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{1-[(2-Morpholin-4-ylethylimino-κ^2N,N')methyl]naphthalen-2-olato-κO}-(thiocyanato-N)nickel(II)

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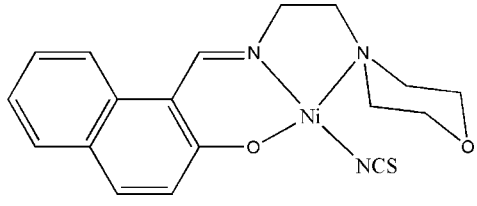
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.063; wR factor = 0.135; data-to-parameter ratio = 17.8.

In the title mononuclear nickel(II) complex, [Ni($C_{17}H_{19}N_2O_2$)(NCS)], the Ni^{II} atom is four-coordinated by the phenolate O, imine N and amine N atoms of one Schiff base ligand, and by the terminal N atom of a thiocyanate ligand, forming a square-planar geometry.

Related literature

For related literature, see: Arıcı *et al.* (2005); Brückner *et al.* (2000); Diao (2007*a*,*b*); Diao, Huang *et al.* (2007); Diao, Shu *et al.* (2007); Harrop *et al.* (2003); Li, Huang *et al.* (2007); Li, Jiang *et al.* (2007); Marganian *et al.* (1995); Ren *et al.* (2002); Usman *et al.* (2003); Van Hecke *et al.* (2007).



Experimental

Crystal data

[Ni($C_{17}H_{19}N_2O_2$)(NCS)]
M_r = 400.13
Orthorhombic, *Pbca*
a = 12.648 (3) Å
b = 12.647 (3) Å
c = 21.915 (4) Å
V = 3505.5 (12) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.24 mm^{-1}
T = 298 (2) K
0.32 × 0.32 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.692, T_{max} = 0.707
28592 measured reflections
4028 independent reflections
3012 reflections with $I > 2\sigma(I)$
R_{int} = 0.065

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.135
S = 1.16
4028 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.828 (2)	Ni1—N3	1.885 (3)
Ni1—N1	1.832 (3)	Ni1—N2	1.959 (3)
O1—Ni1—N1	93.38 (12)	O1—Ni1—N2	176.66 (11)
O1—Ni1—N3	87.57 (11)	N1—Ni1—N2	86.86 (12)
N1—Ni1—N3	171.51 (13)	N3—Ni1—N2	92.69 (12)

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: AT2382).

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supplementary materials

Acta Cryst. (2007). E**63**, m2494 [**doi:10.1107/S1600536807043073**]

{1-[(2-Morpholin-4-ylethylimino-κ^2N,N')methyl]naphthalen-2-olato-κO}(thiocyanato-*N*)nickel(II)

Y.-P. Diao, Y.-Z. Wang, M.-D. Wang and K. Li

Comment

Nickel(II) complexes with Schiff base ligands have received much attention in recent years (Marganian *et al.*, 1995). Some of the complexes have been found to have pharmacological and antitumor properties (Harrop *et al.*, 2003; Brückner *et al.*, 2000; Ren *et al.*, 2002). Nickel is also present in the active sites of several important classes of metalloproteins, as either a homodinuclear or a heterodinuclear species. We have recently reported a few transition metal complexes (Diao, 2007*a*,b; Diao, Huang *et al.*, 2007; Diao, Shu *et al.*, 2007; Li, Huang *et al.*, 2007). In order to further develop the coordination chemistry of such nickel complexes, we report herein the title new nickel(II) compound.

The Ni^{II} atom in the mononuclear complex is four-coordinate in a square-planar geometry with one phenolate O, one imine N, and one amine N atoms of one Schiff base ligand and one terminal N atom of a thiocyanate ligand (Fig. 1). All the bond values (Table 1) subtended at the metal centre are comparable with the values observed in other Schiff base nickel(II) complexes (Arıcı *et al.*, 2005; Usman *et al.*, 2003; Van Hecke *et al.*, 2007; Li, Jiang *et al.*, 2007).

Experimental

2-Hydroxy-1-naphthaldehyde (0.1 mmol, 17.0 mg), 2-morpholin-4-ylethylamine (0.1 mmol, 13.0 mg), ammonium thiocyanate (0.1 mmol, 7.5 mg), and $Ni(NO_3)_2{\cdot}6H_2O$ (0.1 mmol, 29.0 mg) were dissolved in a methanol solution (10 ml). The mixture was stirred at room temperature for 30 min to give a red solution. After keeping the solution in air for 8 days, red block-like crystals were formed.

Refinement

H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

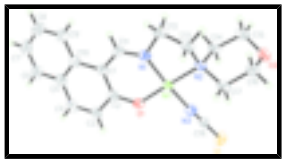


Fig. 1. The structure of the title complex with 30% probability level.

{1-[(2-Morpholin-4-ylethylimino-κ^2*N*,*N*')methyl]naphthalen-2-olato-κ*O*} (thiocyanato-*N*)nickel(II)

Crystal data

[Ni($C_{17}H_{19}N_2O_2$)(NCS)]	F_{000} = 1664
M_r = 400.13	D_x = 1.516 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 3770 reflections
a = 12.648 (3) Å	θ = 2.4–25.0º
b = 12.647 (3) Å	μ = 1.24 mm^{-1}
c = 21.915 (4) Å	*T* = 298 (2) K
V = 3505.5 (12) Å^3	Block, red
Z = 8	0.32 × 0.32 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer	4028 independent reflections
Radiation source: fine-focus sealed tube	3012 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.065
T = 298(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	*h* = −16→16
T_{min} = 0.692, T_{max} = 0.707	*k* = −16→16
28592 measured reflections	*l* = −28→28

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.063	H-atom parameters constrained
$wR(F^2)$ = 0.135	$w = 1/[\sigma^2(F_o^2) + (0.0577P)^2 + 0.5788P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.16	$(\Delta/\sigma)_{max} < 0.001$
4028 reflections	$\Delta\rho_{max}$ = 0.67 e Å^{-3}
226 parameters	$\Delta\rho_{min}$ = −0.36 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 $F^2 > \sigma(F^2)$ 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	0.10083 (3)	0.38201 (3)	0.331471 (19)	0.03927 (16)
S1	−0.00187 (9)	0.45522 (8)	0.13251 (5)	0.0641 (3)
O1	0.02168 (18)	0.49703 (19)	0.35297 (11)	0.0469 (6)
O2	0.2686 (2)	0.1258 (2)	0.21262 (13)	0.0623 (7)
N1	0.1692 (2)	0.3770 (2)	0.40509 (13)	0.0442 (7)
N2	0.17885 (19)	0.2534 (2)	0.30999 (12)	0.0393 (6)
N3	0.0480 (3)	0.3984 (2)	0.25161 (14)	0.0513 (7)
C1	0.1016 (2)	0.5384 (3)	0.44931 (15)	0.0408 (8)
C2	0.0287 (3)	0.5548 (3)	0.40201 (16)	0.0436 (8)
C3	−0.0427 (3)	0.6417 (3)	0.40643 (17)	0.0517 (9)
H3	−0.0959	0.6494	0.3775	0.062*
C4	−0.0344 (3)	0.7124 (3)	0.45163 (18)	0.0544 (10)
H4	−0.0813	0.7690	0.4528	0.065*
C5	0.0436 (3)	0.7039 (3)	0.49775 (18)	0.0513 (9)
C6	0.0570 (4)	0.7847 (4)	0.5416 (2)	0.0680 (12)
H6	0.0126	0.8433	0.5407	0.082*
C7	0.1325 (4)	0.7786 (4)	0.5847 (2)	0.0785 (14)
H7	0.1422	0.8338	0.6122	0.094*
C8	0.1962 (4)	0.6884 (4)	0.5877 (2)	0.0780 (14)
H8	0.2462	0.6826	0.6187	0.094*
C9	0.1860 (3)	0.6079 (3)	0.54553 (17)	0.0615 (11)
H9	0.2294	0.5487	0.5483	0.074*
C10	0.1111 (3)	0.6147 (3)	0.49864 (17)	0.0475 (9)
C11	0.1660 (3)	0.4476 (3)	0.44838 (16)	0.0467 (8)
H11	0.2103	0.4370	0.4817	0.056*
C12	0.2429 (3)	0.2881 (3)	0.41236 (17)	0.0585 (10)
H12A	0.2412	0.2621	0.4540	0.070*
H12B	0.3145	0.3104	0.4030	0.070*
C13	0.2089 (3)	0.2043 (3)	0.36966 (17)	0.0549 (10)
H13A	0.1489	0.1665	0.3865	0.066*
H13B	0.2660	0.1542	0.3635	0.066*
C14	0.2734 (3)	0.2859 (3)	0.27331 (17)	0.0493 (9)
H14A	0.3200	0.3279	0.2988	0.059*
H14B	0.2504	0.3300	0.2396	0.059*
C15	0.3346 (3)	0.1926 (3)	0.24830 (19)	0.0617 (11)
H15A	0.3926	0.2181	0.2234	0.074*
H15B	0.3642	0.1523	0.2819	0.074*
C16	0.1853 (3)	0.0866 (3)	0.24931 (19)	0.0565 (10)

H16A	0.2145	0.0476	0.2835	0.068*
H16B	0.1422	0.0384	0.2255	0.068*
C17	0.1176 (2)	0.1755 (3)	0.27276 (18)	0.0465 (9)
H17A	0.0856	0.2119	0.2384	0.056*
H17B	0.0611	0.1464	0.2975	0.056*
C18	0.0284 (3)	0.4230 (3)	0.20196 (17)	0.0430 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0335 (2)	0.0431 (3)	0.0412 (3)	0.00581 (18)	−0.00355 (18)	0.00764 (19)
S1	0.0890 (8)	0.0573 (6)	0.0461 (6)	0.0087 (6)	−0.0121 (5)	0.0034 (5)
O1	0.0439 (13)	0.0504 (14)	0.0465 (14)	0.0116 (11)	−0.0066 (11)	0.0027 (11)
O2	0.0501 (15)	0.0656 (18)	0.0712 (19)	0.0054 (14)	0.0113 (14)	−0.0084 (14)
N1	0.0367 (15)	0.0514 (17)	0.0446 (16)	0.0023 (13)	−0.0017 (13)	0.0118 (14)
N2	0.0274 (13)	0.0441 (15)	0.0465 (16)	0.0031 (12)	0.0006 (12)	0.0077 (12)
N3	0.0552 (19)	0.0501 (18)	0.0487 (18)	0.0145 (15)	−0.0099 (15)	0.0016 (14)
C1	0.0363 (17)	0.0443 (19)	0.0417 (18)	−0.0075 (15)	0.0050 (15)	0.0078 (15)
C2	0.0400 (18)	0.045 (2)	0.045 (2)	−0.0005 (15)	0.0063 (15)	0.0062 (16)
C3	0.047 (2)	0.058 (2)	0.050 (2)	0.0087 (18)	0.0027 (17)	0.0069 (18)
C4	0.054 (2)	0.049 (2)	0.060 (2)	0.0030 (18)	0.016 (2)	0.0007 (19)
C5	0.049 (2)	0.051 (2)	0.054 (2)	−0.0148 (18)	0.0178 (18)	−0.0001 (18)
C6	0.064 (3)	0.070 (3)	0.069 (3)	−0.015 (2)	0.019 (2)	−0.018 (2)
C7	0.082 (3)	0.087 (3)	0.066 (3)	−0.026 (3)	0.015 (3)	−0.022 (3)
C8	0.066 (3)	0.107 (4)	0.061 (3)	−0.027 (3)	−0.002 (2)	−0.009 (3)
C9	0.053 (2)	0.077 (3)	0.055 (2)	−0.015 (2)	0.0034 (19)	−0.001 (2)
C10	0.0417 (19)	0.057 (2)	0.0439 (19)	−0.0160 (17)	0.0093 (16)	0.0058 (17)
C11	0.0385 (19)	0.060 (2)	0.0421 (19)	−0.0090 (17)	−0.0025 (15)	0.0122 (17)
C12	0.054 (2)	0.068 (2)	0.054 (2)	0.022 (2)	−0.0087 (19)	0.011 (2)
C13	0.054 (2)	0.056 (2)	0.054 (2)	0.0185 (18)	−0.0025 (18)	0.0146 (19)
C14	0.0321 (17)	0.053 (2)	0.063 (2)	−0.0059 (16)	−0.0003 (16)	0.0034 (18)
C15	0.0330 (19)	0.077 (3)	0.075 (3)	0.0027 (18)	0.0057 (19)	0.002 (2)
C16	0.054 (2)	0.043 (2)	0.072 (3)	0.0026 (18)	−0.003 (2)	0.0028 (19)
C17	0.0309 (17)	0.044 (2)	0.065 (2)	0.0000 (15)	0.0008 (16)	0.0087 (17)
C18	0.0428 (18)	0.0341 (17)	0.052 (2)	0.0083 (15)	−0.0041 (17)	−0.0044 (16)

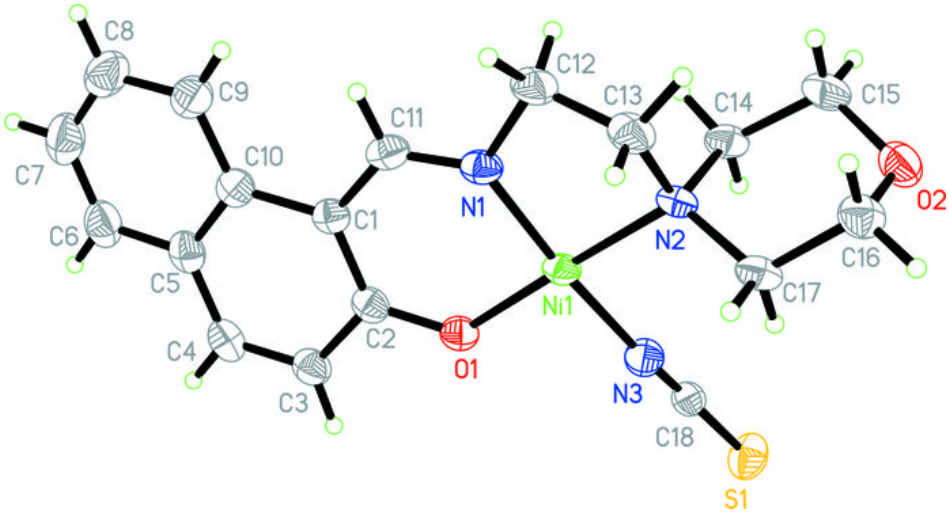
Geometric parameters (Å, °)

Ni1—O1	1.828 (2)	C6—C7	1.345 (6)
Ni1—N1	1.832 (3)	C6—H6	0.9300
Ni1—N3	1.885 (3)	C7—C8	1.398 (7)
Ni1—N2	1.959 (3)	C7—H7	0.9300
S1—C18	1.621 (4)	C8—C9	1.382 (6)
O1—C2	1.302 (4)	C8—H8	0.9300
O2—C16	1.416 (4)	C9—C10	1.401 (5)
O2—C15	1.421 (5)	C9—H9	0.9300
N1—C11	1.303 (4)	C11—H11	0.9300
N1—C12	1.470 (4)	C12—C13	1.478 (5)
N2—C17	1.496 (4)	C12—H12A	0.9700

N2—C13	1.497 (4)	C12—H12B	0.9700
N2—C14	1.498 (4)	C13—H13A	0.9700
N3—C18	1.158 (4)	C13—H13B	0.9700
C1—C2	1.403 (5)	C14—C15	1.514 (5)
C1—C11	1.407 (5)	C14—H14A	0.9700
C1—C10	1.454 (5)	C14—H14B	0.9700
C2—C3	1.426 (5)	C15—H15A	0.9700
C3—C4	1.339 (5)	C15—H15B	0.9700
C3—H3	0.9300	C16—C17	1.504 (5)
C4—C5	1.416 (5)	C16—H16A	0.9700
C4—H4	0.9300	C16—H16B	0.9700
C5—C6	1.413 (5)	C17—H17A	0.9700
C5—C10	1.415 (5)	C17—H17B	0.9700
O1—Ni1—N1	93.38 (12)	C10—C9—H9	119.7
O1—Ni1—N3	87.57 (11)	C9—C10—C5	117.8 (4)
N1—Ni1—N3	171.51 (13)	C9—C10—C1	124.1 (4)
O1—Ni1—N2	176.66 (11)	C5—C10—C1	118.0 (3)
N1—Ni1—N2	86.86 (12)	N1—C11—C1	125.9 (3)
N3—Ni1—N2	92.69 (12)	N1—C11—H11	117.0
C2—O1—Ni1	128.4 (2)	C1—C11—H11	117.0
C16—O2—C15	109.4 (3)	N1—C12—C13	107.2 (3)
C11—N1—C12	117.7 (3)	N1—C12—H12A	110.3
C11—N1—Ni1	127.1 (2)	C13—C12—H12A	110.3
C12—N1—Ni1	114.9 (2)	N1—C12—H12B	110.3
C17—N2—C13	109.5 (3)	C13—C12—H12B	110.3
C17—N2—C14	107.5 (3)	H12A—C12—H12B	108.5
C13—N2—C14	112.3 (3)	C12—C13—N2	109.2 (3)
C17—N2—Ni1	114.65 (18)	C12—C13—H13A	109.8
C13—N2—Ni1	105.2 (2)	N2—C13—H13A	109.8
C14—N2—Ni1	107.7 (2)	C12—C13—H13B	109.8
C18—N3—Ni1	167.9 (3)	N2—C13—H13B	109.8
C2—C1—C11	119.4 (3)	H13A—C13—H13B	108.3
C2—C1—C10	120.3 (3)	N2—C14—C15	112.9 (3)
C11—C1—C10	120.3 (3)	N2—C14—H14A	109.0
O1—C2—C1	124.9 (3)	C15—C14—H14A	109.0
O1—C2—C3	116.4 (3)	N2—C14—H14B	109.0
C1—C2—C3	118.7 (3)	C15—C14—H14B	109.0
C4—C3—C2	121.0 (4)	H14A—C14—H14B	107.8
C4—C3—H3	119.5	O2—C15—C14	111.3 (3)
C2—C3—H3	119.5	O2—C15—H15A	109.4
C3—C4—C5	122.2 (4)	C14—C15—H15A	109.4
C3—C4—H4	118.9	O2—C15—H15B	109.4
C5—C4—H4	118.9	C14—C15—H15B	109.4
C6—C5—C4	120.9 (4)	H15A—C15—H15B	108.0
C6—C5—C10	119.7 (4)	O2—C16—C17	110.8 (3)
C4—C5—C10	119.4 (4)	O2—C16—H16A	109.5
C7—C6—C5	121.4 (5)	C17—C16—H16A	109.5
C7—C6—H6	119.3	O2—C16—H16B	109.5
C5—C6—H6	119.3	C17—C16—H16B	109.5

C6—C7—C8	119.3 (4)	H16A—C16—H16B	108.1
C6—C7—H7	120.3	N2—C17—C16	112.6 (3)
C8—C7—H7	120.3	N2—C17—H17A	109.1
C9—C8—C7	121.0 (4)	C16—C17—H17A	109.1
C9—C8—H8	119.5	N2—C17—H17B	109.1
C7—C8—H8	119.5	C16—C17—H17B	109.1
C8—C9—C10	120.6 (4)	H17A—C17—H17B	107.8
C8—C9—H9	119.7	N3—C18—S1	178.4 (4)

Fig. 1


C8
C9
C10
C7
C6
C5
C4
C3
C2
C1
C11
N1
C12
C13
C14
C15
O2
N2
C16
C17
Ni1
O1
N3
C18
S1