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Bis(2-iminomethyl-5-methoxyphenolato)-nickel(II)

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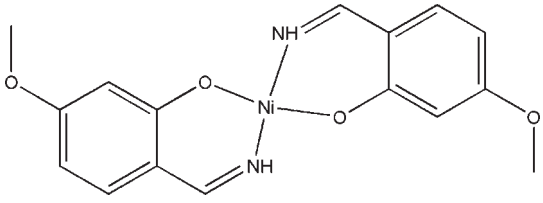
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.028; wR factor = 0.083; data-to-parameter ratio = 14.7.

The title compound, $[Ni(C_8H_8NO_2)_2]$, is a centrosymmetric mononuclear nickel(II) complex. The Ni^{II} ion, lying on an inversion centre, is four-coordinated in a square-planar geometry by two phenolate O and two imine N atoms from two symmetry-related 2-iminomethyl-5-methoxyphenolate ligands. In the crystal, molecules are linked into corrugated layers parallel to (100) by N—H···O hydrogen bonds.

Related literature

For related structures, see: Angulo *et al.* (2001); Dey *et al.* (2004); Edison *et al.* (2004); Ramadevi *et al.* (2005); Suh *et al.* (1996); Tang (2009); Kamenar *et al.* (1990); Costes *et al.* (1994).



Experimental

Crystal data

$[Ni(C_8H_8NO_2)_2]$
M_r = 359.02
Orthorhombic, *Pbca*
a = 7.5704 (16) Å
b = 11.331 (2) Å
c = 17.227 (4) Å
V = 1477.7 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.34 mm^{-1}
T = 298 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} = 0.795, T_{max} = 0.805
7939 measured reflections
1620 independent reflections
1122 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.083
S = 1.01
1620 reflections
110 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.8411 (16)	Ni1—N1	1.8529 (18)
O1^{i}—Ni1—O1	180	O1—Ni1—N1	93.92 (6)
O1—Ni1—N1^{i}	86.08 (6)	N1^{i}—Ni1—N1	180

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{ii}	0.90 (1)	2.391 (18)	3.166 (2)	144 (2)

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

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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2923).

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supporting information

Acta Cryst. (2009). E**65**, m1275 [https://doi.org/10.1107/S1600536809039233]

Bis(2-iminomethyl-5-methoxyphenolato)nickel(II)

Chunbao Tang

S1. Comment

Nickel(II) complexes play an important role in both bioinorganic chemistry and coordination chemistry (Suh *et al.*, 1996; Dey *et al.*, 2004; Angulo *et al.*, 2001; Ramadevi *et al.*, 2005; Edison *et al.*, 2004). Recently, the author has reported a nickel(II) complex (Tang, 2009). As a continuation of this work, the title mononuclear nickel(II) complex (Fig. 1), is reported in this paper.

The title complex is a centrosymmetric mononuclear nickel(II) complex. The Ni^{II} ion, lying on the inversion centre, is four-coordinated in a square-planar geometry, with two phenolate O and two imine N atoms from two 2-(iminomethyl)-5-methoxyphenolate ligands. The coordination bond lengths (Table 1) are comparable to those observed in related complexes (Kamenar *et al.*, 1990; Costes *et al.*, 1994).

In the crytal structure, molecules are linked through intermolecular N—H···O hydrogen bonds (Table 2), forming zigzag layers parallel to the (100) [Fig.2].

S2. Experimental

4-Methoxy-2-hydroxybenzaldehyde (0.2 mmol, 30.5 mg) and nickel(II) nitrate hexahydrate (0.1 mmol, 29.1 mg) were mixed in a methanol solution (20 ml) which contains small quantity of ammonia. The mixture was stirred at room temperature for 30 min to give a red solution. The solution was allowed to stand in air for 8 d, yielding red block-shaped crystals of the title complex. The absorption band indicative of the C═N double bond formation in the IR spectrum of the complex is at 1617 cm^{-1}.

S3. Refinement

Atom H1 was located in a difference Fourier map and refined isotropically, with N-H distance restrained to 0.90 (1) Å and U_{iso} set at 0.08 $Å^2$. Other H atoms were constrained to ideal geometries, with C-H = 0.93–0.96 Å and U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(C8).

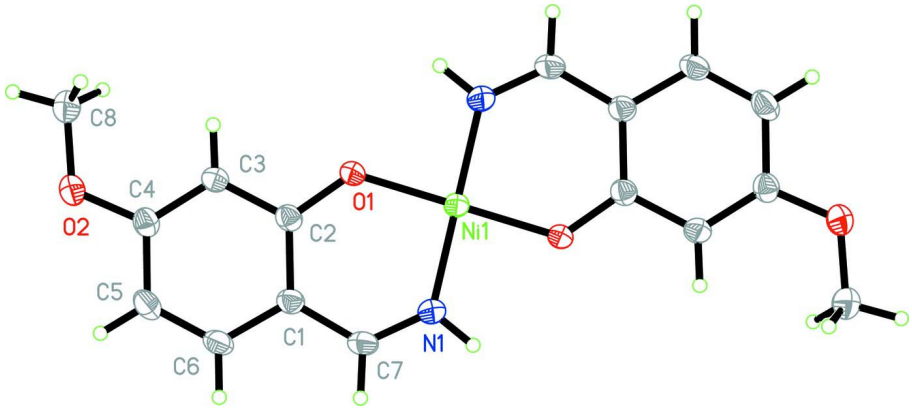

Figure 1

The molecular structure of the title complex. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are at the symmetry position (2-x, -y, 1-z).

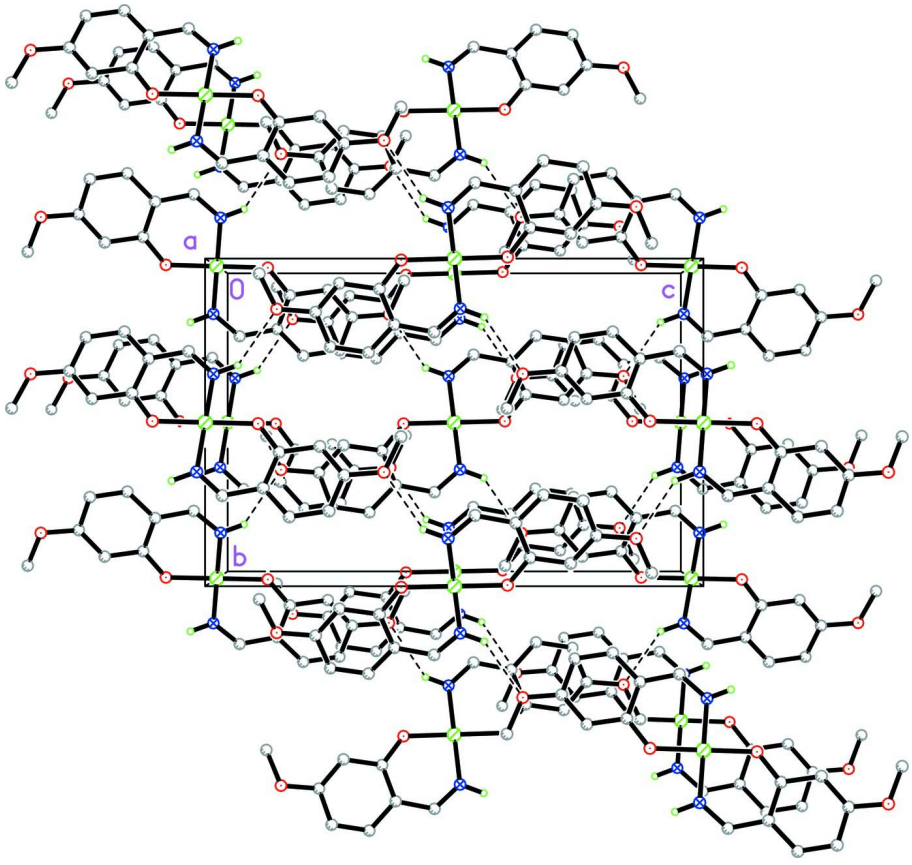

Figure 2

Packing diagram, viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.

Bis(2-iminomethyl-5-methoxyphenolato)nickel(II)

Crystal data

$[Ni(C_8H_8NO_2)_2]$
$M_r = 359.02$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 7.5704$ (16) Å
$b = 11.331$ (2) Å
$c = 17.227$ (4) Å
$V = 1477.7$ (5) Å^3
$Z = 4$
$F(000) = 744$
$D_x = 1.614$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1894 reflections
$\theta = 2.3$–$26.2°$
$\mu = 1.34$ mm^{-1}
$T = 298$ K
Block, red
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)
$T_{min} = 0.795$, $T_{max} = 0.805$
7939 measured reflections
1620 independent reflections
1122 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.4°$
$h = -9 \rightarrow 6$
$k = -11 \rightarrow 14$
$l = -21 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.083$
$S = 1.01$
1620 reflections
110 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
$w = 1/[\sigma^2(F_o^2) + (0.0414P)^2 + 0.384P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	1.0000	0.0000	0.5000	0.03483 (14)
O1	0.98642 (18)	0.00398 (11)	0.39332 (9)	0.0407 (4)
O2	0.8757 (2)	0.14990 (13)	0.13928 (8)	0.0486 (4)
N1	0.9039 (3)	0.14925 (16)	0.51213 (9)	0.0422 (4)

C1	0.8581 (3)	0.19740 (17)	0.37798 (11)	0.0366 (5)
C2	0.9275 (3)	0.08998 (17)	0.34895 (11)	0.0352 (4)
C3	0.9336 (3)	0.07278 (17)	0.26800 (11)	0.0369 (5)
H3	0.9783	0.0026	0.2480	0.044*
C4	0.8738 (3)	0.15895 (18)	0.21830 (11)	0.0380 (5)
C5	0.8038 (3)	0.26481 (18)	0.24643 (12)	0.0457 (5)
H5	0.7634	0.3224	0.2123	0.055*
C6	0.7956 (3)	0.28230 (19)	0.32452 (12)	0.0426 (5)
H6	0.7473	0.3522	0.3433	0.051*
C7	0.8489 (3)	0.22017 (18)	0.45884 (12)	0.0423 (5)
H7	0.7997	0.2915	0.4746	0.051*
C8	0.9403 (4)	0.0435 (2)	0.10637 (13)	0.0547 (6)
H8A	1.0625	0.0338	0.1198	0.082*
H8B	0.9286	0.0467	0.0509	0.082*
H8C	0.8736	−0.0220	0.1261	0.082*
H1	0.897 (3)	0.176 (2)	0.5612 (8)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0469 (2)	0.0262 (2)	0.0314 (2)	0.00123 (15)	−0.00135 (15)	−0.00138 (14)
O1	0.0622 (10)	0.0268 (8)	0.0330 (7)	0.0072 (6)	−0.0022 (6)	0.0002 (5)
O2	0.0658 (10)	0.0432 (9)	0.0367 (8)	0.0046 (7)	−0.0027 (7)	0.0072 (7)
N1	0.0578 (12)	0.0320 (10)	0.0367 (10)	0.0037 (9)	−0.0006 (8)	−0.0044 (7)
C1	0.0413 (11)	0.0290 (10)	0.0395 (11)	−0.0004 (8)	−0.0032 (8)	−0.0019 (9)
C2	0.0384 (11)	0.0289 (11)	0.0382 (11)	−0.0038 (9)	−0.0029 (8)	0.0015 (8)
C3	0.0442 (11)	0.0284 (10)	0.0381 (11)	0.0001 (9)	0.0005 (9)	−0.0001 (8)
C4	0.0402 (12)	0.0361 (11)	0.0378 (11)	−0.0045 (9)	−0.0036 (8)	0.0045 (9)
C5	0.0532 (12)	0.0351 (12)	0.0488 (13)	0.0023 (10)	−0.0072 (10)	0.0107 (10)
C6	0.0499 (13)	0.0279 (11)	0.0500 (13)	0.0058 (9)	−0.0032 (10)	0.0007 (10)
C7	0.0516 (14)	0.0281 (11)	0.0472 (13)	0.0038 (10)	−0.0018 (10)	−0.0050 (9)
C8	0.0743 (16)	0.0515 (14)	0.0382 (12)	0.0055 (13)	−0.0010 (11)	0.0029 (11)

Geometric parameters (Å, º)

Ni1—O1^{i}	1.8411 (16)	C2—C3	1.409 (3)
Ni1—O1	1.8411 (16)	C3—C4	1.375 (3)
Ni1—N1^{i}	1.8529 (18)	C3—H3	0.93
Ni1—N1	1.8529 (18)	C4—C5	1.398 (3)
O1—C2	1.316 (2)	C5—C6	1.361 (3)
O2—C4	1.365 (2)	C5—H5	0.93
O2—C8	1.419 (3)	C6—H6	0.93
N1—C7	1.289 (3)	C7—H7	0.93
N1—H1	0.901 (10)	C8—H8A	0.96
C1—C6	1.413 (3)	C8—H8B	0.96
C1—C2	1.417 (3)	C8—H8C	0.96
C1—C7	1.418 (3)		

O1^{i}—Ni1—O1	180	C2—C3—H3	119.8
O1^{i}—Ni1—N1^{i}	93.92 (6)	O2—C4—C3	124.35 (19)
O1—Ni1—N1^{i}	86.08 (6)	O2—C4—C5	114.44 (18)
O1^{i}—Ni1—N1	86.08 (6)	C3—C4—C5	121.21 (19)
O1—Ni1—N1	93.92 (6)	C6—C5—C4	119.00 (19)
N1^{i}—Ni1—N1	180	C6—C5—H5	120.5
C2—O1—Ni1	128.08 (13)	C4—C5—H5	120.5
C4—O2—C8	117.75 (16)	C5—C6—C1	121.97 (19)
C7—N1—Ni1	127.97 (15)	C5—C6—H6	119.0
C7—N1—H1	116.0 (17)	C1—C6—H6	119.0
Ni1—N1—H1	116.0 (17)	N1—C7—C1	124.78 (19)
C6—C1—C2	118.63 (18)	N1—C7—H7	117.6
C6—C1—C7	119.98 (18)	C1—C7—H7	117.6
C2—C1—C7	121.40 (18)	O2—C8—H8A	109.5
O1—C2—C3	117.48 (18)	O2—C8—H8B	109.5
O1—C2—C1	123.82 (17)	H8A—C8—H8B	109.5
C3—C2—C1	118.69 (18)	O2—C8—H8C	109.5
C4—C3—C2	120.50 (19)	H8A—C8—H8C	109.5
C4—C3—H3	119.8	H8B—C8—H8C	109.5

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{ii}	0.90 (1)	2.39 (2)	3.166 (2)	144 (2)

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