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Azido{2-[2-(piperidin-1-yl)ethyliminomethyl]-1-naphtholato}nickel(II)

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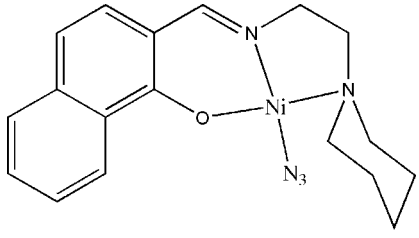
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.039; wR factor = 0.097; data-to-parameter ratio = 17.2.

The title compound, $[Ni(C_{18}H_{21}N_2O)(N_3)]$, was obtained by the reaction of the Schiff base ligand 2-[2-(piperidin-1-yl)ethyliminomethyl]-1-naphthol with sodium azide and nickel(II) nitrate in methanol solution. The Ni atom is four-coordinated by the *N*,*N*,*O*-donor set of the Schiff base ligand and by the terminal N atom of the azide group, forming a square-planar geometry. The piperidine ring adopts a chair conformation and lies nearly perpendicular to the naphthalene system.

Related literature

For related literature, see: Zhu *et al.* (2004); Peng *et al.* (2006); Liu *et al.* (2006); Sun *et al.* (2005); Skovsgaard *et al.* (2005).



Experimental

Crystal data

$[Ni(C_{18}H_{21}N_2O)(N_3)]$
M_r = 382.11
Orthorhombic, *Pbca*
a = 7.5298 (12) Å
b = 13.268 (2) Å
c = 33.912 (5) Å
V = 3387.9 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.16 mm^{-1}
T = 298 (2) K
0.27 × 0.23 × 0.22 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.744, T_{max} = 0.784
19025 measured reflections
3886 independent reflections
2511 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.097
S = 1.03
3886 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); 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: HG2245).

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supplementary materials

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Azido{2-[2-(piperidin-1-yl)ethyliminomethyl]-1-naphtholato}nickel(II)

Z. Zhou and Z.-H. Xiao

Comment

The title compound, (I) (Fig. 1), is a mononuclear nickel(II) complex. The Ni atom is four-coordinated by the NNO donor set of the Schiff base ligand and by the terminal N atom of the azide group, forming a square planar geometry. The piperidine ring adopts chair conformation and lies nearly perpendicular to the naphthalene ring. The bond lengths and bond angles subtended at the metal centre are comparable to the values in other similar nickel(II) complexes (Zhu *et al.*, 2004; Peng *et al.*, 2006; Liu *et al.*, 2006; Sun *et al.*, 2005; Skovsgaard *et al.*, 2005).

Experimental

2-Hydroxy-1-naphthaldehyde (0.1 mmol, 17.2 mg), 2-piperidin-1-ylethylamine (0.1 mmol, 12.8 mg), sodium azide (0.1 mmol, 6.5 mg) and nickel nitrate (0.1 mmol, 29.1 mg) were mixed in a methanol solution (10 ml). The mixture was stirred at room temperature for 30 min to give an orange solution. Red block-like crystals were formed by slow evaporation of the solution in air.

Refinement

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.97 Å and with U_{iso}(H) = 1.2 times U_{eq}(C).

Figures

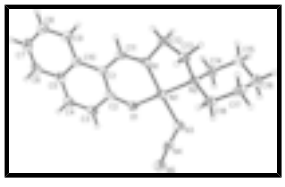

Fig. 1. The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

Azido{2-[2-(piperidin-1-yl)ethyliminomethyl]-1-naphtholato}nickel(II)

Crystal data

$[Ni(C_{18}H_{21}N_2O)(N_3)]$	F_{000} = 1600
M_r = 382.11	D_x = 1.498 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 2636 reflections
a = 7.5298 (12) Å	θ = 2.4–24.9º
b = 13.268 (2) Å	μ = 1.16 mm^{-1}

c = 33.912 (5) Å	T = 298 (2) K
V = 3387.9 (9) Å^3	Block, red
Z = 8	0.27 × 0.23 × 0.22 mm

Data collection

Bruker SMART APEXII area-detector diffractometer	3886 independent reflections
Radiation source: fine-focus sealed tube	2511 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.057
T = 298(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 2.4º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	$h = -9 \rightarrow 9$
T_{min} = 0.744, T_{max} = 0.784	$k = -17 \rightarrow 9$
19025 measured reflections	$l = -42 \rightarrow 44$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.039	H-atom parameters constrained
$wR(F^2)$ = 0.097	$w = 1/[\sigma^2(F_o^2) + (0.0408P)^2 + 0.3939P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
3886 reflections	$\Delta\rho_{max}$ = 0.31 e Å^{-3}
226 parameters	$\Delta\rho_{min}$ = −0.29 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 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	0.11052 (4)	1.01754 (2)	0.126498 (9)	0.03627 (12)
O1	0.0701 (2)	1.11144 (12)	0.16469 (5)	0.0406 (4)

N1	0.2013 (3)	0.92459 (14)	0.16125 (6)	0.0355 (5)
N2	0.1609 (3)	0.91868 (15)	0.08457 (6)	0.0394 (5)
N3	0.0296 (3)	1.11223 (18)	0.08820 (6)	0.0517 (6)
N4	−0.0786 (3)	1.17598 (18)	0.09472 (6)	0.0435 (6)
N5	−0.1800 (4)	1.2398 (2)	0.09892 (7)	0.0638 (7)
C1	0.1479 (3)	1.01488 (18)	0.22235 (8)	0.0334 (6)
C2	0.0797 (3)	1.10007 (19)	0.20300 (8)	0.0355 (6)
C3	0.0174 (3)	1.1829 (2)	0.22607 (8)	0.0420 (6)
H3	−0.0281	1.2396	0.2135	0.050*
C4	0.0235 (3)	1.1799 (2)	0.26581 (8)	0.0458 (7)
H4	−0.0180	1.2350	0.2800	0.055*
C5	0.0913 (3)	1.0955 (2)	0.28661 (7)	0.0400 (6)
C6	0.0994 (4)	1.0939 (2)	0.32823 (8)	0.0519 (8)
H6	0.0596	1.1495	0.3424	0.062*
C7	0.1640 (4)	1.0127 (3)	0.34801 (9)	0.0575 (8)
H7	0.1690	1.0131	0.3754	0.069*
C8	0.2227 (4)	0.9288 (2)	0.32689 (8)	0.0502 (7)
H8	0.2662	0.8729	0.3403	0.060*
C9	0.2169 (3)	0.9282 (2)	0.28642 (8)	0.0435 (7)
H9	0.2562	0.8716	0.2728	0.052*
C10	0.1528 (3)	1.01158 (19)	0.26501 (8)	0.0363 (6)
C11	0.2107 (3)	0.93247 (18)	0.19959 (7)	0.0362 (6)
H11	0.2632	0.8794	0.2132	0.043*
C12	0.2765 (4)	0.83414 (19)	0.14273 (7)	0.0441 (7)
H12A	0.2627	0.7762	0.1599	0.053*
H12B	0.4020	0.8436	0.1373	0.053*
C13	0.1756 (4)	0.81910 (19)	0.10506 (8)	0.0461 (7)
H13A	0.2372	0.7712	0.0883	0.055*
H13B	0.0581	0.7927	0.1107	0.055*
C14	0.3328 (4)	0.9506 (2)	0.06614 (8)	0.0490 (7)
H14A	0.4244	0.9505	0.0862	0.059*
H14B	0.3204	1.0191	0.0566	0.059*
C15	0.3927 (4)	0.8840 (3)	0.03216 (8)	0.0623 (9)
H15A	0.5006	0.9113	0.0208	0.075*
H15B	0.4186	0.8169	0.0419	0.075*
C16	0.2506 (5)	0.8780 (3)	0.00090 (9)	0.0736 (10)
H16A	0.2867	0.8308	−0.0194	0.088*
H16B	0.2352	0.9436	−0.0112	0.088*
C17	0.0771 (5)	0.8439 (2)	0.01886 (9)	0.0711 (10)
H17A	0.0892	0.7752	0.0282	0.085*
H17B	−0.0149	0.8449	−0.0012	0.085*
C18	0.0223 (4)	0.9118 (2)	0.05305 (8)	0.0517 (7)
H18A	−0.0019	0.9788	0.0430	0.062*
H18B	−0.0867	0.8860	0.0645	0.062*

Atomic displacement parameters (Å^2)

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

Ni1	0.0394 (2)	0.02563 (18)	0.0438 (2)	0.00147 (14)	−0.00179 (15)	0.00165 (15)
O1	0.0522 (11)	0.0259 (9)	0.0437 (10)	0.0041 (8)	−0.0025 (8)	0.0024 (8)
N1	0.0340 (12)	0.0249 (11)	0.0475 (13)	0.0028 (9)	−0.0028 (9)	−0.0006 (10)
N2	0.0427 (13)	0.0313 (12)	0.0442 (12)	0.0014 (10)	−0.0093 (10)	−0.0003 (10)
N3	0.0725 (17)	0.0371 (13)	0.0456 (13)	0.0140 (13)	0.0023 (12)	0.0045 (12)
N4	0.0570 (16)	0.0361 (13)	0.0374 (13)	−0.0015 (12)	−0.0060 (11)	0.0044 (11)
N5	0.0761 (18)	0.0562 (17)	0.0591 (17)	0.0239 (15)	−0.0021 (14)	0.0058 (14)
C1	0.0281 (12)	0.0263 (12)	0.0458 (15)	−0.0040 (10)	−0.0017 (10)	0.0009 (12)
C2	0.0304 (14)	0.0276 (13)	0.0483 (16)	−0.0045 (11)	0.0023 (11)	−0.0031 (12)
C3	0.0359 (15)	0.0303 (14)	0.0597 (18)	0.0005 (12)	0.0027 (13)	−0.0022 (13)
C4	0.0400 (16)	0.0369 (16)	0.0604 (19)	−0.0019 (13)	0.0088 (13)	−0.0112 (14)
C5	0.0302 (14)	0.0440 (16)	0.0458 (16)	−0.0085 (12)	0.0033 (11)	−0.0058 (13)
C6	0.0425 (17)	0.058 (2)	0.0548 (18)	−0.0080 (15)	0.0060 (14)	−0.0114 (16)
C7	0.0463 (17)	0.080 (2)	0.0462 (18)	−0.0157 (17)	0.0027 (14)	−0.0036 (17)
C8	0.0406 (16)	0.0568 (19)	0.0531 (18)	−0.0119 (14)	−0.0061 (13)	0.0124 (16)
C9	0.0387 (15)	0.0418 (16)	0.0498 (17)	−0.0079 (13)	−0.0022 (12)	0.0032 (14)
C10	0.0275 (13)	0.0358 (14)	0.0457 (15)	−0.0101 (11)	0.0003 (10)	−0.0009 (12)
C11	0.0319 (14)	0.0289 (14)	0.0479 (16)	−0.0030 (11)	−0.0033 (11)	0.0057 (12)
C12	0.0549 (17)	0.0287 (14)	0.0487 (16)	0.0092 (13)	−0.0058 (13)	0.0003 (13)
C13	0.0609 (18)	0.0265 (14)	0.0509 (17)	0.0031 (13)	−0.0034 (14)	−0.0037 (13)
C14	0.0471 (16)	0.0543 (18)	0.0458 (16)	−0.0012 (14)	−0.0020 (13)	−0.0019 (15)
C15	0.066 (2)	0.072 (2)	0.0486 (17)	0.0199 (18)	0.0024 (15)	−0.0048 (17)
C16	0.099 (3)	0.075 (2)	0.0468 (18)	0.031 (2)	−0.0117 (19)	−0.0095 (18)
C17	0.096 (3)	0.051 (2)	0.066 (2)	0.0106 (19)	−0.043 (2)	−0.0147 (17)
C18	0.0501 (18)	0.0435 (17)	0.0613 (18)	0.0003 (14)	−0.0202 (14)	−0.0029 (15)

Geometric parameters (Å, °)

Ni1—O1	1.8226 (17)	C7—H7	0.9300
Ni1—N1	1.838 (2)	C8—C9	1.373 (4)
Ni1—N3	1.907 (2)	C8—H8	0.9300
Ni1—N2	1.971 (2)	C9—C10	1.408 (3)
O1—C2	1.310 (3)	C9—H9	0.9300
N1—C11	1.306 (3)	C11—H11	0.9300
N1—C12	1.468 (3)	C12—C13	1.500 (4)
N2—C18	1.497 (3)	C12—H12A	0.9700
N2—C13	1.497 (3)	C12—H12B	0.9700
N2—C14	1.499 (3)	C13—H13A	0.9700
N3—N4	1.195 (3)	C13—H13B	0.9700
N4—N5	1.149 (3)	C14—C15	1.520 (4)
C1—C2	1.404 (3)	C14—H14A	0.9700
C1—C11	1.419 (3)	C14—H14B	0.9700
C1—C10	1.448 (4)	C15—C16	1.508 (4)
C2—C3	1.428 (3)	C15—H15A	0.9700
C3—C4	1.349 (3)	C15—H15B	0.9700
C3—H3	0.9300	C16—C17	1.511 (5)
C4—C5	1.419 (4)	C16—H16A	0.9700
C4—H4	0.9300	C16—H16B	0.9700
C5—C10	1.410 (3)	C17—C18	1.525 (4)

C5—C6	1.413 (4)	C17—H17A	0.9700
C6—C7	1.359 (4)	C17—H17B	0.9700
C6—H6	0.9300	C18—H18A	0.9700
C7—C8	1.396 (4)	C18—H18B	0.9700
O1—Ni1—N1	93.73 (8)	C5—C10—C1	119.1 (2)
O1—Ni1—N3	88.87 (9)	N1—C11—C1	125.8 (2)
N1—Ni1—N3	176.16 (10)	N1—C11—H11	117.1
O1—Ni1—N2	178.12 (8)	C1—C11—H11	117.1
N1—Ni1—N2	86.82 (9)	N1—C12—C13	106.1 (2)
N3—Ni1—N2	90.49 (9)	N1—C12—H12A	110.5
C2—O1—Ni1	128.09 (16)	C13—C12—H12A	110.5
C11—N1—C12	118.1 (2)	N1—C12—H12B	110.5
C11—N1—Ni1	127.20 (17)	C13—C12—H12B	110.5
C12—N1—Ni1	114.69 (16)	H12A—C12—H12B	108.7
C18—N2—C13	109.2 (2)	N2—C13—C12	108.4 (2)
C18—N2—C14	108.8 (2)	N2—C13—H13A	110.0
C13—N2—C14	112.3 (2)	C12—C13—H13A	110.0
C18—N2—Ni1	114.96 (16)	N2—C13—H13B	110.0
C13—N2—Ni1	105.47 (15)	C12—C13—H13B	110.0
C14—N2—Ni1	106.21 (15)	H13A—C13—H13B	108.4
N4—N3—Ni1	123.93 (19)	N2—C14—C15	114.1 (2)
N5—N4—N3	176.0 (3)	N2—C14—H14A	108.7
C2—C1—C11	119.2 (2)	C15—C14—H14A	108.7
C2—C1—C10	120.0 (2)	N2—C14—H14B	108.7
C11—C1—C10	120.8 (2)	C15—C14—H14B	108.7
O1—C2—C1	125.2 (2)	H14A—C14—H14B	107.6
O1—C2—C3	115.9 (2)	C16—C15—C14	110.7 (3)
C1—C2—C3	118.9 (2)	C16—C15—H15A	109.5
C4—C3—C2	120.9 (3)	C14—C15—H15A	109.5
C4—C3—H3	119.5	C16—C15—H15B	109.5
C2—C3—H3	119.5	C14—C15—H15B	109.5
C3—C4—C5	122.1 (3)	H15A—C15—H15B	108.1
C3—C4—H4	118.9	C15—C16—C17	110.3 (3)
C5—C4—H4	118.9	C15—C16—H16A	109.6
C10—C5—C6	119.5 (3)	C17—C16—H16A	109.6
C10—C5—C4	118.9 (2)	C15—C16—H16B	109.6
C6—C5—C4	121.6 (3)	C17—C16—H16B	109.6
C7—C6—C5	121.4 (3)	H16A—C16—H16B	108.1
C7—C6—H6	119.3	C16—C17—C18	111.3 (3)
C5—C6—H6	119.3	C16—C17—H17A	109.4
C6—C7—C8	119.5 (3)	C18—C17—H17A	109.4
C6—C7—H7	120.3	C16—C17—H17B	109.4
C8—C7—H7	120.3	C18—C17—H17B	109.4
C9—C8—C7	120.5 (3)	H17A—C17—H17B	108.0
C9—C8—H8	119.8	N2—C18—C17	113.0 (2)
C7—C8—H8	119.8	N2—C18—H18A	109.0
C8—C9—C10	121.5 (3)	C17—C18—H18A	109.0
C8—C9—H9	119.3	N2—C18—H18B	109.0
C10—C9—H9	119.3	C17—C18—H18B	109.0

C9—C10—C5	117.7 (2)	H18A—C18—H18B	107.8
C9—C10—C1	123.2 (2)		

Fig. 1