	122.03 (17)	C11—C10—C9	122.97 (14)
C1—C2—H2A	119.0	C15—C10—C9	118.38 (15)
C3—C2—H2A	119.0	C10—C11—C12	120.43 (16)
C4—C3—C2	117.38 (17)	C10—C11—H11A	119.8
C4—C3—C7	121.88 (18)	C12—C11—H11A	119.8
C2—C3—C7	120.74 (17)	C13—C12—C11	120.70 (16)
C3—C4—C5	122.16 (17)	C13—C12—H12A	119.6
C3—C4—H4A	118.9	C11—C12—H12A	119.6
C5—C4—H4A	118.9	C12—C13—C14	119.18 (17)
C4—C5—C6	120.06 (16)	C12—C13—H13A	120.4
C4—C5—C8	119.30 (16)	C14—C13—H13A	120.4
C6—C5—C8	120.59 (15)	C13—C14—C15	120.46 (16)
O1—C6—C5	123.54 (16)	C13—C14—H14A	119.8
O1—C6—C1	119.03 (16)	C15—C14—H14A	119.8
C5—C6—C1	117.42 (16)	C14—C15—C10	120.65 (16)
C3—C7—H7A	109.5	C14—C15—H15A	119.7
C3—C7—H7B	109.5	C10—C15—H15A	119.7
H7A—C7—H7B	109.5		

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*.

Fig. 1