Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(2-hydroxyiminomethyl-6-methoxyphenolato-κ^2O^1,N)nickel(II)

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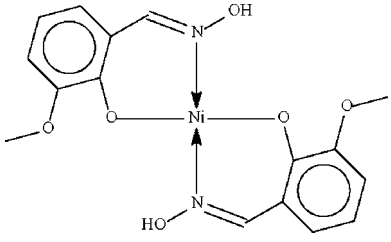
Received 18 February 2009; accepted 19 February 2009

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; R factor = 0.036; wR factor = 0.105; data-to-parameter ratio = 12.0.

The Ni atom in the title compound, $[Ni(C_8H_8NO_3)_2]$, lies on a center of inversion in a square-planar coordination environment. The hydroxyl group of one anion forms a short hydrogen bond to the metal-coordinated O atom of the other anion.

Related literature

For the structure of *o*-vanillin oxime, see: Xu *et al.* (2004). For the structure of bis(salicylaldoximato)nickel, see: Srivastava *et al.* (1967). The title compound is expected to form complexes with nitrogen-donor ligands as bis(salicylaldoxinato)nickel forms such adducts; see, for example, Hultgren *et al.* (2001); Lalia-Kantouri *et al.* (1999); Ma *et al.* (2007*a*,*b*).



Experimental

Crystal data

$[Ni(C_8H_8NO_3)_2]$
M_r = 391.02
Monoclinic, $P2_1/n$
a = 8.3464 (8) Å
b = 4.8596 (4) Å
c = 18.735 (2) Å
β = 95.376 (2)°
V = 756.5 (1) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.32 mm^{-1}
T = 173 K
0.48 × 0.16 × 0.15 mm

Data collection

Bruker APEX2 diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.570, T_{max} = 0.826
3461 measured reflections
1405 independent reflections
1178 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.105
S = 1.13
1405 reflections
117 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—O1	1.827 (2)	Ni1—N1	1.866 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O1^{i}	0.84	1.86	2.492 (3)	131

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

We thank the Natural Science Foundation of Guangxi, Guangxi Normal University and the University of Malaya for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2577).

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supporting information

Acta Cryst. (2009). E**65**, m318 [doi:10.1107/S1600536809005996]

Bis(2-hydroxyiminomethyl-6-methoxyphenolato-κ^2O^1,N)nickel(II)

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S1. Experimental

Nickel perchlorate hexahydrate (0.36 g, 1 mmol), 3-methoxysalicylaldoxime (0.17 g, 1 mmol) and DMF (8 ml) were placed in a 15 ml Teflon-lined autoclave. The autoclave was heated at 353 K for 3 days. The autoclave was cooled over a period of 8 h at a rate of 10 K per hour. Green crystals were collected by filtration, washed with methanol, and dried in air; yield 30% based on Ni.

S2. Refinement

Carbon-bound H atoms were placed at calculated positions (C–H 0.95 to 0.98 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2–1.5 times U_{eq}(C).

The crystal was original measured in the triclinic setting; the raw data when processed for absorption effects in the correct monoclinic setting had somewhat fewer reflections.

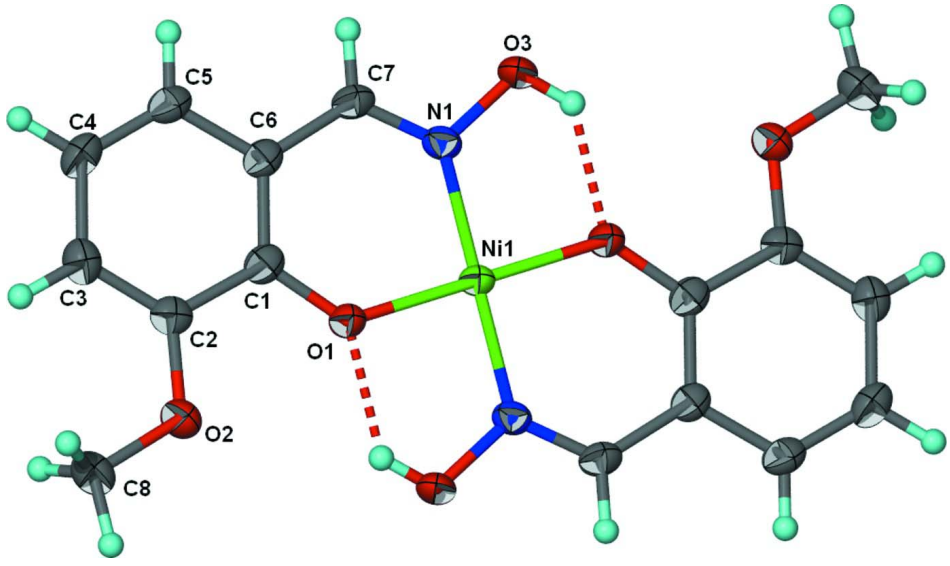

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $Ni(C_8H_8NO_3)_2$. Displacement ellipsoids are drawn at the 70% probability level, and H atoms as spheres of arbitrary radius. The dashed lines denote hydrogen bonds.

Bis(2-hydroxyiminomethyl-6-methoxyphenolato-κ^2O^1,N)nickel(II)

Crystal data

$[Ni(C_8H_8NO_3)_2]$
$M_r = 391.02$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 8.3464$ (8) Å
$b = 4.8596$ (4) Å
$c = 18.735$ (2) Å
$\beta = 95.376$ (2)°
$V = 756.5$ (1) Å^3
$Z = 2$
$F(000) = 404$
$D_x = 1.717$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1702 reflections
$\theta = 2.6$–$26.0°$
$\mu = 1.32$ mm^{-1}
$T = 173$ K
Prism, green
0.48 × 0.16 × 0.15 mm

Data collection

Bruker APEX2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.570$, $T_{max} = 0.826$
3461 measured reflections
1405 independent reflections
1178 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.2°$
$h = -8 \rightarrow 10$
$k = -5 \rightarrow 4$
$l = -14 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.105$
$S = 1.13$
1405 reflections
117 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
$w = 1/[\sigma^2(F_o^2) + (0.0656P)^2 + 0.2378P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.67$ e Å^{-3}

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	0.0169 (2)
O1	0.5102 (2)	0.2294 (4)	0.43290 (9)	0.0214 (4)
O2	0.5912 (2)	−0.1173 (5)	0.33768 (9)	0.0262 (5)
O3	0.2047 (2)	0.6111 (5)	0.55486 (10)	0.0257 (5)
H3	0.2703	0.7276	0.5735	0.039*
N1	0.2806 (3)	0.4473 (5)	0.50729 (11)	0.0192 (5)
C1	0.3919 (3)	0.0737 (6)	0.40274 (13)	0.0210 (6)
C2	0.4326 (3)	−0.1201 (6)	0.35041 (12)	0.0207 (6)
C3	0.3162 (3)	−0.2898 (6)	0.31716 (13)	0.0247 (6)
H3A	0.3443	−0.4196	0.2825	0.030*
C4	0.1567 (3)	−0.2720 (6)	0.33415 (13)	0.0249 (6)
H4	0.0773	−0.3896	0.3109	0.030*
C5	0.1144 (3)	−0.0863 (6)	0.38401 (13)	0.0227 (6)

H5	0.0057	−0.0748	0.3949	0.027*
C6	0.2328 (3)	0.0897 (6)	0.41955 (13)	0.0201 (6)
C7	0.1836 (3)	0.2781 (6)	0.47199 (12)	0.0212 (6)
H7	0.0737	0.2788	0.4814	0.025*
C8	0.6428 (4)	−0.3281 (6)	0.29197 (14)	0.0280 (7)
H8A	0.7599	−0.3188	0.2912	0.042*
H8B	0.5910	−0.3019	0.2433	0.042*
H8C	0.6128	−0.5084	0.3100	0.042*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0126 (3)	0.0189 (3)	0.0194 (3)	0.00116 (19)	0.00209 (17)	−0.00161 (17)
O1	0.0155 (10)	0.0228 (11)	0.0263 (8)	−0.0005 (8)	0.0032 (7)	−0.0067 (7)
O2	0.0226 (11)	0.0263 (12)	0.0304 (10)	0.0010 (9)	0.0063 (8)	−0.0080 (9)
O3	0.0148 (10)	0.0342 (13)	0.0288 (9)	0.0006 (9)	0.0055 (7)	−0.0106 (9)
N1	0.0151 (12)	0.0226 (14)	0.0201 (10)	0.0038 (9)	0.0021 (8)	−0.0004 (8)
C1	0.0201 (14)	0.0205 (15)	0.0220 (12)	−0.0015 (11)	−0.0004 (10)	0.0023 (10)
C2	0.0205 (14)	0.0220 (15)	0.0197 (11)	0.0016 (12)	0.0021 (9)	0.0038 (10)
C3	0.0293 (16)	0.0220 (16)	0.0225 (11)	0.0004 (12)	0.0016 (10)	−0.0021 (11)
C4	0.0235 (15)	0.0253 (17)	0.0248 (12)	−0.0053 (12)	−0.0039 (10)	0.0023 (11)
C5	0.0186 (14)	0.0259 (16)	0.0235 (12)	−0.0039 (12)	0.0011 (10)	0.0040 (11)
C6	0.0190 (14)	0.0199 (14)	0.0210 (11)	−0.0014 (11)	−0.0001 (10)	0.0024 (10)
C7	0.0140 (13)	0.0253 (15)	0.0242 (12)	0.0014 (11)	0.0006 (9)	0.0019 (11)
C8	0.0287 (16)	0.0283 (18)	0.0278 (13)	0.0033 (12)	0.0065 (11)	−0.0041 (11)

Geometric parameters (Å, º)

Ni1—O1	1.827 (2)	C2—C3	1.378 (4)
Ni1—O1^{i}	1.827 (2)	C3—C4	1.400 (4)
Ni1—N1	1.866 (2)	C3—H3A	0.9500
Ni1—N1^{i}	1.866 (2)	C4—C5	1.369 (4)
O1—C1	1.328 (3)	C4—H4	0.9500
O2—C2	1.367 (3)	C5—C6	1.424 (4)
O2—C8	1.427 (3)	C5—H5	0.9500
O3—N1	1.391 (3)	C6—C7	1.431 (4)
O3—H3	0.8400	C7—H7	0.9500
N1—C7	1.292 (3)	C8—H8A	0.9800
C1—C6	1.395 (4)	C8—H8B	0.9800
C1—C2	1.423 (4)	C8—H8C	0.9800
O1—Ni1—O1^{i}	180.00 (7)	C4—C3—H3A	119.8
O1—Ni1—N1	93.50 (9)	C5—C4—C3	120.5 (3)
O1^{i}—Ni1—N1	86.50 (9)	C5—C4—H4	119.7
O1—Ni1—N1^{i}	86.50 (9)	C3—C4—H4	119.7
O1^{i}—Ni1—N1^{i}	93.50 (9)	C4—C5—C6	120.2 (3)
N1—Ni1—N1^{i}	180.00 (12)	C4—C5—H5	119.9
C1—O1—Ni1	128.47 (17)	C6—C5—H5	119.9

C2—O2—C8	116.7 (2)	C1—C6—C5	119.7 (3)
N1—O3—H3	109.5	C1—C6—C7	122.1 (3)
C7—N1—O3	113.0 (2)	C5—C6—C7	118.3 (2)
C7—N1—Ni1	128.46 (19)	N1—C7—C6	123.5 (2)
O3—N1—Ni1	118.51 (16)	N1—C7—H7	118.2
O1—C1—C6	123.9 (2)	C6—C7—H7	118.2
O1—C1—C2	117.0 (2)	O2—C8—H8A	109.5
C6—C1—C2	119.1 (3)	O2—C8—H8B	109.5
O2—C2—C3	125.5 (2)	H8A—C8—H8B	109.5
O2—C2—C1	114.3 (2)	O2—C8—H8C	109.5
C3—C2—C1	120.2 (2)	H8A—C8—H8C	109.5
C2—C3—C4	120.4 (3)	H8B—C8—H8C	109.5
C2—C3—H3A	119.8		

N1—Ni1—O1—C1	2.2 (2)	O2—C2—C3—C4	−179.3 (2)
N1^{i}—Ni1—O1—C1	−177.8 (2)	C1—C2—C3—C4	0.4 (4)
O1—Ni1—N1—C7	−2.1 (2)	C2—C3—C4—C5	−0.1 (4)
O1^{i}—Ni1—N1—C7	177.9 (2)	C3—C4—C5—C6	−0.4 (4)
O1—Ni1—N1—O3	179.66 (18)	O1—C1—C6—C5	179.9 (2)
O1^{i}—Ni1—N1—O3	−0.34 (18)	C2—C1—C6—C5	−0.3 (4)
Ni1—O1—C1—C6	−1.4 (4)	O1—C1—C6—C7	−0.3 (4)
Ni1—O1—C1—C2	178.79 (17)	C2—C1—C6—C7	179.5 (2)
C8—O2—C2—C3	−7.2 (4)	C4—C5—C6—C1	0.6 (4)
C8—O2—C2—C1	173.0 (2)	C4—C5—C6—C7	−179.2 (2)
O1—C1—C2—O2	−0.6 (3)	O3—N1—C7—C6	179.5 (2)
C6—C1—C2—O2	179.6 (2)	Ni1—N1—C7—C6	1.3 (4)
O1—C1—C2—C3	179.6 (2)	C1—C6—C7—N1	0.4 (4)
C6—C1—C2—C3	−0.2 (4)	C5—C6—C7—N1	−179.8 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O1^{i}	0.84	1.86	2.492 (3)	131

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