Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{2,2′-[4-Chloro-5-methyl-*o*-phenylenebis(nitrilomethylidyne)]diphenolato}-nickel(II)

Haixia Wang

Department of Chemistry and Environmental Science, Henan Normal University, Xinxiang 453007, People's Republic of China
Correspondence e-mail: xxhxwang@126.com

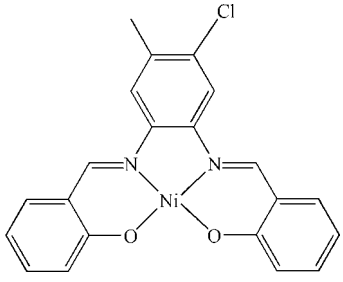
Received 31 October 2010; accepted 9 November 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.052; wR factor = 0.153; data-to-parameter ratio = 11.9.

In the title complex, $[Ni(C_{21}H_{15}ClN_2O_2)]$, the Ni^{II} ion is coordinated by two N and two O atoms from the tetradentate Schiff base ligand in a distorted square geometry. The crystal packing exhibits short intermolecular Ni···Ni distances of 3.273 (3) Å.

Related literature

For related structures, see: Ali *et al.* (2010); Hernandez-Molina *et al.* (1997); Niu *et al.* (2009); Radha *et al.* (1985).



Experimental

Crystal data

$[Ni(C_{21}H_{15}ClN_2O_2)]$
M_r = 421.51
Monoclinic, $P2_1/c$
a = 11.0451 (10) Å
b = 8.0202 (7) Å
c = 19.5959 (17) Å
β = 106.37°
V = 1665.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.35 mm^{-1}
T = 293 K
0.34 × 0.29 × 0.23 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.658, T_{max} = 0.747
7946 measured reflections
2917 independent reflections
2155 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.153
S = 1.03
2917 reflections
245 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.91 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2792).

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supporting information

Acta Cryst. (2010). E**66**, m1571 [https://doi.org/10.1107/S1600536810046088]

{2,2′-[4-Chloro-5-methyl-*o*-phenylenebis(nitrilomethylidyne)]diphenolato}nickel(II)

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S1. Comment

Schiff-base ligands, due to their excellent coordination ability, have been widely introduced into the coordination chemistry. Here, we report a new nickel complex based on a tetradentate Schiff-base ligand.

In the title compound (Fig. 1), the whole molecule is essentially planar with the mean deviation 0.0523 Å from the plane formed by all non-hydrogen atoms. The Ni^{II} ion is four-coordinated by two N atoms and two O atoms of the Schiff base ligand. The Ni—O and Ni—N bond lengths are all consistent with those found in other reported tetradentate Schiff base Ni complexes (Ali, *et al.*, 2010; Hernandez-Molina, *et al.*, 1997; Niu, *et al.*, 2009; Radha, *et al.*, 1985).

S2. Experimental

The synthesis of the title complex was carried out by reaction of $Ni(ClO_4)_2.6H_2O$ and the Schiff-base ligand with the molar ratio 1:1 in methanol under the stirring condition at room temperature. The filtrated solution was left to slowly evaperate in air to obtain single-crystal suitable for X-ray diffraction with the yield about 56%.

S3. Refinement

C-bound H atoms were placed in idealized positions with C—H distances of 0.93 and 0.96 Å, and were refined as riding atoms, with U_{iso}(H) = 1.2-1.5 U_{eq}(C).

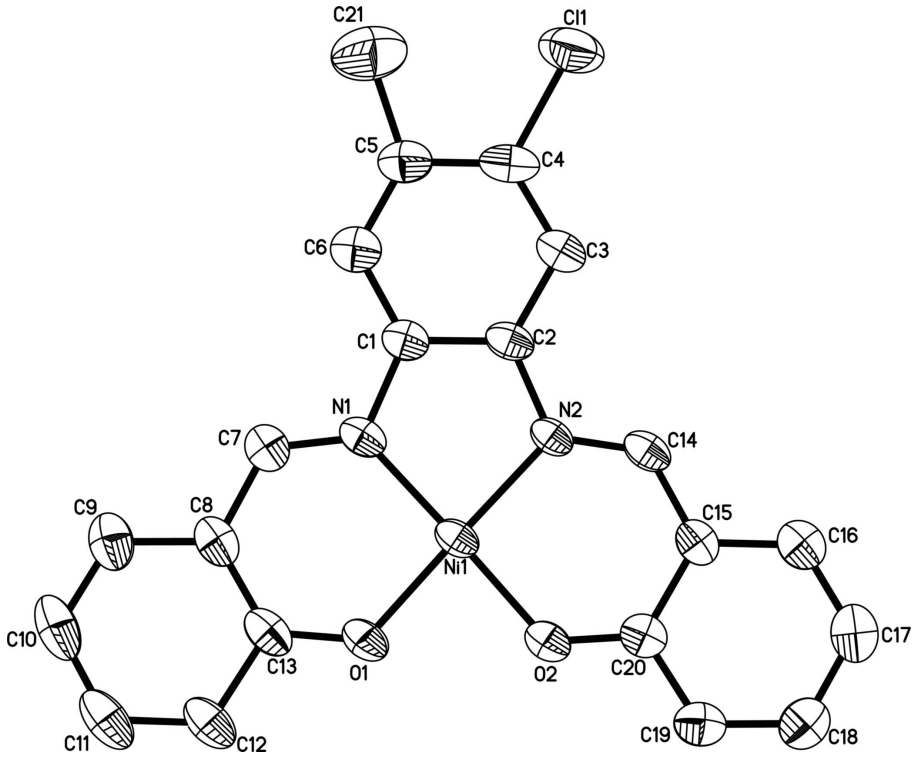

Figure 1

The molecular structure of the title complex with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms omitted for clarity.

{2,2′-[4-Chloro-5-methyl-*o*- phenylenebis(nitrilomethylidyne)]diphenolato}nickel(II)

Crystal data

$[Ni(C_{21}H_{15}ClN_2O_2)]$
$M_r = 421.51$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.0451\ (10)$ Å
$b = 8.0202\ (7)$ Å
$c = 19.5959\ (17)$ Å
$\beta = 106.37°$
$V = 1665.5\ (3)$ Å^3
$Z = 4$
$F(000) = 864$
$D_x = 1.681$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2314 reflections
$\theta = 2.5–27.0°$
$\mu = 1.35$ mm^{-1}
$T = 293$ K
Block, red-brown
0.34 × 0.29 × 0.23 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
$T_{min} = 0.658$, $T_{max} = 0.747$
7946 measured reflections
2917 independent reflections
2155 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$
$h = -13\rightarrow13$
$k = -9\rightarrow9$
$l = -23\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.153$
$S = 1.03$
2917 reflections
245 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
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.018$
$\Delta\rho_{max} = 0.67$ e Å^{-3}
$\Delta\rho_{min} = -0.91$ 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	0.45347 (5)	0.83377 (6)	0.03397 (2)	0.0490 (2)
Cl1	0.13615 (17)	0.8003 (2)	−0.31318 (8)	0.1129 (6)
O1	0.4706 (3)	0.9080 (4)	0.12480 (13)	0.0619 (7)
O2	0.6066 (3)	0.7335 (4)	0.07528 (14)	0.0582 (7)
N1	0.2996 (3)	0.9374 (4)	−0.00538 (16)	0.0520 (8)
N2	0.4388 (3)	0.7559 (4)	−0.05774 (15)	0.0471 (8)
C1	0.2514 (4)	0.9118 (5)	−0.0800 (2)	0.0541 (10)
C2	0.3286 (4)	0.8106 (5)	−0.1080 (2)	0.0531 (10)
C3	0.2928 (4)	0.7764 (6)	−0.1805 (2)	0.0627 (11)
H3	0.3430	0.7089	−0.1999	0.075*
C4	0.1837 (5)	0.8422 (6)	−0.2230 (2)	0.0732 (14)
C5	0.1058 (5)	0.9433 (6)	−0.1956 (3)	0.0721 (13)
C6	0.1415 (4)	0.9765 (6)	−0.1252 (2)	0.0689 (12)
H6	0.0908	1.0449	−0.1065	0.083*
C7	0.2348 (4)	1.0221 (5)	0.0289 (2)	0.0583 (11)
H7	0.1561	1.0618	0.0031	0.070*
C8	0.2758 (4)	1.0584 (5)	0.1032 (2)	0.0606 (11)
C9	0.1979 (6)	1.1596 (6)	0.1325 (3)	0.0792 (15)
H9	0.1203	1.1955	0.1035	0.095*
C10	0.2337 (7)	1.2052 (7)	0.2016 (3)	0.0926 (18)
H10	0.1801	1.2683	0.2204	0.111*
C11	0.3516 (7)	1.1567 (7)	0.2444 (3)	0.0880 (18)
H11	0.3779	1.1922	0.2915	0.106*
C12	0.4299 (5)	1.0572 (6)	0.2186 (2)	0.0756 (14)
H12	0.5079	1.0253	0.2484	0.091*

C13	0.3926 (5)	1.0026 (5)	0.1465 (2)	0.0598 (11)
C14	0.5194 (4)	0.6572 (5)	−0.0743 (2)	0.0530 (10)
H14	0.4997	0.6228	−0.1215	0.064*
C15	0.6325 (4)	0.5970 (5)	−0.0291 (2)	0.0529 (10)
C16	0.7113 (5)	0.4956 (5)	−0.0562 (3)	0.0669 (12)
H16	0.6855	0.4652	−0.1039	0.080*
C17	0.8255 (5)	0.4398 (6)	−0.0143 (3)	0.0774 (14)
H17	0.8756	0.3714	−0.0334	0.093*
C18	0.8657 (5)	0.4859 (6)	0.0564 (3)	0.0752 (13)
H18	0.9440	0.4507	0.0847	0.090*
C19	0.7894 (4)	0.5848 (6)	0.0855 (2)	0.0676 (12)
H19	0.8173	0.6124	0.1335	0.081*
C20	0.6729 (4)	0.6436 (5)	0.0451 (2)	0.0529 (10)
C21	0.0008 (6)	1.0115 (12)	−0.2558 (4)	0.132 (3)
H21A	−0.0784	0.9956	−0.2455	0.199*
H21B	−0.0005	0.9539	−0.2989	0.199*
H21C	0.0144	1.1283	−0.2613	0.199*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0643 (4)	0.0489 (4)	0.0354 (3)	−0.0117 (2)	0.0164 (2)	−0.0002 (2)
Cl1	0.1186 (13)	0.1466 (16)	0.0594 (9)	−0.0027 (10)	0.0020 (8)	−0.0031 (8)
O1	0.081 (2)	0.0689 (19)	0.0377 (15)	−0.0039 (16)	0.0190 (14)	−0.0014 (14)
O2	0.0714 (19)	0.0603 (17)	0.0423 (15)	−0.0052 (15)	0.0147 (14)	−0.0016 (13)
N1	0.072 (2)	0.0443 (18)	0.0400 (17)	−0.0150 (16)	0.0156 (15)	0.0010 (14)
N2	0.063 (2)	0.0462 (18)	0.0342 (16)	−0.0094 (16)	0.0174 (15)	0.0023 (14)
C1	0.062 (3)	0.051 (2)	0.049 (2)	−0.011 (2)	0.014 (2)	0.0046 (19)
C2	0.065 (3)	0.052 (2)	0.040 (2)	−0.0162 (19)	0.0116 (19)	0.0027 (17)
C3	0.076 (3)	0.065 (3)	0.046 (2)	−0.012 (2)	0.016 (2)	−0.003 (2)
C4	0.079 (3)	0.079 (3)	0.050 (3)	−0.019 (3)	−0.001 (2)	0.013 (2)
C5	0.074 (3)	0.071 (3)	0.062 (3)	−0.007 (3)	0.003 (2)	0.004 (2)
C6	0.073 (3)	0.065 (3)	0.066 (3)	−0.008 (2)	0.016 (2)	0.003 (2)
C7	0.070 (3)	0.049 (2)	0.061 (3)	−0.010 (2)	0.026 (2)	0.001 (2)
C8	0.086 (3)	0.048 (2)	0.057 (3)	−0.013 (2)	0.035 (2)	−0.001 (2)
C9	0.103 (4)	0.065 (3)	0.082 (4)	0.001 (3)	0.047 (3)	−0.002 (2)
C10	0.142 (6)	0.073 (3)	0.085 (4)	−0.008 (4)	0.068 (4)	−0.017 (3)
C11	0.141 (5)	0.077 (4)	0.061 (3)	−0.028 (3)	0.053 (4)	−0.017 (3)
C12	0.111 (4)	0.075 (3)	0.047 (2)	−0.019 (3)	0.035 (3)	−0.008 (2)
C13	0.090 (3)	0.050 (2)	0.046 (2)	−0.021 (2)	0.032 (2)	−0.0019 (19)
C14	0.075 (3)	0.047 (2)	0.039 (2)	−0.016 (2)	0.019 (2)	0.0006 (17)
C15	0.067 (3)	0.044 (2)	0.053 (2)	−0.0125 (19)	0.027 (2)	0.0010 (18)
C16	0.084 (3)	0.055 (3)	0.065 (3)	−0.007 (2)	0.028 (3)	0.005 (2)
C17	0.090 (4)	0.059 (3)	0.094 (4)	−0.004 (3)	0.044 (3)	0.003 (3)
C18	0.069 (3)	0.069 (3)	0.088 (4)	−0.004 (2)	0.022 (3)	0.009 (3)
C19	0.071 (3)	0.069 (3)	0.060 (3)	−0.012 (2)	0.013 (2)	0.005 (2)
C20	0.064 (3)	0.044 (2)	0.053 (2)	−0.0135 (19)	0.020 (2)	0.0092 (18)
C21	0.099 (5)	0.161 (8)	0.116 (5)	−0.012 (4)	−0.004 (4)	0.020 (4)

Geometric parameters (Å, º)

Ni1—O1	1.835 (3)	C9—C10	1.349 (8)
Ni1—O2	1.841 (3)	C9—H9	0.9300
Ni1—N1	1.854 (3)	C10—C11	1.391 (8)
Ni1—N2	1.866 (3)	C10—H10	0.9300
Cl1—C4	1.729 (5)	C11—C12	1.375 (7)
O1—C13	1.306 (5)	C11—H11	0.9300
O2—C20	1.285 (5)	C12—C13	1.425 (6)
N1—C7	1.302 (5)	C12—H12	0.9300
N1—C1	1.422 (5)	C14—C15	1.398 (6)
N2—C14	1.298 (5)	C14—H14	0.9300
N2—C2	1.403 (5)	C15—C16	1.400 (6)
C1—C6	1.386 (6)	C15—C20	1.444 (6)
C1—C2	1.397 (6)	C16—C17	1.372 (7)
C2—C3	1.390 (6)	C16—H16	0.9300
C3—C4	1.363 (6)	C17—C18	1.381 (7)
C3—H3	0.9300	C17—H17	0.9300
C4—C5	1.395 (7)	C18—C19	1.390 (7)
C5—C6	1.349 (6)	C18—H18	0.9300
C5—C21	1.505 (8)	C19—C20	1.390 (6)
C6—H6	0.9300	C19—H19	0.9300
C7—C8	1.428 (6)	C21—H21A	0.9600
C7—H7	0.9300	C21—H21B	0.9600
C8—C13	1.402 (6)	C21—H21C	0.9600
C8—C9	1.417 (6)		
O1—Ni1—O2	83.34 (13)	C8—C9—H9	119.3
O1—Ni1—N1	95.17 (14)	C9—C10—C11	119.3 (5)
O2—Ni1—N1	178.50 (13)	C9—C10—H10	120.3
O1—Ni1—N2	178.89 (14)	C11—C10—H10	120.3
O2—Ni1—N2	95.55 (14)	C12—C11—C10	121.3 (5)
N1—Ni1—N2	85.94 (14)	C12—C11—H11	119.4
C13—O1—Ni1	127.3 (3)	C10—C11—H11	119.4
C20—O2—Ni1	127.9 (3)	C11—C12—C13	120.5 (5)
C7—N1—C1	120.3 (4)	C11—C12—H12	119.7
C7—N1—Ni1	126.3 (3)	C13—C12—H12	119.7
C1—N1—Ni1	113.4 (3)	O1—C13—C8	124.6 (4)
C14—N2—C2	122.4 (3)	O1—C13—C12	117.9 (5)
C14—N2—Ni1	124.4 (3)	C8—C13—C12	117.5 (4)
C2—N2—Ni1	113.2 (3)	N2—C14—C15	127.2 (4)
C6—C1—C2	119.2 (4)	N2—C14—H14	116.4
C6—C1—N1	127.6 (4)	C15—C14—H14	116.4
C2—C1—N1	113.2 (4)	C14—C15—C16	120.0 (4)
C3—C2—C1	119.1 (4)	C14—C15—C20	121.0 (4)
C3—C2—N2	126.6 (4)	C16—C15—C20	118.9 (4)
C1—C2—N2	114.3 (3)	C17—C16—C15	121.8 (5)
C4—C3—C2	119.8 (5)	C17—C16—H16	119.1

C4—C3—H3	120.1	C15—C16—H16	119.1
C2—C3—H3	120.1	C16—C17—C18	119.6 (5)
C3—C4—C5	121.6 (4)	C16—C17—H17	120.2
C3—C4—Cl1	120.7 (4)	C18—C17—H17	120.2
C5—C4—Cl1	117.6 (4)	C17—C18—C19	120.2 (5)
C6—C5—C4	118.3 (5)	C17—C18—H18	119.9
C6—C5—C21	131.9 (6)	C19—C18—H18	119.9
C4—C5—C21	109.4 (5)	C18—C19—C20	122.0 (5)
C5—C6—C1	122.1 (5)	C18—C19—H19	119.0
C5—C6—H6	119.0	C20—C19—H19	119.0
C1—C6—H6	119.0	O2—C20—C19	119.0 (4)
N1—C7—C8	124.8 (4)	O2—C20—C15	123.6 (4)
N1—C7—H7	117.6	C19—C20—C15	117.4 (4)
C8—C7—H7	117.6	C5—C21—H21A	109.5
C13—C8—C9	119.9 (4)	C5—C21—H21B	109.5
C13—C8—C7	121.6 (4)	H21A—C21—H21B	109.5
C9—C8—C7	118.4 (5)	C5—C21—H21C	109.5
C10—C9—C8	121.4 (6)	H21A—C21—H21C	109.5
C10—C9—H9	119.3	H21B—C21—H21C	109.5