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{2-[2-(Piperidin-1-yl)ethyliminomethyl]-phenolato-κ^3N,N',O}(thiocyanato-κN)-nickel(II)

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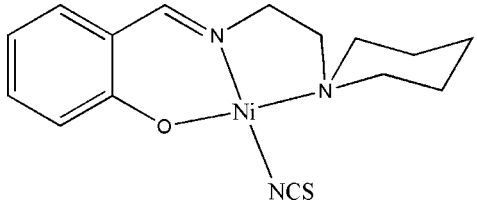
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.043; wR factor = 0.107; data-to-parameter ratio = 18.9.

In the title compound, [Ni($C_{14}H_{19}N_2O$)(NCS)], a mononuclear Schiff base nickel(II) complex, the Ni atom is four-coordinated by one imine N atom, one amine N atom and one phenolate O atom of the Schiff base ligand, and by one terminal N atom of the thiocyanate ligand, forming a square-planar geometry. The piperidine ring adopts a chair conformation. No significant hydrogen bonding or π–π interactions are observed in the crystal structure.

Related literature

For related literature, see: Costes *et al.* (2005); Di Bella *et al.* (1997); Fu *et al.* (2007); Kraihanzel *et al.* (1981); Liu *et al.* (2006); Loeb *et al.* (1984); Mukhopadhyay *et al.* (2003); Wang (2007); Zhu *et al.* (2004).



Experimental

Crystal data

[Ni($C_{14}H_{19}N_2O$)(NCS)]
M_r = 348.10
Orthorhombic, *Pbca*
a = 12.997 (3) Å
b = 12.525 (3) Å
c = 19.386 (4) Å
V = 3155.8 (11) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.36 mm^{-1}
T = 298 (2) K
0.37 × 0.32 × 0.30 mm

Data collection

Bruker SMART APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.618, T_{max} = 0.670
18388 measured reflections
3587 independent reflections
2494 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.107
S = 1.02
3587 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.8344 (19)	Ni1—N3	1.877 (3)
Ni1—N1	1.840 (2)	Ni1—N2	1.965 (2)
O1—Ni1—N1	94.26 (10)	O1—Ni1—N2	178.33 (9)
O1—Ni1—N3	86.63 (9)	N1—Ni1—N2	86.94 (10)
N1—Ni1—N3	176.32 (10)	N3—Ni1—N2	92.09 (10)

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2396).

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supplementary materials

Acta Cryst. (2007). E**63**, m1946 [**doi:10.1107/S1600536807029340**]

{2-[2-(Piperidin-1-yl)ethyliminomethyl]phenolato-κ^3N,N',O}(thiocyanato-κN)nickel(II)

S.-X. Wang

Comment

Nickel(II) complexes derived from Schiff base ligands have been studied extensively due to their interesting structures and numerous applications (Mukhopadhyay *et al.*, 2003; Kraihanzel *et al.*, 1981; Di Bella *et al.*, 1997; Loeb *et al.*, 1984; Costes *et al.*, 2005). Previously, the author has reported the crystal structure of a Schiff base zinc(II) complex (Wang, 2007). As part of a further investigation of Schiff base complexes, the structure of the title compound, a mononuclear nickel(II) complex, is reported here.

The square-planar coordination environment of Ni^{II} atom in the title compound is formed by one imine N atom, one amine N atom, and one phenolate O atom of the Schiff base ligand, and by one terminal N atom of the thiocyanate ligand (Fig. 1). The coordination bond distances (Table 1) are typical and comparable with the values in similar nickel(II) complexes (Zhu *et al.*, 2004; Liu *et al.*, 2006; Fu *et al.*, 2007).

Experimental

The title compound was obtained by stirring of salicylaldehyde (0.1 mmol, 12.1 mg), 2-piperidin-1-ylethylamine (0.1 mmol, 12.8 mg), ammonium thiocyanate (0.1 mmol, 7.6 mg), and nickel(II) nitrate (0.1 mmol, 29.1 mg) in methanol (20 ml) for 30 min. The reaction mixture was then filtered. Red block-shaped single crystals suitable for X-ray diffraction were formed from the filtrate after 5 d.

Refinement

H atoms were positioned geometrically (C—H = 0.93 or 0.97 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

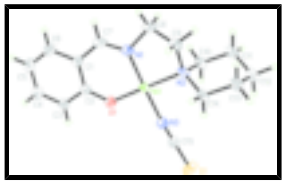

Fig. 1. The molecular structure of title compound, showing the numbering scheme and displacement ellipsoids drawn at the 30% probability level

{2-[2-(Piperidin-1-yl)ethyliminomethyl]phenolato-κ^3N,N',O}(thiocyanato- κN)nickel(II)

Crystal data

$[Ni(C_{14}H_{19}N_2O)(NCS)]$	$F_{000} = 1456$
$M_r = 348.10$	$D_x = 1.465$ Mg m^{-3}

Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 3068 reflections
a = 12.997 (3) Å	θ = 2.5–25.4º
b = 12.525 (3) Å	μ = 1.36 mm^{-1}
c = 19.386 (4) Å	*T* = 298 (2) K
V = 3155.8 (11) Å^3	Block, red
Z = 8	0.37 × 0.32 × 0.30 mm

Data collection

Bruker SMART APEX area-detector diffractometer	3587 independent reflections
Radiation source: fine-focus sealed tube	2494 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.054
T = 298(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −16→16
T_{min} = 0.618, T_{max} = 0.670	*k* = −16→16
18388 measured reflections	*l* = −16→25

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.043	H-atom parameters constrained
$wR(F^2)$ = 0.107	$w = 1/[\sigma^2(F_o^2) + (0.0516P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.001
3587 reflections	$\Delta\rho_{max}$ = 0.51 e Å^{-3}
190 parameters	$\Delta\rho_{min}$ = −0.35 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	0.11596 (2)	0.56364 (3)	0.162861 (19)	0.03658 (13)
S1	−0.00585 (8)	0.49582 (7)	0.38329 (4)	0.0652 (3)
O1	0.05319 (15)	0.43892 (14)	0.13658 (11)	0.0459 (5)
N1	0.18173 (17)	0.58278 (17)	0.07974 (12)	0.0409 (6)
N2	0.18420 (15)	0.69534 (17)	0.19361 (12)	0.0373 (5)
N3	0.05700 (18)	0.54126 (18)	0.25004 (14)	0.0465 (6)
C1	0.1120 (2)	0.4304 (2)	0.01950 (16)	0.0428 (7)
C2	0.0550 (2)	0.3924 (2)	0.07622 (15)	0.0382 (6)
C3	−0.0010 (2)	0.2974 (2)	0.06736 (16)	0.0455 (7)
H3	−0.0393	0.2707	0.1040	0.055*
C4	−0.0004 (2)	0.2436 (2)	0.00622 (16)	0.0508 (8)
H4	−0.0379	0.1807	0.0021	0.061*
C5	0.0552 (2)	0.2813 (3)	−0.05009 (17)	0.0563 (9)
H5	0.0552	0.2442	−0.0917	0.068*
C6	0.1096 (2)	0.3739 (3)	−0.04300 (16)	0.0523 (8)
H6	0.1461	0.4001	−0.0806	0.063*
C7	0.1740 (2)	0.5242 (2)	0.02556 (16)	0.0462 (7)
H7	0.2119	0.5446	−0.0129	0.055*
C8	0.2543 (2)	0.6728 (2)	0.07842 (17)	0.0511 (8)
H8A	0.2566	0.7043	0.0327	0.061*
H8B	0.3229	0.6487	0.0905	0.061*
C9	0.2168 (2)	0.7523 (2)	0.12972 (14)	0.0475 (7)
H9A	0.1591	0.7917	0.1107	0.057*
H9B	0.2712	0.8026	0.1405	0.057*
C10	0.2741 (2)	0.6595 (2)	0.23558 (16)	0.0450 (7)
H10A	0.3201	0.6186	0.2063	0.054*
H10B	0.2497	0.6123	0.2718	0.054*
C11	0.3344 (2)	0.7504 (3)	0.26836 (16)	0.0535 (8)
H11A	0.3669	0.7925	0.2325	0.064*
H11B	0.3881	0.7212	0.2975	0.064*
C12	0.2646 (2)	0.8218 (3)	0.31126 (18)	0.0597 (9)
H12A	0.2378	0.7822	0.3503	0.072*
H12B	0.3035	0.8822	0.3287	0.072*
C13	0.1766 (2)	0.8611 (2)	0.26675 (17)	0.0512 (8)
H13A	0.1302	0.9040	0.2945	0.061*
H13B	0.2034	0.9058	0.2301	0.061*
C14	0.11822 (19)	0.7684 (2)	0.23584 (16)	0.0422 (7)
H14A	0.0868	0.7277	0.2728	0.051*
H14B	0.0634	0.7961	0.2070	0.051*
C15	0.0307 (2)	0.5216 (2)	0.30525 (16)	0.0405 (7)

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

Ni1	0.0351 (2)	0.0358 (2)	0.0388 (2)	−0.00503 (14)	0.00431 (15)	0.00423 (16)
S1	0.0955 (7)	0.0548 (5)	0.0454 (5)	0.0077 (5)	0.0229 (5)	0.0067 (4)
O1	0.0569 (13)	0.0419 (11)	0.0388 (12)	−0.0127 (9)	0.0085 (10)	0.0004 (9)
N1	0.0376 (12)	0.0401 (13)	0.0448 (15)	−0.0040 (10)	0.0058 (11)	0.0084 (11)
N2	0.0307 (11)	0.0364 (12)	0.0448 (14)	−0.0035 (9)	0.0010 (10)	0.0048 (11)
N3	0.0522 (15)	0.0421 (14)	0.0451 (16)	−0.0119 (11)	0.0063 (12)	0.0000 (12)
C1	0.0447 (16)	0.0452 (17)	0.0386 (17)	0.0032 (13)	0.0001 (13)	0.0036 (14)
C2	0.0373 (14)	0.0391 (15)	0.0380 (17)	0.0060 (12)	−0.0026 (12)	0.0036 (13)
C3	0.0475 (16)	0.0443 (16)	0.0448 (18)	−0.0041 (13)	−0.0035 (14)	0.0025 (15)
C4	0.0528 (17)	0.0485 (18)	0.051 (2)	−0.0015 (15)	−0.0117 (16)	−0.0030 (16)
C5	0.066 (2)	0.060 (2)	0.042 (2)	0.0033 (17)	−0.0084 (16)	−0.0080 (16)
C6	0.0557 (18)	0.064 (2)	0.0369 (18)	0.0027 (16)	0.0013 (14)	0.0019 (16)
C7	0.0455 (17)	0.0488 (17)	0.0441 (18)	0.0010 (14)	0.0128 (14)	0.0110 (15)
C8	0.0512 (17)	0.0498 (19)	0.052 (2)	−0.0133 (14)	0.0111 (15)	0.0096 (15)
C9	0.0443 (16)	0.0425 (16)	0.056 (2)	−0.0094 (13)	0.0004 (14)	0.0098 (16)
C10	0.0353 (14)	0.0427 (16)	0.057 (2)	0.0033 (12)	−0.0036 (13)	0.0043 (14)
C11	0.0348 (14)	0.063 (2)	0.062 (2)	−0.0071 (14)	−0.0099 (14)	0.0069 (18)
C12	0.0524 (19)	0.061 (2)	0.066 (2)	−0.0174 (16)	−0.0054 (16)	−0.0108 (17)
C13	0.0463 (16)	0.0372 (16)	0.070 (2)	−0.0025 (13)	0.0010 (16)	−0.0051 (15)
C14	0.0330 (13)	0.0384 (16)	0.055 (2)	0.0009 (11)	−0.0015 (13)	−0.0005 (14)
C15	0.0441 (15)	0.0291 (14)	0.0484 (19)	−0.0019 (12)	0.0036 (14)	−0.0033 (14)

Geometric parameters (Å, °)

Ni1—O1	1.8344 (19)	C6—H6	0.93
Ni1—N1	1.840 (2)	C7—H7	0.93
Ni1—N3	1.877 (3)	C8—C9	1.490 (4)
Ni1—N2	1.965 (2)	C8—H8A	0.97
S1—C15	1.619 (3)	C8—H8B	0.97
O1—C2	1.307 (3)	C9—H9A	0.97
N1—C7	1.285 (4)	C9—H9B	0.97
N1—C8	1.470 (3)	C10—C11	1.521 (4)
N2—C9	1.491 (3)	C10—H10A	0.97
N2—C10	1.493 (3)	C10—H10B	0.97
N2—C14	1.498 (3)	C11—C12	1.522 (4)
N3—C15	1.150 (3)	C11—H11A	0.97
C1—C6	1.404 (4)	C11—H11B	0.97
C1—C2	1.409 (4)	C12—C13	1.515 (4)
C1—C7	1.429 (4)	C12—H12A	0.97
C2—C3	1.405 (4)	C12—H12B	0.97
C3—C4	1.363 (4)	C13—C14	1.511 (4)
C3—H3	0.93	C13—H13A	0.97
C4—C5	1.392 (4)	C13—H13B	0.97
C4—H4	0.93	C14—H14A	0.97
C5—C6	1.365 (4)	C14—H14B	0.97
C5—H5	0.93		
O1—Ni1—N1	94.26 (10)	N1—C8—H8B	110.3
O1—Ni1—N3	86.63 (9)	C9—C8—H8B	110.3
N1—Ni1—N3	176.32 (10)	H8A—C8—H8B	108.6

O1—Ni1—N2	178.33 (9)	C8—C9—N2	109.1 (2)
N1—Ni1—N2	86.94 (10)	C8—C9—H9A	109.9
N3—Ni1—N2	92.09 (10)	N2—C9—H9A	109.9
C2—O1—Ni1	128.31 (18)	C8—C9—H9B	109.9
C7—N1—C8	118.3 (2)	N2—C9—H9B	109.9
C7—N1—Ni1	127.2 (2)	H9A—C9—H9B	108.3
C8—N1—Ni1	114.41 (19)	N2—C10—C11	113.9 (2)
C9—N2—C10	112.0 (2)	N2—C10—H10A	108.8
C9—N2—C14	108.9 (2)	C11—C10—H10A	108.8
C10—N2—C14	109.5 (2)	N2—C10—H10B	108.8
C9—N2—Ni1	106.12 (17)	C11—C10—H10B	108.8
C10—N2—Ni1	105.41 (16)	H10A—C10—H10B	107.7
C14—N2—Ni1	114.86 (15)	C10—C11—C12	111.2 (2)
C15—N3—Ni1	172.4 (2)	C10—C11—H11A	109.4
C6—C1—C2	119.4 (3)	C12—C11—H11A	109.4
C6—C1—C7	119.9 (3)	C10—C11—H11B	109.4
C2—C1—C7	120.7 (3)	C12—C11—H11B	109.4
O1—C2—C3	118.5 (3)	H11A—C11—H11B	108.0
O1—C2—C1	123.9 (3)	C13—C12—C11	109.3 (3)
C3—C2—C1	117.6 (3)	C13—C12—H12A	109.8
C4—C3—C2	121.5 (3)	C11—C12—H12A	109.8
C4—C3—H3	119.3	C13—C12—H12B	109.8
C2—C3—H3	119.3	C11—C12—H12B	109.8
C3—C4—C5	121.1 (3)	H12A—C12—H12B	108.3
C3—C4—H4	119.4	C14—C13—C12	110.8 (2)
C5—C4—H4	119.4	C14—C13—H13A	109.5
C6—C5—C4	118.6 (3)	C12—C13—H13A	109.5
C6—C5—H5	120.7	C14—C13—H13B	109.5
C4—C5—H5	120.7	C12—C13—H13B	109.5
C5—C6—C1	121.8 (3)	H13A—C13—H13B	108.1
C5—C6—H6	119.1	N2—C14—C13	113.5 (2)
C1—C6—H6	119.1	N2—C14—H14A	108.9
N1—C7—C1	125.5 (3)	C13—C14—H14A	108.9
N1—C7—H7	117.3	N2—C14—H14B	108.9
C1—C7—H7	117.3	C13—C14—H14B	108.9
N1—C8—C9	106.9 (2)	H14A—C14—H14B	107.7
N1—C8—H8A	110.3	N3—C15—S1	179.2 (3)
C9—C8—H8A	110.3		

Fig. 1