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Bis[4-chloro-2-(iminomethyl)phenolato]-nickel(II)

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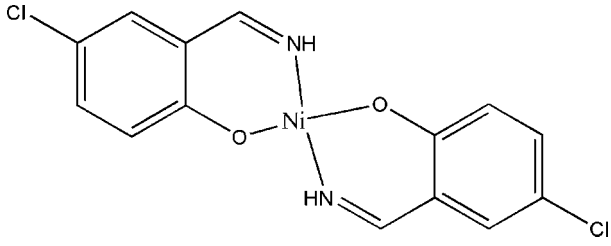
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.030; wR factor = 0.084; data-to-parameter ratio = 15.3.

In the title centrosymmetric mononuclear nickel(II) complex, $[Ni(C_7H_5ClNO)_2]$, the Ni^{II} ion, lying on an inversion center, is four-coordinated by two O and two imine N atoms from two 4-chloro-2-iminomethylphenolate ligands, forming a distorted square-planar geometry. In the crystal structure, molecules are linked into a two-dimensional network parallel to the *bc* plane by C—H···O hydrogen bonds.

Related literature

For related structures, see: Hong (2007); Kamenar *et al.* (1990); Li *et al.* (2005, 2007); Zhou *et al.* (2004).



Experimental

Crystal data

$[Ni(C_7H_5ClNO)_2]$
M_r = 367.85
Monoclinic, $P2_1/c$
a = 15.775 (6) Å
b = 5.685 (2) Å
c = 7.894 (3) Å
β = 93.864 (18)°
V = 706.3 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.76 mm^{-1}
T = 298 (2) K
0.18 × 0.17 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.743, T_{max} = 0.755
4102 measured reflections
1532 independent reflections
1296 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.084
S = 1.04
1532 reflections
100 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O1^{i}	0.93	2.54	3.318 (3)	142

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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: CI2768).

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supporting information

Acta Cryst. (2009). E**65**, m273 [doi:10.1107/S1600536809004279]

Bis[4-chloro-2-(iminomethyl)phenolato]nickel(II)

Zhe Hong

S1. Comment

Recently, the author has reported the crystal structure of a Schiff base nickel(II) complex (Hong, 2007). As an extension of the work on the structural investigation of nickel(II) complexes, the title complex is reported here.

The title compound is a centrosymmetric mononuclear nickel(II) complex (Fig. 1), which is similar to those reported previously (Kamenar *et al.*, 1990). The Ni atom, lying on the inversion center, is four-coordinated by two O and two imine N atoms from two 4-chloro-2-iminomethylphenol ligands, forming a square-planar geometry. The bond lengths (Table 1) related to the metal centre are comparable to the values in similar nickel(II) complexes (Zhou *et al.*, 2004; Li *et al.*, 2005; Li *et al.*, 2007).

In the crystal structure, the molecules are linked into a two-dimensional network parallel to the *bc* plane by C—H···O hydrogen bonds (Table 1).

S2. Experimental

5-Chlorosalicylaldehyde (1.0 mmol, 156.6 mg) and $Ni(CH_3COO)_2.4H_2O$ (0.5 mmol, 125.0 mg) were dissolved in methanol solution containing a small quantity of ammonia (30 ml). The mixture was stirred at room temperature for 30 min to give a clear brown solution. After keeping the solution in air for a few days, brown block-shaped crystals were formed.

S3. Refinement

Atom H1 was located from a difference Fourier map and refined isotropically, with the N1–H1 distance restrained to 0.90 (1) Å. Other H atoms were placed in idealized positions and constrained to ride on their parent atoms with C–H distances of 0.93 Å, and with U_{iso}(H) set to 1.2U_{eq}(C).

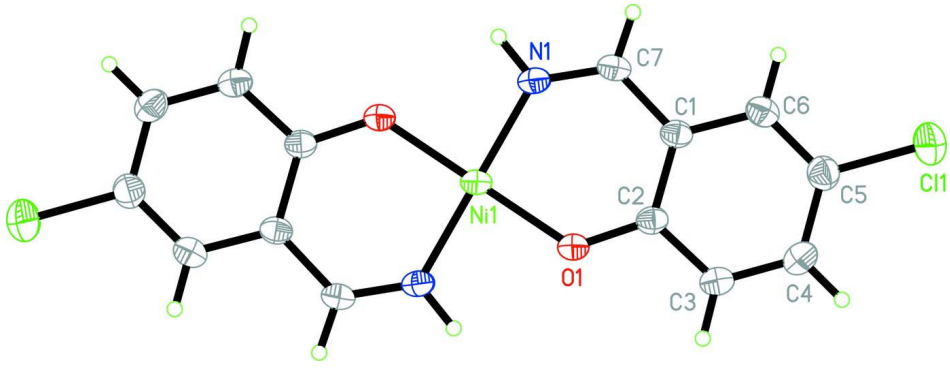

Figure 1

The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. Unlabelled atoms are related to labelled atoms by the symmetry operation (1 - x, 1 - y, - z).

Bis[4-chloro-2-(iminomethyl)phenolato]nickel(II)

Crystal data

$[Ni(C_7H_5ClNO)_2]$
$M_r = 367.85$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 15.775$ (6) Å
$b = 5.685$ (2) Å
$c = 7.894$ (3) Å
$\beta = 93.864$ (18)°
$V = 706.3$ (5) Å^3
$Z = 2$
$F(000) = 372$
$D_x = 1.730$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1954 reflections
$\theta = 2.8$–27.6°
$\mu = 1.76$ mm^{-1}
$T = 298$ K
Block, brown
0.18 × 0.17 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.743$, $T_{max} = 0.755$
4102 measured reflections
1532 independent reflections
1296 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.6°$
$h = -20\rightarrow18$
$k = -7\rightarrow7$
$l = -10\rightarrow9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.084$
$S = 1.04$
1532 reflections
100 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2 + 0.0905P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Ni1	0.5000	0.5000	0.0000	0.03469 (15)
Cl1	0.06466 (4)	0.34882 (15)	0.19374 (11)	0.0778 (3)
N1	0.45858 (11)	0.2416 (3)	0.1094 (2)	0.0421 (4)

O1	0.39683 (9)	0.6527 (2)	−0.01584 (18)	0.0411 (3)
C1	0.31247 (13)	0.3565 (3)	0.1140 (3)	0.0374 (4)
C2	0.32363 (13)	0.5745 (4)	0.0315 (3)	0.0369 (4)
C3	0.25045 (14)	0.7137 (4)	−0.0045 (3)	0.0445 (5)
H3	0.2554	0.8554	−0.0619	0.053*
C4	0.17234 (15)	0.6450 (4)	0.0433 (3)	0.0501 (6)
H4	0.1252	0.7403	0.0189	0.060*
C5	0.16322 (14)	0.4331 (5)	0.1283 (3)	0.0493 (6)
C6	0.23191 (14)	0.2906 (4)	0.1628 (3)	0.0439 (5)
H6	0.2252	0.1487	0.2190	0.053*
C7	0.38261 (14)	0.1990 (4)	0.1480 (3)	0.0412 (5)
H7	0.3722	0.0571	0.2015	0.049*
H1	0.4993 (14)	0.133 (4)	0.131 (4)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0430 (2)	0.0274 (2)	0.0335 (2)	0.00107 (14)	0.00128 (15)	0.00308 (13)
Cl1	0.0488 (4)	0.0872 (6)	0.0994 (6)	−0.0016 (3)	0.0197 (3)	0.0169 (4)
N1	0.0470 (10)	0.0325 (9)	0.0465 (10)	0.0054 (7)	0.0023 (8)	0.0076 (7)
O1	0.0437 (8)	0.0314 (7)	0.0483 (9)	0.0025 (6)	0.0049 (6)	0.0063 (6)
C1	0.0467 (11)	0.0305 (10)	0.0348 (10)	−0.0012 (8)	0.0020 (8)	−0.0010 (8)
C2	0.0447 (11)	0.0312 (9)	0.0345 (10)	0.0018 (8)	0.0017 (8)	−0.0021 (8)
C3	0.0510 (12)	0.0351 (11)	0.0469 (13)	0.0042 (9)	0.0004 (10)	0.0025 (9)
C4	0.0470 (12)	0.0463 (14)	0.0565 (14)	0.0086 (10)	−0.0006 (10)	−0.0021 (10)
C5	0.0454 (13)	0.0497 (13)	0.0530 (14)	−0.0026 (10)	0.0052 (10)	−0.0009 (11)
C6	0.0517 (12)	0.0379 (11)	0.0424 (12)	−0.0045 (10)	0.0060 (9)	0.0008 (9)
C7	0.0513 (12)	0.0316 (10)	0.0406 (11)	−0.0007 (9)	0.0037 (9)	0.0066 (8)

Geometric parameters (Å, º)

Ni1—O1^{i}	1.8414 (15)	C1—C7	1.434 (3)
Ni1—O1	1.8414 (15)	C2—C3	1.412 (3)
Ni1—N1^{i}	1.8455 (18)	C3—C4	1.370 (3)
Ni1—N1	1.8455 (18)	C3—H3	0.93
Cl1—C5	1.738 (2)	C4—C5	1.391 (4)
N1—C7	1.280 (3)	C4—H4	0.93
N1—H1	0.897 (10)	C5—C6	1.365 (3)
O1—C2	1.315 (2)	C6—H6	0.93
C1—C6	1.403 (3)	C7—H7	0.93
C1—C2	1.417 (3)		
O1^{i}—Ni1—O1	180.00 (4)	C4—C3—C2	121.5 (2)
O1^{i}—Ni1—N1^{i}	93.89 (7)	C4—C3—H3	119.2
O1—Ni1—N1^{i}	86.11 (7)	C2—C3—H3	119.2
O1^{i}—Ni1—N1	86.11 (7)	C3—C4—C5	120.3 (2)
O1—Ni1—N1	93.89 (7)	C3—C4—H4	119.9
N1^{i}—Ni1—N1	180.00 (10)	C5—C4—H4	119.9

C7—N1—Ni1	128.97 (15)	C6—C5—C4	120.2 (2)
C7—N1—H1	120 (2)	C6—C5—Cl1	119.4 (2)
Ni1—N1—H1	111 (2)	C4—C5—Cl1	120.37 (19)
C2—O1—Ni1	127.63 (13)	C5—C6—C1	120.6 (2)
C6—C1—C2	120.15 (18)	C5—C6—H6	119.7
C6—C1—C7	118.94 (19)	C1—C6—H6	119.7
C2—C1—C7	120.91 (19)	N1—C7—C1	124.10 (19)
O1—C2—C3	118.37 (19)	N1—C7—H7	118.0
O1—C2—C1	124.41 (18)	C1—C7—H7	118.0
C3—C2—C1	117.21 (19)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O1^{ii}	0.93	2.54	3.318 (3)	142

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