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Bis{2-[imino(phenyl)methyl]-5-methoxyphenolato-κ^2N,O^1}nickel(II)

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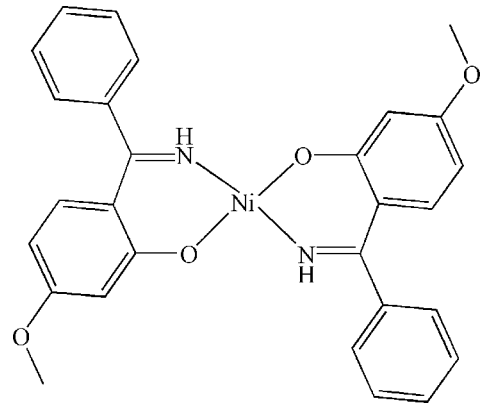
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.025; wR factor = 0.064; data-to-parameter ratio = 12.5.

The title complex, $[Ni(C_{14}H_{12}NO_2)_2]$, lies about an inversion center. The Ni^{II} atom is coordinated in a slightly distorted square-planar geometry by two O atoms and two N atoms from two 2-[imino(phenyl)methyl]-5-methoxyphenolate ligands. The dihedral angle between the symmetry-unique phenyl and benzene rings is 73.2 (1)°.

Related literature

For background to 2-imino(methyl)phenol compounds, see: Zhang *et al.* (2008, 2009); Jiang *et al.* (2003); Liu *et al.* (2009). For a related structure, see: Bernès (2010).



Experimental

Crystal data

$[Ni(C_{14}H_{12}NO_2)_2]$
M_r = 511.20
Monoclinic, $P2_1/n$
a = 11.882 (2) Å
b = 5.4983 (10) Å
c = 17.494 (3) Å
β = 91.913 (2)°
V = 1142.3 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.89 mm^{-1}
T = 296 K
0.24 × 0.15 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.244, T_{max} = 0.453
5526 measured reflections
2010 independent reflections
1680 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.064
S = 1.03
2010 reflections
161 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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: LH5543).

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supporting information

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Bis{2-[imino(phenyl)methyl]-5-methoxyphenolato-κ^2N,O^1}nickel(II)

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S1. Comment

2-Imino(methyl)phenol compounds have been studied for many years (Jiang *et al.*, 2003; Zhang *et al.*, 2008, 2009; Bernés 2010; Liu *et al.*, 2009) and have attracted interest because of their magnetic properties. The crystal structure of the title compound (I) is presented herein.

The molecular structure of (I) is shown in Fig .1. The Ni^{II} ion lies on a centre of inversion and is coordinated by two O atoms and two N atoms from two bidentate ligands, forming a slightly distorted square-planar geometry. The dihedral angle between the symmetry unique phenyl and benzene rings is 73.2 (1) °.

S2. Experimental

Complex (I) was prepared from a mixture of 2-hydroxy-4-methoxy benzophenone (1 mmol, 0.228 g), ammonia (25%, 0.5 ml), triethylamine (0.5 ml), nickel(II) acetate tetrahydrate (0.5 mmol, 0.127 g) and methanol(8 mL) sealed in a 15 mL teflon-lined stainless steel bomb, and kept at 393 K for 120 h under autogenous pressure. After the reaction was slowly cooled to room temperature, green rectangular plates were produced (yield: 63%, based on Nickel). Anal. Calcd for $C_{28}H_{24}N_2NiO_4$(%): C, 65.78; H, 4.73; N, 5.48. Found(%): C, 65.72; H, 4.76; N, 5.53.

S3. Refinement

H atoms were positioned geometrically and refined with a riding model, with distances 0.86(N—H), 0.96(CH_3) or 0.93 Å (aromatic ring), and with U_{iso}(H) = 1.2 U_{eq}(aromatic ring, N—H) or U_{iso}(H) = 1.5 U_{eq}(CH_3).

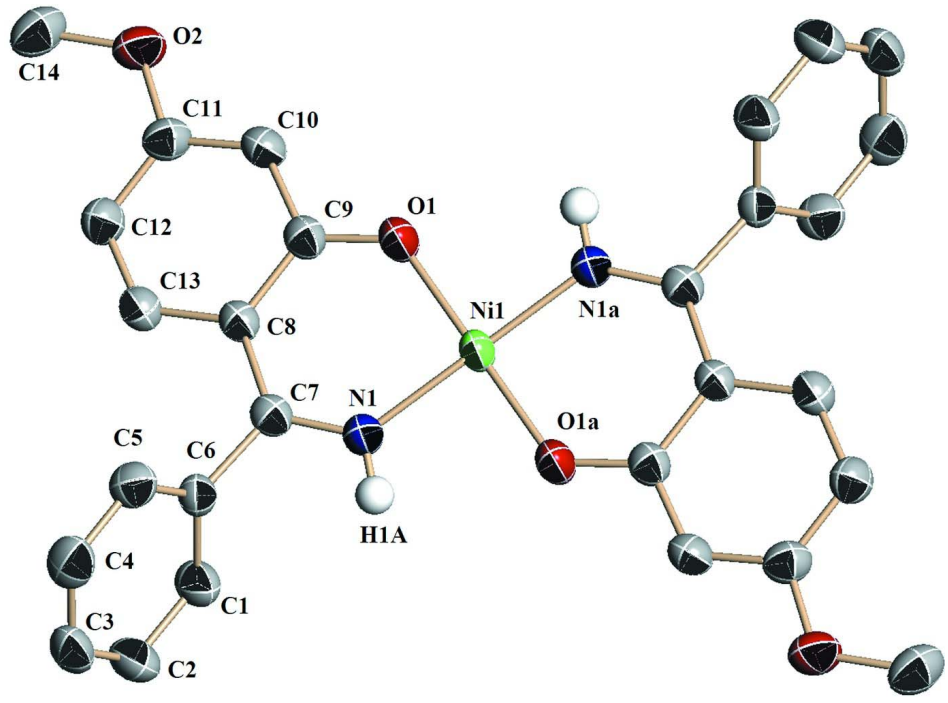

Figure 1

The molecular structure of (I), showing 30 % probability displacement ellipsoids. H atoms bonded to atoms are not shown. Symmetry code (a); 1-x, -y, 2-z.

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Crystal data

$[Ni(C_{14}H_{12}NO_2)_2]$
$M_r = 511.20$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 11.882$ (2) Å
$b = 5.4983$ (10) Å
$c = 17.494$ (3) Å
$\beta = 91.913$ (2)°
$V = 1142.3$ (4) Å^3
$Z = 2$
$F(000) = 532$
$D_x = 1.486$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2010 reflections
$\theta = 2.0$–$25.0°$
$\mu = 0.89$ mm^{-1}
$T = 296$ K
Plate, green
0.24 × 0.15 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.244$, $T_{max} = 0.453$
5526 measured reflections
2010 independent reflections
1680 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.0°$
$h = -14 \rightarrow 11$
$k = -6 \rightarrow 6$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.064$
$S = 1.03$
2010 reflections
161 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0308P)^2 + 0.224P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$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}
C1	0.47072 (17)	0.1107 (4)	0.71936 (11)	0.0451 (5)
H1	0.5182	−0.0211	0.7290	0.054*
C2	0.41390 (18)	0.1315 (4)	0.64899 (11)	0.0538 (5)
H2	0.4237	0.0140	0.6116	0.065*
C3	0.34319 (17)	0.3250 (4)	0.63443 (11)	0.0514 (5)
H3	0.3044	0.3374	0.5875	0.062*
C4	0.33005 (16)	0.4994 (4)	0.68923 (12)	0.0495 (5)
H4	0.2828	0.6311	0.6792	0.059*
C5	0.38659 (15)	0.4814 (3)	0.75956 (11)	0.0428 (5)
H5	0.3773	0.6012	0.7963	0.051*
C6	0.45685 (14)	0.2859 (3)	0.77523 (9)	0.0338 (4)
C7	0.50867 (14)	0.2546 (3)	0.85404 (9)	0.0346 (4)
C8	0.59499 (14)	0.4187 (3)	0.88197 (9)	0.0336 (4)
C9	0.63412 (15)	0.4204 (3)	0.96059 (10)	0.0359 (4)
C10	0.71438 (15)	0.5983 (4)	0.98239 (10)	0.0410 (4)
H10	0.7376	0.6093	1.0336	0.049*
C11	0.75958 (15)	0.7561 (4)	0.93082 (11)	0.0411 (4)
C12	0.72465 (16)	0.7507 (4)	0.85333 (10)	0.0428 (5)
H12	0.7555	0.8556	0.8180	0.051*
C13	0.64357 (15)	0.5853 (4)	0.83168 (10)	0.0389 (4)
H13	0.6191	0.5830	0.7806	0.047*
C14	0.88453 (18)	1.0924 (4)	0.91151 (13)	0.0564 (6)
H14A	0.9237	1.0160	0.8708	0.085*
H14B	0.9358	1.1940	0.9406	0.085*
H14C	0.8241	1.1898	0.8904	0.085*

Ni1	0.5000	0.0000	1.0000	0.03463 (12)
N1	0.47005 (13)	0.0801 (3)	0.89494 (8)	0.0404 (4)
H1A	0.4234	−0.0153	0.8712	0.048*
O2	0.84011 (12)	0.9107 (3)	0.96004 (8)	0.0573 (4)
O1	0.60041 (10)	0.2698 (2)	1.01257 (7)	0.0437 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0554 (12)	0.0395 (11)	0.0399 (10)	0.0065 (10)	−0.0067 (9)	0.0015 (9)
C2	0.0702 (14)	0.0538 (14)	0.0369 (11)	−0.0003 (12)	−0.0086 (10)	−0.0047 (10)
C3	0.0531 (12)	0.0599 (14)	0.0401 (11)	−0.0120 (11)	−0.0150 (9)	0.0128 (10)
C4	0.0407 (11)	0.0483 (12)	0.0587 (13)	0.0024 (10)	−0.0116 (9)	0.0105 (11)
C5	0.0416 (10)	0.0390 (11)	0.0475 (11)	0.0029 (9)	−0.0031 (8)	−0.0009 (9)
C6	0.0330 (9)	0.0353 (10)	0.0329 (9)	−0.0041 (8)	−0.0017 (7)	0.0061 (8)
C7	0.0343 (9)	0.0371 (10)	0.0322 (9)	0.0030 (8)	0.0011 (7)	−0.0004 (8)
C8	0.0350 (10)	0.0356 (9)	0.0301 (9)	0.0030 (8)	−0.0002 (7)	0.0006 (7)
C9	0.0369 (10)	0.0369 (10)	0.0339 (9)	0.0031 (8)	0.0009 (8)	0.0010 (8)
C10	0.0449 (11)	0.0458 (11)	0.0320 (9)	−0.0028 (9)	−0.0037 (8)	−0.0015 (9)
C11	0.0365 (10)	0.0430 (11)	0.0439 (10)	−0.0048 (9)	0.0016 (8)	−0.0052 (9)
C12	0.0426 (10)	0.0463 (12)	0.0397 (10)	−0.0081 (9)	0.0045 (8)	0.0035 (9)
C13	0.0400 (10)	0.0433 (11)	0.0334 (10)	0.0005 (9)	0.0001 (8)	0.0030 (8)
C14	0.0523 (13)	0.0493 (12)	0.0680 (14)	−0.0138 (11)	0.0090 (11)	−0.0067 (11)
Ni1	0.0386 (2)	0.0381 (2)	0.02698 (17)	−0.00429 (15)	−0.00215 (12)	0.00705 (14)
N1	0.0476 (9)	0.0416 (9)	0.0316 (7)	−0.0113 (7)	−0.0048 (7)	0.0054 (7)
O2	0.0616 (9)	0.0619 (9)	0.0483 (8)	−0.0262 (8)	−0.0007 (7)	−0.0050 (7)
O1	0.0501 (8)	0.0482 (8)	0.0323 (6)	−0.0107 (6)	−0.0051 (5)	0.0080 (6)

Geometric parameters (Å, º)

C1—C6	1.387 (3)	C9—C10	1.410 (3)
C1—C2	1.389 (3)	C10—C11	1.374 (3)
C1—H1	0.9300	C10—H10	0.9300
C2—C3	1.374 (3)	C11—O2	1.366 (2)
C2—H2	0.9300	C11—C12	1.405 (3)
C3—C4	1.369 (3)	C12—C13	1.369 (3)
C3—H3	0.9300	C12—H12	0.9300
C4—C5	1.385 (3)	C13—H13	0.9300
C4—H4	0.9300	C14—O2	1.424 (3)
C5—C6	1.383 (2)	C14—H14A	0.9600
C5—H5	0.9300	C14—H14B	0.9600
C6—C7	1.501 (2)	C14—H14C	0.9600
C7—N1	1.290 (2)	Ni1—N1	1.9118 (14)
C7—C8	1.439 (2)	Ni1—N1^{i}	1.9118 (14)
C8—C13	1.407 (3)	Ni1—O1	1.9120 (13)
C8—C9	1.437 (2)	Ni1—O1^{i}	1.9120 (13)
C9—O1	1.303 (2)	N1—H1A	0.8600

C6—C1—C2	120.12 (19)	C11—C10—H10	118.8
C6—C1—H1	119.9	C9—C10—H10	118.8
C2—C1—H1	119.9	O2—C11—C10	115.56 (16)
C3—C2—C1	120.3 (2)	O2—C11—C12	123.72 (17)
C3—C2—H2	119.9	C10—C11—C12	120.71 (17)
C1—C2—H2	119.9	C13—C12—C11	117.63 (17)
C4—C3—C2	119.73 (18)	C13—C12—H12	121.2
C4—C3—H3	120.1	C11—C12—H12	121.2
C2—C3—H3	120.1	C12—C13—C8	123.98 (16)
C3—C4—C5	120.59 (19)	C12—C13—H13	118.0
C3—C4—H4	119.7	C8—C13—H13	118.0
C5—C4—H4	119.7	O2—C14—H14A	109.5
C6—C5—C4	120.21 (18)	O2—C14—H14B	109.5
C6—C5—H5	119.9	H14A—C14—H14B	109.5
C4—C5—H5	119.9	O2—C14—H14C	109.5
C5—C6—C1	119.06 (16)	H14A—C14—H14C	109.5
C5—C6—C7	119.85 (16)	H14B—C14—H14C	109.5
C1—C6—C7	120.87 (16)	N1—Ni1—N1^{i}	180.00 (2)
N1—C7—C8	122.72 (15)	N1—Ni1—O1	91.56 (6)
N1—C7—C6	116.88 (15)	N1^{i}—Ni1—O1	88.44 (6)
C8—C7—C6	120.39 (15)	N1—Ni1—O1^{i}	88.44 (6)
C13—C8—C9	117.89 (16)	N1^{i}—Ni1—O1^{i}	91.56 (6)
C13—C8—C7	119.90 (15)	O1—Ni1—O1^{i}	180.0
C9—C8—C7	122.21 (16)	C7—N1—Ni1	130.26 (13)
O1—C9—C10	118.23 (15)	C7—N1—H1A	114.9
O1—C9—C8	124.53 (16)	Ni1—N1—H1A	114.9
C10—C9—C8	117.24 (16)	C11—O2—C14	118.83 (16)
C11—C10—C9	122.44 (17)	C9—O1—Ni1	128.17 (11)

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