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# Bis[2-(3-cyanophenyliminomethyl)-phenolato]nickel(II)

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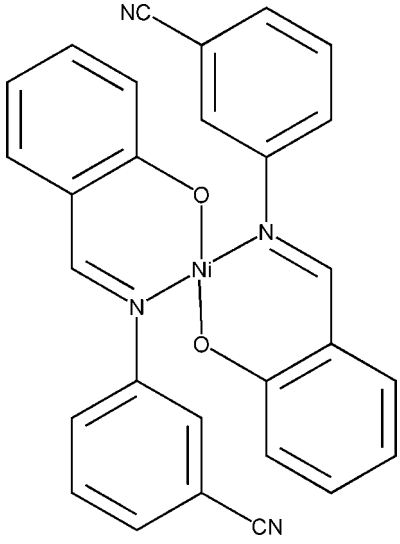
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.034; $wR$ factor = 0.090; data-to-parameter ratio = 15.9.

In the title complex, $[Ni(C_{14}H_9N_2O)_2]$, the $Ni^{II}$ atom lies on an inversion center and is coordinated by the O atom and an N atom of two Schiff base 2-(3-cyanophenyliminomethyl)-phenolate ligands in a square-planar geometry. The dihedral angle between the cyanophenyl and phenolate rings is 47.62 (7)°.

## Related literature

For related literature, see: Adams *et al.* (2004); Bian *et al.* (2004); Brückner *et al.* (2000); Harrop *et al.* (2003); Marganian *et al.* (1995); Akkurt *et al.* (2006); Peng *et al.* (2006).




## Experimental

### Crystal data

$[Ni(C_{14}H_9N_2O)_2]$
$M_r$ = 501.17
Monoclinic, $P2_1/c$
$a$ = 9.0294 (18) Å
$b$ = 8.0856 (16) Å
$c$ = 15.644 (3) Å
$\beta$ = 104.01 (3)°
$V$ = 1108.1 (4) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.91 mm$^{-1}$
$T$ = 293 (2) K
0.25 × 0.18 × 0.18 mm

### Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min}$ = 0.852, $T_{max}$ = 1.00
(expected range = 0.723–0.849)
11052 measured reflections
2540 independent reflections
2246 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.035

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.090
$S$ = 1.10
2540 reflections
160 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.35 e Å$^{-3}$

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2310).

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# supplementary materials

*Acta Cryst.* (2008). E**64**, m494 [ **doi:10.1107/S1600536808004765** ]

# Bis[2-(3-cyanophenyliminomethyl)phenolato]nickel(II)

**X.-X. Gong, R. Xia and H.-J. Xu**

## Comment

Schiff bases have been used extensively as ligands in the field of coordination chemistry. These complexes play an important role in the development of pharmacological and catalytic properties (Harrop *et al.*, 2003; Brückner *et al.*, 2000). Nickel(II) compounds with Schiff bases have received much attention in recent years (Marganian *et al.*, 1995). Here we report the molecular and crystal structure of nickel (II) complex with a Schiff base ligand.

The $Ni^{II}$ atom in (I) lies on an inversion center and is coordinated by the two imine N and two phenolateO atoms of the two Schiff base ligands in a square-planar geometry (Fig.1). The dihedral angle between the cyanophenyl and phenyl rings is 47.62 (7)°.. The Ni—O and Ni—N bond lengths agree with the values reported for related complexes(Peng, *et al.*, (2006); Adams *et al.*, 2004; Bian *et al.*, 2004).

## Experimental

2-(3-cyanophenyliminomethyl)phenol was prepared according to the literature (Akkurt *et al.*, 2006). $NiCl_2·6H_2O$(23.7 mg, 0.1 mmol) in methanol (5 ml) was added to the solution of 2-(3-cyanophenyliminomethyl)phenol (22.2 mg, 0.1 mmol)in the methanol (5 ml), the pH was then adjusted to 8–9 and the mixture was stirred for 4 h. The filtrate was kept at room temperature for about two weeks, and blue block shaped crystals of (I) suitable for for X-ray single-crystal analyses were obtained.

## Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

## Figures

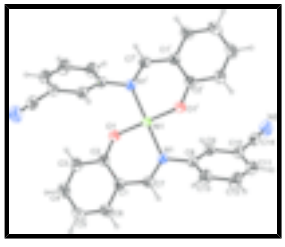


Fig. 1. Molecular view of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii. [Symmetry code: (i) $1-x$, $1-y$, $1-z$]

## Bis[2-(3-cyanophenyliminomethyl)phenolato]nickel(II)

*Crystal data*

$[Ni(C_{14}H_9N_2O_1)_2]$ $F_{000} = 516$

| | |
|---|---|
| $M_r$ = 501.17 | $D_x$ = 1.502 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 10336 reflections |
| $a$ = 9.0294 (18) Å | θ = 3.1–27.4º |
| $b$ = 8.0856 (16) Å | μ = 0.91 mm$^{-1}$ |
| $c$ = 15.644 (3) Å | $T$ = 293 (2) K |
| β = 104.01 (3)º | Block, blue |
| $V$ = 1108.1 (4) Å$^3$ | 0.25 × 0.18 × 0.18 mm |
| $Z$ = 2 | |

*Data collection*

| | |
|---|---|
| Rigaku Mercury2 diffractometer | 2540 independent reflections |
| Radiation source: fine-focus sealed tube | 2246 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.035 |
| Detector resolution: 13.6612 pixels mm$^{-1}$ | $\theta_{max}$ = 27.5º |
| $T$ = 293(2) K | $\theta_{min}$ = 3.1º |
| ω scans | $h$ = −11→11 |
| Absorption correction: multi-scan (CrystalClear; Rigaku, 2005) | $k$ = −10→10 |
| $T_{min}$ = 0.852, $T_{max}$ = 1.00 | $l$ = −20→20 |
| 11052 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.034 | H-atom parameters constrained |
| $wR(F^2)$ = 0.090 | $w = 1/[\sigma^2(F_o^2) + (0.0403P)^2 + 0.5389P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.10 | $(\Delta/\sigma)_{max} < 0.001$ |
| 2540 reflections | $\Delta\rho_{max}$ = 0.32 e Å$^{-3}$ |
| 160 parameters | $\Delta\rho_{min}$ = −0.35 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 $F^2 > 2\text{sigma}(F^2)$ is used only for calculat-

ing *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 | 0.5000 | 0.02514 (11) |
| O1 | 0.66446 (15) | 0.36034 (17) | 0.52053 (9) | 0.0349 (3) |
| N1 | 0.41172 (16) | 0.38940 (18) | 0.58415 (10) | 0.0266 (3) |
| C9 | 0.3215 (2) | 0.6210 (2) | 0.65595 (12) | 0.0302 (4) |
| H9 | 0.4159 | 0.6714 | 0.6613 | 0.036* |
| C14 | 0.2380 (2) | 0.8635 (3) | 0.72431 (15) | 0.0401 (5) |
| C1 | 0.5678 (2) | 0.1429 (2) | 0.59534 (12) | 0.0283 (4) |
| C10 | 0.2087 (2) | 0.6997 (2) | 0.68770 (12) | 0.0318 (4) |
| C8 | 0.2929 (2) | 0.4678 (2) | 0.61652 (12) | 0.0274 (4) |
| C11 | 0.0679 (2) | 0.6238 (3) | 0.68133 (14) | 0.0395 (5) |
| H11 | −0.0069 | 0.6759 | 0.7034 | 0.047* |
| C3 | 0.7949 (2) | 0.1080 (3) | 0.54150 (14) | 0.0383 (5) |
| H3 | 0.8663 | 0.1492 | 0.5130 | 0.046* |
| C2 | 0.6729 (2) | 0.2098 (2) | 0.55130 (11) | 0.0286 (4) |
| C13 | 0.1528 (2) | 0.3938 (3) | 0.60894 (15) | 0.0404 (5) |
| H13 | 0.1329 | 0.2914 | 0.5815 | 0.048* |
| C7 | 0.4475 (2) | 0.2409 (2) | 0.61321 (12) | 0.0297 (4) |
| H7 | 0.3897 | 0.1942 | 0.6488 | 0.036* |
| C5 | 0.7059 (3) | −0.1167 (3) | 0.61697 (15) | 0.0432 (5) |
| H5 | 0.7169 | −0.2245 | 0.6382 | 0.052* |
| N2 | 0.2618 (3) | 0.9944 (2) | 0.75059 (17) | 0.0570 (6) |
| C12 | 0.0409 (2) | 0.4716 (3) | 0.64212 (17) | 0.0461 (6) |
| H12 | −0.0527 | 0.4199 | 0.6377 | 0.055* |
| C4 | 0.8094 (3) | −0.0502 (3) | 0.57343 (15) | 0.0430 (5) |
| H4 | 0.8904 | −0.1149 | 0.5658 | 0.052* |
| C6 | 0.5875 (3) | −0.0197 (2) | 0.62794 (14) | 0.0366 (4) |
| H6 | 0.5184 | −0.0625 | 0.6577 | 0.044* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ni1 | 0.02507 (18) | 0.02233 (17) | 0.03093 (19) | 0.00178 (12) | 0.01241 (13) | 0.00362 (12) |
| O1 | 0.0309 (7) | 0.0327 (7) | 0.0458 (8) | 0.0070 (6) | 0.0182 (6) | 0.0125 (6) |
| N1 | 0.0262 (7) | 0.0245 (7) | 0.0319 (7) | −0.0009 (6) | 0.0124 (6) | −0.0003 (6) |
| C9 | 0.0294 (9) | 0.0286 (9) | 0.0360 (9) | −0.0003 (7) | 0.0146 (8) | 0.0016 (7) |
| C14 | 0.0431 (12) | 0.0363 (12) | 0.0480 (12) | 0.0067 (9) | 0.0247 (10) | 0.0000 (9) |
| C1 | 0.0305 (9) | 0.0236 (9) | 0.0309 (9) | 0.0009 (7) | 0.0075 (7) | 0.0007 (7) |
| C10 | 0.0348 (10) | 0.0305 (9) | 0.0332 (9) | 0.0058 (8) | 0.0140 (8) | 0.0022 (8) |
| C8 | 0.0282 (9) | 0.0272 (9) | 0.0300 (9) | 0.0015 (7) | 0.0133 (7) | 0.0023 (7) |
| C11 | 0.0327 (10) | 0.0449 (12) | 0.0461 (11) | 0.0093 (9) | 0.0194 (9) | 0.0032 (9) |
| C3 | 0.0335 (10) | 0.0412 (11) | 0.0425 (11) | 0.0088 (9) | 0.0134 (9) | 0.0043 (9) |
| C2 | 0.0294 (9) | 0.0282 (9) | 0.0278 (9) | 0.0036 (7) | 0.0064 (7) | 0.0020 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C13 | 0.0348 (10) | 0.0378 (11) | 0.0521 (12) | −0.0068 (9) | 0.0174 (9) | −0.0090 (9) |
| C7 | 0.0315 (9) | 0.0263 (9) | 0.0335 (9) | −0.0034 (7) | 0.0122 (7) | 0.0022 (7) |
| C5 | 0.0491 (13) | 0.0250 (10) | 0.0528 (13) | 0.0073 (9) | 0.0070 (10) | 0.0048 (9) |
| N2 | 0.0685 (15) | 0.0369 (11) | 0.0762 (15) | −0.0001 (9) | 0.0379 (12) | −0.0109 (10) |
| C12 | 0.0294 (10) | 0.0550 (14) | 0.0592 (14) | −0.0081 (9) | 0.0212 (10) | −0.0084 (11) |
| C4 | 0.0407 (12) | 0.0397 (11) | 0.0476 (12) | 0.0173 (9) | 0.0085 (9) | 0.0018 (10) |
| C6 | 0.0398 (11) | 0.0266 (10) | 0.0437 (11) | −0.0013 (8) | 0.0104 (9) | 0.0045 (8) |

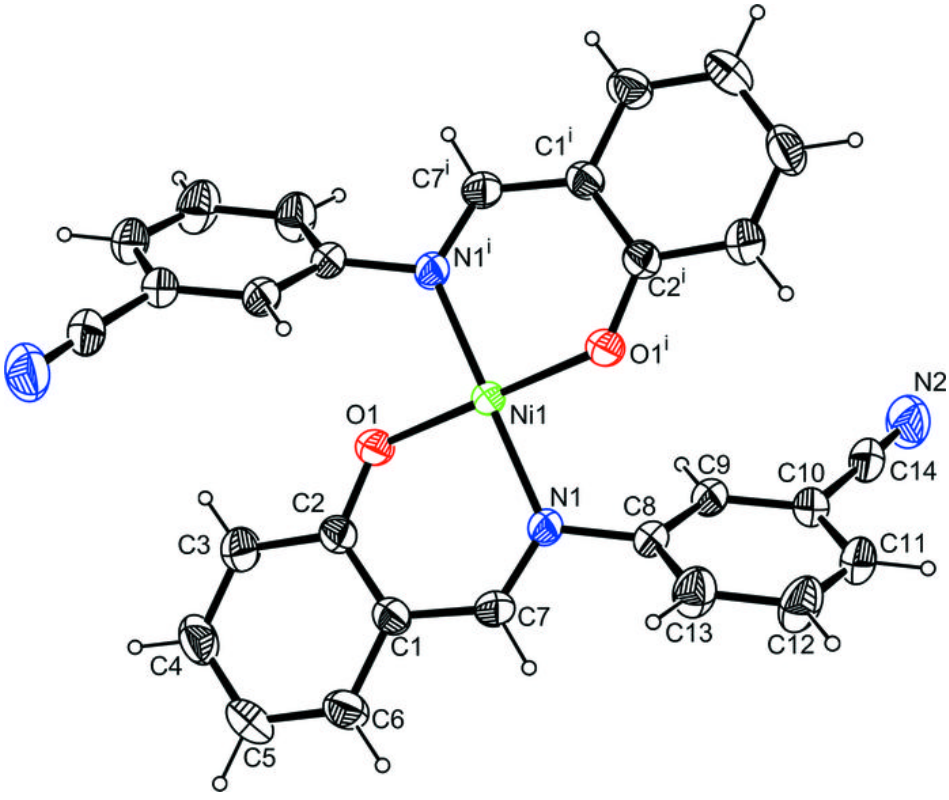
*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Ni1—O1$^{i}$ | 1.8310 (14) | C8—C13 | 1.378 (3) |
| Ni1—O1 | 1.8310 (14) | C11—C12 | 1.371 (3) |
| Ni1—N1$^{i}$ | 1.9174 (15) | C11—H11 | 0.9300 |
| Ni1—N1 | 1.9174 (15) | C3—C4 | 1.368 (3) |
| O1—C2 | 1.304 (2) | C3—C2 | 1.413 (3) |
| N1—C7 | 1.297 (2) | C3—H3 | 0.9300 |
| N1—C8 | 1.440 (2) | C13—C12 | 1.393 (3) |
| C9—C8 | 1.380 (3) | C13—H13 | 0.9300 |
| C9—C10 | 1.391 (3) | C7—H7 | 0.9300 |
| C9—H9 | 0.9300 | C5—C6 | 1.370 (3) |
| C14—N2 | 1.137 (3) | C5—C4 | 1.390 (3) |
| C14—C10 | 1.442 (3) | C5—H5 | 0.9300 |
| C1—C6 | 1.406 (2) | C12—H12 | 0.9300 |
| C1—C2 | 1.409 (3) | C4—H4 | 0.9300 |
| C1—C7 | 1.426 (3) | C6—H6 | 0.9300 |
| C10—C11 | 1.393 (3) | | |
| O1$^{i}$—Ni1—O1 | 180.000 (1) | C10—C11—H11 | 120.4 |
| O1$^{i}$—Ni1—N1$^{i}$ | 92.65 (6) | C4—C3—C2 | 120.89 (19) |
| O1—Ni1—N1$^{i}$ | 87.35 (6) | C4—C3—H3 | 119.6 |
| O1$^{i}$—Ni1—N1 | 87.35 (6) | C2—C3—H3 | 119.6 |
| O1—Ni1—N1 | 92.65 (6) | O1—C2—C1 | 123.56 (17) |
| N1$^{i}$—Ni1—N1 | 180.000 (1) | O1—C2—C3 | 118.75 (17) |
| C2—O1—Ni1 | 127.78 (12) | C1—C2—C3 | 117.68 (17) |
| C7—N1—C8 | 115.34 (15) | C8—C13—C12 | 120.4 (2) |
| C7—N1—Ni1 | 124.25 (13) | C8—C13—H13 | 119.8 |
| C8—N1—Ni1 | 120.35 (12) | C12—C13—H13 | 119.8 |
| C8—C9—C10 | 119.75 (18) | N1—C7—C1 | 125.63 (17) |
| C8—C9—H9 | 120.1 | N1—C7—H7 | 117.2 |
| C10—C9—H9 | 120.1 | C1—C7—H7 | 117.2 |
| N2—C14—C10 | 177.8 (2) | C6—C5—C4 | 118.5 (2) |
| C6—C1—C2 | 119.71 (18) | C6—C5—H5 | 120.7 |
| C6—C1—C7 | 118.93 (18) | C4—C5—H5 | 120.7 |
| C2—C1—C7 | 121.21 (16) | C11—C12—C13 | 120.4 (2) |
| C9—C10—C11 | 120.51 (18) | C11—C12—H12 | 119.8 |
| C9—C10—C14 | 118.81 (18) | C13—C12—H12 | 119.8 |
| C11—C10—C14 | 120.64 (18) | C3—C4—C5 | 121.6 (2) |
| C13—C8—C9 | 119.78 (17) | C3—C4—H4 | 119.2 |

| | | | |
|---|---|---|---|
| C13—C8—N1 | 121.69 (17) | C5—C4—H4 | 119.2 |
| C9—C8—N1 | 118.53 (16) | C5—C6—C1 | 121.6 (2) |
| C12—C11—C10 | 119.20 (19) | C5—C6—H6 | 119.2 |
| C12—C11—H11 | 120.4 | C1—C6—H6 | 119.2 |

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

**Fig. 1**


C1i
C7i
N1i
C2i
O1i
N2
O1
Ni1
C9
C10
C14
C2
N1
C8
C3
C11
C7
C13
C12
C1
C4
C6
C5