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{1-[2-(Piperidin-1-yl)ethyliminomethyl]-2-naphtholato}thiocyanatonickel(II)

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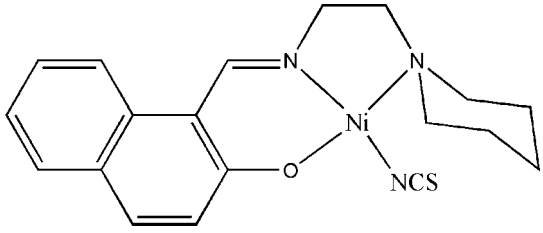
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.008 Å; R factor = 0.072; wR factor = 0.179; data-to-parameter ratio = 18.3.

In the title mononuclear nickel(II) complex, [Ni($C_{18}H_{21}N_2O$)(NCS)], the Ni^{II} atom is four-coordinated by the phenolate O, imine N and amine N atoms of the Schiff base ligand, and by the terminal N atom of a thiocyanate anion in a square-planar geometry.

Related literature

For the coordination chemistry and biological properties of nickel(II) complexes with Schiff base ligands, see Brückner *et al.* (2000); Harrop *et al.* (2003); Marganian *et al.* (1995); Ren *et al.* (2002). For related structures, see Arıcı *et al.* (2005); Diao (2007); Diao *et al.* (2007); Li, Huang *et al.* (2007); Li, Jiang *et al.* (2007); Usman *et al.* (2003); Van Hecke *et al.* (2007).



Experimental

Crystal data

[Ni($C_{18}H_{21}N_2O$)(NCS)]
M_r = 398.16
Monoclinic, $P2_1/c$
a = 11.663 (2) Å
b = 12.530 (3) Å
c = 13.484 (3) Å
β = 111.77 (3)°
V = 1830.0 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.19 mm^{-1}
T = 298 (2) K
0.20 × 0.20 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.797, T_{max} = 0.824
15376 measured reflections
4144 independent reflections
2157 reflections with $I > 2\sigma(I)$
R_{int} = 0.134

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.072
$wR(F^2)$ = 0.179
S = 0.97
4144 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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: SJ2338).

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supplementary materials

Acta Cryst. (2007). E**63**, m2426 [**doi:10.1107/S1600536807041505**]

{1-[2-(Piperidin-1-yl)ethyliminomethyl]-2-naphtholato}thiocyanatonickel(II)

Y.-P. Diao, K. Li, S.-S. Huang, L. Lu and K.-X. Liu

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 (Brückner *et al.*, 2000; Harrop *et al.*, 2003; 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. As part of our research programme on metal complexes of Schiff base ligands (Diao *et al.*, 2007; Diao, 2007; Li, Huang *et al.*, 2007) we report here the structure of the title compound (I) Fig.1.

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 atom of the Schiff base ligand and one terminal N atom of a thiocyanate anion in the coordination sphere (Fig. 1). Bond lengths and angles about the Ni(II) centre are comparable with the values observed in other Schiff base Ni(II) complexes (Arıcı *et al.*, 2005; Li, Jiang *et al.*, 2007; Li, Huang *et al.*, 2007; Usman *et al.*, 2003; Van Hecke *et al.*, 2007).

Experimental

2-Hydroxy-1-naphthaldehyde (0.1 mmol, 17.0 mg), 2-piperidin-1-ylethylamine (0.1 mmol, 12.7 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 a week, 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

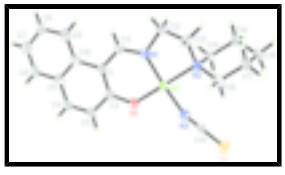


Fig. 1. The structure of the complex with displacement parameters drawn at the 30% probability level.

{1-[2-(Piperidin-1-yl)ethyliminomethyl]-2-naphtholato}thiocyanatonickel(II)

Crystal data

$[Ni(C_{18}H_{21}N_2O)(NCS)]$ $F_{000} = 832$

M_r = 398.16	D_x = 1.445 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 539 reflections
a = 11.663 (2) Å	θ = 2.3–24.5º
b = 12.530 (3) Å	μ = 1.19 mm^{-1}
c = 13.484 (3) Å	T = 298 (2) K
β = 111.77 (3)º	Block, red
V = 1830.0 (6) Å^3	0.20 × 0.20 × 0.17 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	4144 independent reflections
Radiation source: fine-focus sealed tube	2157 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.134
T = 298(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	h = −14→15
T_{min} = 0.797, T_{max} = 0.824	k = −15→16
15376 measured reflections	l = −17→17

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.072	H-atom parameters constrained
$wR(F^2)$ = 0.179	$w = 1/[\sigma^2(F_o^2) + (0.0415P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.97	$(\Delta/\sigma)_{max} < 0.001$
4144 reflections	$\Delta\rho_{max}$ = 0.36 e Å^{-3}
226 parameters	$\Delta\rho_{min}$ = −0.34 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	0.81734 (6)	0.61182 (5)	0.21941 (5)	0.0371 (2)
S1	1.23098 (15)	0.52220 (16)	0.36976 (15)	0.0681 (5)
O1	0.7816 (3)	0.5295 (3)	0.0990 (3)	0.0444 (10)
N1	0.6722 (4)	0.6864 (3)	0.1645 (3)	0.0389 (11)
N2	0.8531 (4)	0.6987 (3)	0.3496 (3)	0.0361 (10)
N3	0.9770 (5)	0.5519 (4)	0.2725 (4)	0.0507 (13)
C1	0.5878 (4)	0.6076 (4)	−0.0116 (4)	0.0335 (12)
C2	0.6857 (5)	0.5347 (4)	0.0089 (4)	0.0360 (12)
C3	0.6827 (5)	0.4611 (5)	−0.0724 (5)	0.0478 (15)
H3	0.7444	0.4097	−0.0578	0.057*
C4	0.5922 (5)	0.4642 (5)	−0.1701 (5)	0.0476 (15)
H4	0.5945	0.4159	−0.2217	0.057*
C5	0.4938 (5)	0.5387 (4)	−0.1970 (4)	0.0438 (14)
C6	0.4020 (6)	0.5438 (5)	−0.3007 (5)	0.0590 (18)
H6	0.4058	0.4970	−0.3529	0.071*
C7	0.3085 (7)	0.6156 (6)	−0.3258 (6)	0.074 (2)
H7	0.2492	0.6186	−0.3946	0.089*
C8	0.3022 (6)	0.6849 (6)	−0.2471 (6)	0.071 (2)
H8	0.2371	0.7330	−0.2635	0.085*
C9	0.3904 (5)	0.6832 (5)	−0.1457 (5)	0.0532 (16)
H9	0.3845	0.7310	−0.0950	0.064*
C10	0.4894 (5)	0.6110 (4)	−0.1168 (4)	0.0404 (13)
C11	0.5856 (5)	0.6796 (4)	0.0688 (4)	0.0396 (13)
H11	0.5181	0.7252	0.0527	0.048*
C12	0.6534 (5)	0.7687 (5)	0.2368 (5)	0.0501 (16)
H12A	0.5671	0.7723	0.2280	0.060*
H12B	0.6789	0.8384	0.2211	0.060*
C13	0.7314 (5)	0.7350 (5)	0.3487 (5)	0.0517 (16)
H13A	0.7425	0.7945	0.3974	0.062*
H13B	0.6912	0.6775	0.3715	0.062*
C14	0.9339 (5)	0.7901 (4)	0.3413 (4)	0.0392 (13)
H14A	1.0082	0.7611	0.3355	0.047*
H14B	0.8903	0.8297	0.2764	0.047*
C15	0.9699 (5)	0.8657 (4)	0.4346 (4)	0.0470 (15)
H15A	0.8968	0.9023	0.4349	0.056*
H15B	1.0260	0.9190	0.4262	0.056*
C16	1.0315 (6)	0.8091 (4)	0.5405 (4)	0.0506 (16)
H16A	1.0434	0.8589	0.5985	0.061*
H16B	1.1120	0.7831	0.5458	0.061*
C17	0.9519 (6)	0.7147 (5)	0.5505 (4)	0.0524 (16)
H17A	0.9968	0.6744	0.6146	0.063*
H17B	0.8768	0.7415	0.5565	0.063*

C18	0.9195 (6)	0.6420 (4)	0.4537 (4)	0.0483 (15)
H18A	0.9947	0.6108	0.4519	0.058*
H18B	0.8678	0.5843	0.4612	0.058*
C19	1.0826 (6)	0.5392 (4)	0.3121 (4)	0.0397 (14)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0348 (4)	0.0382 (4)	0.0377 (4)	0.0019 (3)	0.0127 (3)	−0.0044 (3)
S1	0.0411 (10)	0.0882 (14)	0.0700 (12)	0.0021 (9)	0.0149 (9)	−0.0089 (10)
O1	0.037 (2)	0.047 (2)	0.045 (2)	0.0026 (18)	0.0097 (19)	−0.0137 (18)
N1	0.040 (3)	0.039 (3)	0.036 (3)	0.004 (2)	0.012 (2)	−0.003 (2)
N2	0.037 (3)	0.037 (3)	0.040 (3)	−0.002 (2)	0.020 (2)	−0.004 (2)
N3	0.039 (3)	0.061 (3)	0.042 (3)	0.012 (3)	0.004 (2)	−0.009 (2)
C1	0.033 (3)	0.033 (3)	0.034 (3)	−0.004 (3)	0.012 (2)	0.001 (2)
C2	0.036 (3)	0.036 (3)	0.039 (3)	−0.005 (3)	0.017 (3)	−0.004 (2)
C3	0.046 (4)	0.048 (4)	0.054 (4)	0.001 (3)	0.023 (3)	−0.012 (3)
C4	0.049 (4)	0.049 (4)	0.045 (4)	−0.006 (3)	0.017 (3)	−0.017 (3)
C5	0.051 (4)	0.040 (3)	0.042 (3)	−0.012 (3)	0.019 (3)	−0.002 (3)
C6	0.068 (5)	0.056 (4)	0.039 (4)	−0.019 (4)	0.003 (3)	−0.004 (3)
C7	0.069 (5)	0.067 (5)	0.061 (5)	−0.014 (4)	−0.005 (4)	0.005 (4)
C8	0.065 (5)	0.062 (5)	0.063 (5)	0.004 (4)	−0.003 (4)	0.007 (4)
C9	0.055 (4)	0.056 (4)	0.042 (4)	−0.007 (3)	0.010 (3)	0.003 (3)
C10	0.041 (3)	0.039 (3)	0.046 (3)	−0.004 (3)	0.021 (3)	0.006 (3)
C11	0.039 (3)	0.038 (3)	0.043 (3)	0.003 (3)	0.015 (3)	0.003 (3)
C12	0.045 (4)	0.046 (4)	0.061 (4)	0.005 (3)	0.022 (3)	−0.021 (3)
C13	0.046 (4)	0.062 (4)	0.053 (4)	−0.003 (3)	0.024 (3)	−0.015 (3)
C14	0.043 (3)	0.039 (3)	0.039 (3)	−0.006 (3)	0.018 (3)	−0.002 (3)
C15	0.048 (4)	0.043 (4)	0.044 (3)	−0.002 (3)	0.010 (3)	−0.003 (3)
C16	0.064 (4)	0.040 (3)	0.040 (4)	−0.007 (3)	0.010 (3)	−0.006 (3)
C17	0.072 (4)	0.050 (4)	0.038 (3)	−0.002 (3)	0.023 (3)	−0.004 (3)
C18	0.062 (4)	0.044 (4)	0.041 (3)	−0.007 (3)	0.022 (3)	0.008 (3)
C19	0.053 (4)	0.035 (3)	0.029 (3)	0.007 (3)	0.013 (3)	−0.007 (2)

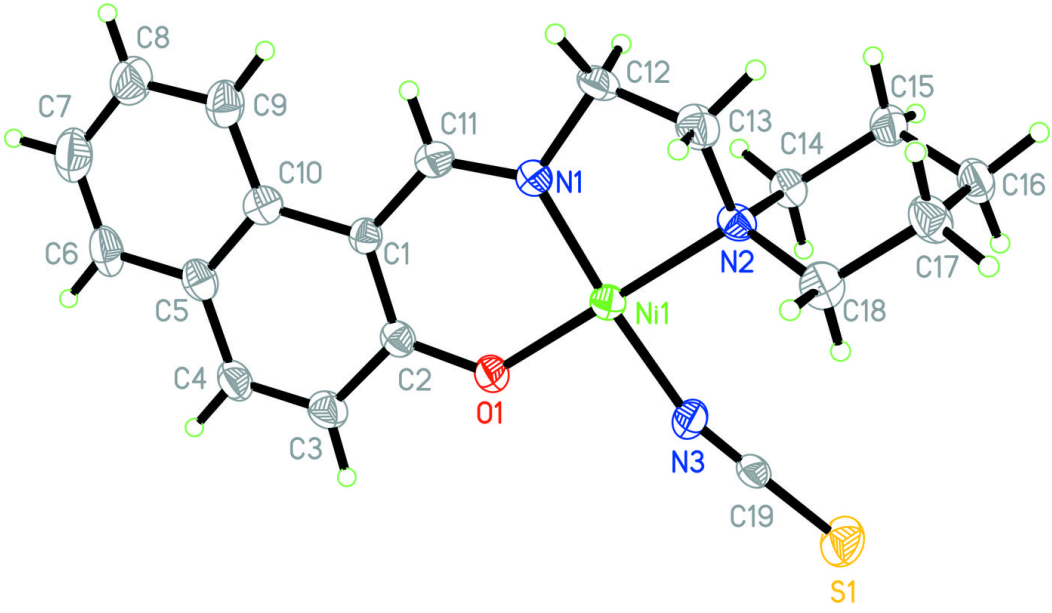
Geometric parameters (Å, °)

Ni1—N1	1.832 (4)	C7—H7	0.9300
Ni1—O1	1.836 (3)	C8—C9	1.373 (8)
Ni1—N3	1.886 (5)	C8—H8	0.9300
Ni1—N2	1.975 (4)	C9—C10	1.404 (8)
S1—C19	1.627 (6)	C9—H9	0.9300
O1—C2	1.314 (6)	C11—H11	0.9300
N1—C11	1.314 (6)	C12—C13	1.505 (8)
N1—C12	1.489 (6)	C12—H12A	0.9700
N2—C13	1.486 (7)	C12—H12B	0.9700
N2—C18	1.506 (6)	C13—H13A	0.9700
N2—C14	1.513 (6)	C13—H13B	0.9700
N3—C19	1.157 (7)	C14—C15	1.505 (7)
C1—C2	1.407 (7)	C14—H14A	0.9700

C1—C11	1.418 (7)	C14—H14B	0.9700
C1—C10	1.457 (7)	C15—C16	1.516 (7)
C2—C3	1.423 (7)	C15—H15A	0.9700
C3—C4	1.349 (7)	C15—H15B	0.9700
C3—H3	0.9300	C16—C17	1.540 (8)
C4—C5	1.418 (8)	C16—H16A	0.9700
C4—H4	0.9300	C16—H16B	0.9700
C5—C6	1.412 (8)	C17—C18	1.519 (7)
C5—C10	1.425 (7)	C17—H17A	0.9700
C6—C7	1.357 (9)	C17—H17B	0.9700
C6—H6	0.9300	C18—H18A	0.9700
C7—C8	1.394 (10)	C18—H18B	0.9700
N1—Ni1—O1	93.25 (18)	N1—C11—C1	124.5 (5)
N1—Ni1—N3	172.3 (2)	N1—C11—H11	117.7
O1—Ni1—N3	88.87 (18)	C1—C11—H11	117.7
N1—Ni1—N2	86.38 (18)	N1—C12—C13	106.3 (4)
O1—Ni1—N2	178.83 (17)	N1—C12—H12A	110.5
N3—Ni1—N2	91.64 (19)	C13—C12—H12A	110.5
C2—O1—Ni1	128.8 (3)	N1—C12—H12B	110.5
C11—N1—C12	116.2 (4)	C13—C12—H12B	110.5
C11—N1—Ni1	128.5 (4)	H12A—C12—H12B	108.7
C12—N1—Ni1	115.3 (3)	N2—C13—C12	108.4 (4)
C13—N2—C18	108.1 (4)	N2—C13—H13A	110.0
C13—N2—C14	112.8 (4)	C12—C13—H13A	110.0
C18—N2—C14	107.9 (4)	N2—C13—H13B	110.0
C13—N2—Ni1	106.0 (3)	C12—C13—H13B	110.0
C18—N2—Ni1	115.8 (3)	H13A—C13—H13B	108.4
C14—N2—Ni1	106.5 (3)	C15—C14—N2	113.8 (4)
C19—N3—Ni1	164.1 (5)	C15—C14—H14A	108.8
C2—C1—C11	120.4 (5)	N2—C14—H14A	108.8
C2—C1—C10	119.9 (5)	C15—C14—H14B	108.8
C11—C1—C10	119.7 (5)	N2—C14—H14B	108.8
O1—C2—C1	124.4 (5)	H14A—C14—H14B	107.7
O1—C2—C3	116.7 (5)	C14—C15—C16	112.4 (5)
C1—C2—C3	118.9 (5)	C14—C15—H15A	109.1
C4—C3—C2	121.3 (5)	C16—C15—H15A	109.1
C4—C3—H3	119.3	C14—C15—H15B	109.1
C2—C3—H3	119.3	C16—C15—H15B	109.1
C3—C4—C5	122.3 (5)	H15A—C15—H15B	107.9
C3—C4—H4	118.8	C15—C16—C17	110.6 (5)
C5—C4—H4	118.8	C15—C16—H16A	109.5
C6—C5—C4	121.8 (6)	C17—C16—H16A	109.5
C6—C5—C10	119.7 (6)	C15—C16—H16B	109.5
C4—C5—C10	118.5 (5)	C17—C16—H16B	109.5
C7—C6—C5	121.4 (6)	H16A—C16—H16B	108.1
C7—C6—H6	119.3	C18—C17—C16	110.6 (5)
C5—C6—H6	119.3	C18—C17—H17A	109.5
C6—C7—C8	119.1 (6)	C16—C17—H17A	109.5
C6—C7—H7	120.4	C18—C17—H17B	109.5

C8—C7—H7	120.4	C16—C17—H17B	109.5
C9—C8—C7	121.2 (7)	H17A—C17—H17B	108.1
C9—C8—H8	119.4	N2—C18—C17	113.3 (5)
C7—C8—H8	119.4	N2—C18—H18A	108.9
C8—C9—C10	121.4 (6)	C17—C18—H18A	108.9
C8—C9—H9	119.3	N2—C18—H18B	108.9
C10—C9—H9	119.3	C17—C18—H18B	108.9
C9—C10—C5	117.2 (5)	H18A—C18—H18B	107.7
C9—C10—C1	123.9 (5)	N3—C19—S1	179.0 (5)
C5—C10—C1	118.9 (5)		

Fig. 1


C8
C7
C9
C10
C11
C12
C13
C14
C15
C16
C17
C18
C6
C5
C4
C3
C2
C1
N1
N2
Ni1
O1
N3
C19
S1