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Bis[2-(benzyliminomethyl)-4-chlorophenolato-κ^2N,O]nickel(II)

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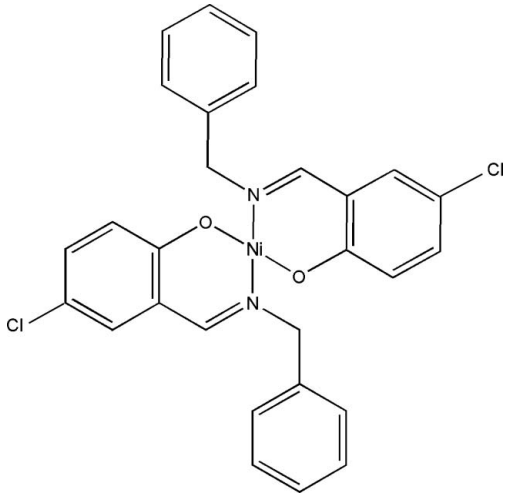
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.043; wR factor = 0.124; data-to-parameter ratio = 13.2.

In the mononuclear centrosymmetric title compound, $[Ni(C_{14}H_{11}ClNO)_2]$, the Ni^{II} atom, lying on a center of symmetry, is four-coordinated by two O atoms and two N atoms from two Schiff base ligands, forming a slightly distorted square-planar environment. The dihedral angle between the two aromatic rings of the ligand is 72.0 (2)°. No significant hydrogen bonding or π–π stacking interactions are observed.

Related literature

For bond-length data, see: Allen *et al.* (1987). For related literature, see: Christensen *et al.* (1997); Costes *et al.* (2005); Hu *et al.* (2005); Liu *et al.* (2006); Wallis & Cummings (1974); Yu (2006).



Experimental

Crystal data

$[Ni(C_{14}H_{11}ClNO)_2]$
M_r = 548.09
Monoclinic, $P2_1/c$
a = 13.6785 (17) Å
b = 10.5986 (14) Å
c = 8.6560 (13) Å
β = 107.529 (2)°
V = 1196.6 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.06 mm^{-1}
T = 298 (2) K
0.56 × 0.44 × 0.32 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.587, T_{max} = 0.727
5718 measured reflections
2110 independent reflections
1506 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.124
S = 1.08
2110 reflections
160 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.817 (2)	Ni1—N1	1.926 (3)
O1—Ni1—O1^{i}	180	O1—Ni1—N1	92.61 (11)
O1—Ni1—N1^{i}	87.39 (11)		

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); 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: CI2496).

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Acta Cryst. (2008). E**64**, m202 [https://doi.org/10.1107/S1600536807054943]

Bis[2-(benzyliminomethyl)-4-chlorophenolato-κ^2N,O]nickel(II)

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S1. Comment

Recently, we have reported a Schiff base nickel(II) complex (Hu *et al.*, 2005). Owing to the nickel complexes derived from Schiff base ligands possess interesting structures and wide applications (Costes *et al.*, 2005; Wallis & Cummings, 1974; Christensen *et al.*, 1997; Liu *et al.*, 2006); Yu, 2006), we report here the crystal structure of a new Schiff base nickel(II) complex, title compound, (I),

Compound (I) is a mononuclear centrosymmetric Ni^{II} complex (Fig. 1) The Ni atom, lying on the center of symmetry, is four-coordainated by two O atoms and two N atoms from two Schiff base ligands, forming a slightly distorted square-planar environment (Table 1). The bond lengths and angles of the ligands show normal values (Allen *et al.*, 1987). The dihedral angle between the two aromatic rings of the ligand is 72.0 (2)°. No significant hydrogen bonding or π-π stacking interactions are observed.

S2. Experimental

5-Chlorosalicylaldehyde (0.1 mmol, 15.7 mg), $Ni(NO_3)_2.6H_2O$ (0.1 mmol, 29.0 mg) and benzylamine (0.1 mmol, 10.7 mg) were dissolved in methanol (10 ml). The mixture was stirred for 30 min at room temperature to give a clear brown solution. After allowing the resulting solution to stand in air for 11 d, brown block-shaped crystals of compound (I) were formed on slow evaporation of the solvent. The crystals were collected, washed with methanol and dried in a vacuum desiccator using anhydrous $CaCl_2$ (yield 54%). Analysis found: C 61.30, H 4.0%; calculated for $Ni(C_{14}H_{11}Cl_O)_2$: C 61.34, H 4.01%.

S3. Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

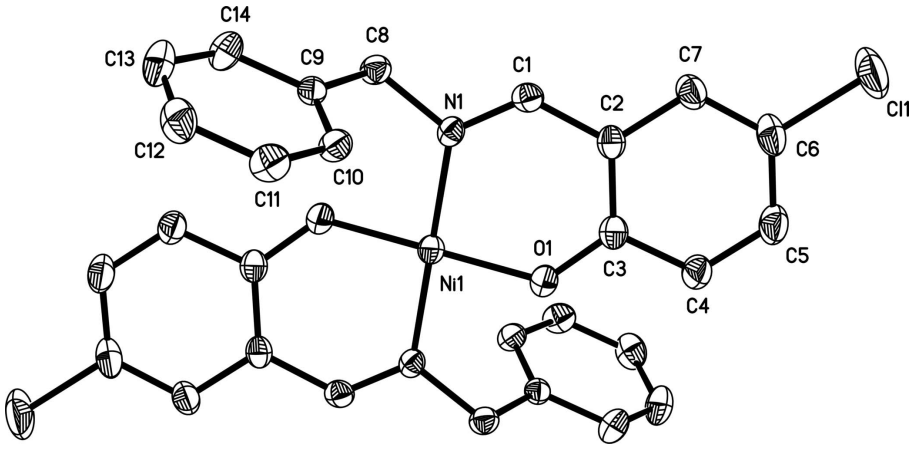

Figure 1

The molecular structure of (I), showing 30% probability displacement ellipsoids. H atoms have been omitted for clarity. Unlabelled atoms are related to other labelled atoms by the symmetry operation (*-x*, 1 - *y*, *-z*).

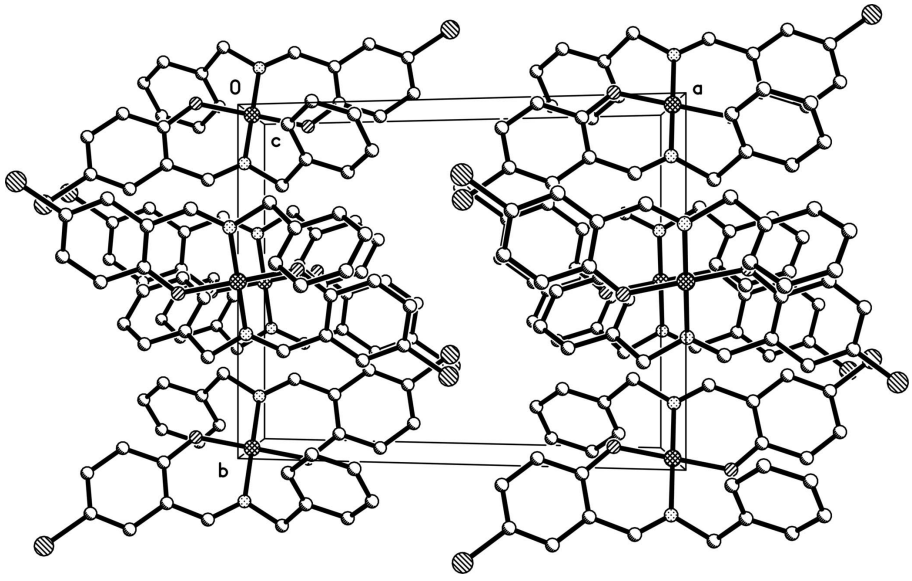

Figure 2

The crystal packing of (I), viewed along the *c* axis.

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Crystal data

$[Ni(C_{14}H_{11}ClNO)_2]$
M_r = 548.09
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
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b = 10.5986 (14) Å
c = 8.6560 (13) Å
β = 107.529 (2)°
V = 1196.6 (3) Å^3
Z = 2
$F(000)$ = 564
D_x = 1.521 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1825 reflections
θ = 2.5–25.2°
μ = 1.06 mm^{-1}
T = 298 K
Rhombus, green
0.56 × 0.44 × 0.32 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.587, T_{max} = 0.727
5718 measured reflections
2110 independent reflections
1506 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 25.0°, θ_{min} = 2.5°
h = −16→12
k = −12→8
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.124
S = 1.08
2110 reflections
160 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.057P)^2 + 0.6708P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Ni1	0.0000	0.5000	0.0000	0.0329 (2)
Cl1	0.48272 (9)	0.77502 (16)	0.44350 (18)	0.0919 (6)
N1	0.0104 (2)	0.6504 (3)	0.1288 (3)	0.0316 (7)
O1	0.13607 (19)	0.4664 (3)	0.0829 (3)	0.0472 (7)
C1	0.0949 (3)	0.7006 (4)	0.2141 (4)	0.0354 (8)
H1	0.0899	0.7737	0.2705	0.043*
C2	0.1963 (3)	0.6549 (4)	0.2309 (4)	0.0359 (9)
C3	0.2107 (3)	0.5393 (4)	0.1629 (4)	0.0365 (9)
C4	0.3123 (3)	0.4982 (4)	0.1878 (5)	0.0467 (10)
H4	0.3240	0.4208	0.1461	0.056*
C5	0.3939 (3)	0.5699 (5)	0.2720 (5)	0.0528 (11)
H5	0.4603	0.5418	0.2855	0.063*
C6	0.3779 (3)	0.6840 (5)	0.3372 (5)	0.0520 (11)
C7	0.2809 (3)	0.7283 (4)	0.3197 (5)	0.0451 (10)
H7	0.2710	0.8048	0.3653	0.054*
C8	−0.0831 (3)	0.7179 (4)	0.1351 (4)	0.0369 (9)

H8A	−0.1254	0.7353	0.0253	0.044*
H8B	−0.0633	0.7982	0.1893	0.044*
C9	−0.1461 (2)	0.6457 (3)	0.2219 (4)	0.0316 (8)
C10	−0.1084 (3)	0.5490 (4)	0.3262 (4)	0.0393 (9)
H10	−0.0411	0.5225	0.3438	0.047*
C11	−0.1688 (3)	0.4897 (4)	0.4064 (5)	0.0469 (10)
H11	−0.1422	0.4233	0.4767	0.056*
C12	−0.2678 (3)	0.5281 (4)	0.3827 (5)	0.0533 (12)
H12	−0.3087	0.4878	0.4361	0.064*
C13	−0.3059 (3)	0.6264 (5)	0.2799 (5)	0.0553 (12)
H13	−0.3725	0.6544	0.2651	0.066*
C14	−0.2457 (3)	0.6839 (4)	0.1983 (5)	0.0458 (10)
H14	−0.2727	0.7493	0.1265	0.055*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0295 (4)	0.0348 (4)	0.0367 (4)	−0.0008 (3)	0.0133 (3)	−0.0002 (3)
Cl1	0.0415 (7)	0.1240 (14)	0.1083 (11)	−0.0314 (7)	0.0197 (7)	−0.0503 (10)
N1	0.0291 (15)	0.0328 (17)	0.0363 (16)	0.0014 (13)	0.0152 (13)	0.0075 (13)
O1	0.0307 (14)	0.0475 (19)	0.0590 (17)	0.0032 (11)	0.0070 (13)	−0.0124 (13)
C1	0.040 (2)	0.031 (2)	0.040 (2)	−0.0020 (16)	0.0191 (17)	0.0023 (16)
C2	0.0311 (19)	0.043 (2)	0.035 (2)	−0.0034 (17)	0.0123 (15)	0.0036 (18)
C3	0.033 (2)	0.045 (2)	0.035 (2)	−0.0018 (16)	0.0137 (17)	0.0024 (17)
C4	0.035 (2)	0.053 (3)	0.054 (2)	0.0008 (19)	0.0156 (18)	−0.010 (2)
C5	0.031 (2)	0.069 (3)	0.059 (3)	−0.001 (2)	0.0156 (19)	−0.005 (2)
C6	0.034 (2)	0.073 (3)	0.050 (2)	−0.014 (2)	0.0137 (18)	−0.008 (2)
C7	0.037 (2)	0.049 (3)	0.051 (2)	−0.0103 (18)	0.0162 (18)	−0.008 (2)
C8	0.038 (2)	0.032 (2)	0.043 (2)	0.0018 (16)	0.0163 (17)	0.0026 (17)
C9	0.0308 (18)	0.033 (2)	0.0309 (19)	−0.0009 (15)	0.0095 (15)	−0.0046 (16)
C10	0.039 (2)	0.037 (2)	0.043 (2)	0.0046 (17)	0.0142 (17)	0.0024 (18)
C11	0.055 (3)	0.043 (2)	0.047 (2)	0.003 (2)	0.0222 (19)	0.009 (2)
C12	0.049 (2)	0.067 (3)	0.053 (2)	−0.012 (2)	0.029 (2)	−0.001 (2)
C13	0.035 (2)	0.079 (4)	0.055 (3)	0.005 (2)	0.019 (2)	0.002 (2)
C14	0.040 (2)	0.055 (3)	0.043 (2)	0.0121 (19)	0.0139 (18)	0.010 (2)

Geometric parameters (Å, º)

Ni1—O1	1.817 (2)	C6—C7	1.372 (5)
Ni1—O1^{i}	1.817 (2)	C7—H7	0.93
Ni1—N1^{i}	1.926 (3)	C8—C9	1.510 (5)
Ni1—N1	1.926 (3)	C8—H8A	0.97
Cl1—C6	1.743 (4)	C8—H8B	0.97
N1—C1	1.284 (4)	C9—C10	1.361 (5)
N1—C8	1.480 (4)	C9—C14	1.377 (5)
O1—C3	1.301 (4)	C10—C11	1.380 (5)
C1—C2	1.434 (5)	C10—H10	0.93
C1—H1	0.93	C11—C12	1.369 (6)

C2—C3	1.399 (5)	C11—H11	0.93
C2—C7	1.414 (5)	C12—C13	1.367 (6)
C3—C4	1.409 (5)	C12—H12	0.93
C4—C5	1.365 (6)	C13—C14	1.378 (6)
C4—H4	0.93	C13—H13	0.93
C5—C6	1.379 (6)	C14—H14	0.93
C5—H5	0.93		

O1—Ni1—O1^{i}	180	C6—C7—C2	118.6 (4)
O1—Ni1—N1^{i}	87.39 (11)	C6—C7—H7	120.7
O1^{i}—Ni1—N1^{i}	92.61 (11)	C2—C7—H7	120.7
O1—Ni1—N1	92.61 (11)	N1—C8—C9	113.7 (3)
O1^{i}—Ni1—N1	87.39 (11)	N1—C8—H8A	108.8
N1^{i}—Ni1—N1	180.00 (14)	C9—C8—H8A	108.8
C1—N1—C8	114.6 (3)	N1—C8—H8B	108.8
C1—N1—Ni1	124.9 (2)	C9—C8—H8B	108.8
C8—N1—Ni1	120.5 (2)	H8A—C8—H8B	107.7
C3—O1—Ni1	129.8 (3)	C10—C9—C14	118.7 (3)
N1—C1—C2	126.4 (4)	C10—C9—C8	123.5 (3)
N1—C1—H1	116.8	C14—C9—C8	117.7 (3)
C2—C1—H1	116.8	C9—C10—C11	120.8 (3)
C3—C2—C7	120.9 (3)	C9—C10—H10	119.6
C3—C2—C1	120.5 (3)	C11—C10—H10	119.6
C7—C2—C1	118.5 (4)	C12—C11—C10	120.3 (4)
O1—C3—C2	123.8 (3)	C12—C11—H11	119.9
O1—C3—C4	118.5 (4)	C10—C11—H11	119.9
C2—C3—C4	117.6 (3)	C13—C12—C11	119.4 (4)
C5—C4—C3	121.3 (4)	C13—C12—H12	120.3
C5—C4—H4	119.3	C11—C12—H12	120.3
C3—C4—H4	119.3	C12—C13—C14	120.1 (4)
C4—C5—C6	120.1 (4)	C12—C13—H13	120.0
C4—C5—H5	120.0	C14—C13—H13	120.0
C6—C5—H5	120.0	C9—C14—C13	120.7 (4)
C7—C6—C5	121.4 (4)	C9—C14—H14	119.6
C7—C6—Cl1	118.9 (4)	C13—C14—H14	119.6
C5—C6—Cl1	119.6 (3)		

O1—Ni1—N1—C1	9.0 (3)	C4—C5—C6—C7	0.0 (7)
O1^{i}—Ni1—N1—C1	−171.0 (3)	C4—C5—C6—Cl1	−179.7 (3)
O1—Ni1—N1—C8	−171.1 (2)	C5—C6—C7—C2	−0.8 (6)
O1^{i}—Ni1—N1—C8	8.9 (2)	Cl1—C6—C7—C2	178.9 (3)
N1^{i}—Ni1—O1—C3	164.0 (3)	C3—C2—C7—C6	0.4 (5)
N1—Ni1—O1—C3	−16.0 (3)	C1—C2—C7—C6	179.3 (3)
C8—N1—C1—C2	179.6 (3)	C1—N1—C8—C9	−111.5 (3)
Ni1—N1—C1—C2	−0.4 (5)	Ni1—N1—C8—C9	68.5 (3)
N1—C1—C2—C3	−6.1 (6)	N1—C8—C9—C10	19.2 (5)
N1—C1—C2—C7	174.9 (3)	N1—C8—C9—C14	−163.5 (3)
Ni1—O1—C3—C2	14.1 (5)	C14—C9—C10—C11	0.4 (6)

Ni1—O1—C3—C4	−168.2 (3)	C8—C9—C10—C11	177.6 (4)
C7—C2—C3—O1	178.5 (3)	C9—C10—C11—C12	−0.5 (6)
C1—C2—C3—O1	−0.5 (5)	C10—C11—C12—C13	−0.5 (6)
C7—C2—C3—C4	0.7 (5)	C11—C12—C13—C14	1.5 (7)
C1—C2—C3—C4	−178.2 (3)	C10—C9—C14—C13	0.7 (6)
O1—C3—C4—C5	−179.4 (4)	C8—C9—C14—C13	−176.8 (4)
C2—C3—C4—C5	−1.5 (6)	C12—C13—C14—C9	−1.6 (7)
C3—C4—C5—C6	1.1 (6)		

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