Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Azido{1-[(2-diethylaminoethylimino-κ^2N,N')methyl]naphthalen-2-olato-κO}-nickel(II)

Yun-Peng Diao,[a] Shan-Shan Huang,[a] Bao-Jing Zhang[a] and Kun Li[b]*

[a]School of Pharmacy, Dalian Medical University, Dalian 116027, People's Republic of China, and [b]College of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian 116029, People's Republic of China
Correspondence e-mail: diaoyiwen@126.com

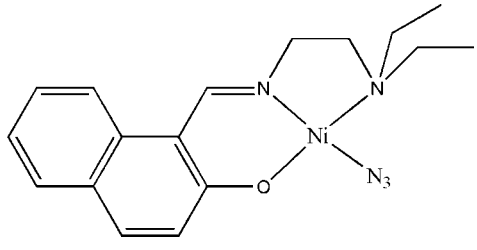
Received 21 August 2007; accepted 3 September 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.055; wR factor = 0.152; data-to-parameter ratio = 18.5.

In the title mononuclear nickel(II) complex, $[Ni(C_{17}H_{21}N_2O)(N_3)]$, 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 an azido 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

$[Ni(C_{17}H_{21}N_2O)(N_3)]$
M_r = 370.10
Orthorhombic, *Pbca*
a = 7.220 (2) Å
b = 13.873 (2) Å
c = 33.630 (5) Å
V = 3368.5 (12) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.17 mm^{-1}
T = 293 (2) K
0.21 × 0.17 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.792, T_{max} = 0.826
27240 measured reflections
4062 independent reflections
2839 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.152
S = 1.03
4062 reflections
219 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.94 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 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*.

This project was financially supported by a research grant from Dalian Medical University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2384).

References

Arıcı, C., Yüzer, D., Atakol, O., Fuess, H. & Svoboda, I. (2005). *Acta Cryst.* E**61**, m919–m921.
Brückner, C., Rettig, S. J. & Dolphin, D. (2000). *Inorg. Chem.* **39**, 6100–6106.
Bruker (2000). *SMART* (Version 5.625), *SAINT* (Version 6.01), *SHELXTL* (Version 6.10) and *SADABS* (Version 2.03). Bruker AXS Inc., Madison, Wisconsin, USA.
Diao, Y.-P. (2007*a*). *Acta Cryst.* E**63**, m1081–m1083.
Diao, Y.-P. (2007*b*). *Acta Cryst.* E**63**, m1453–m1454.
Diao, Y.-P., Huang, S.-S., Zhang, H.-L., Deng, S. & Liu, K.-X. (2007). *Acta Cryst.* E**63**, m1694.
Diao, Y.-P., Shu, X.-H., Zhang, B.-J., Zhen, Y.-H. & Kang, T.-G. (2007). *Acta Cryst.* E**63**, m1816.
Harrop, T. C., Olmstead, M. M. & Mascharak, P. K. (2003). *Chem. Commun.* pp. 410–411.
Li, J.-M., Jiang, Y.-M., Li, C.-Z. & Zhang, S.-H. (2007). *Acta Cryst.* E**63**, m447–m449.
Li, K., Huang, S.-S., Zhang, B.-J., Meng, D.-L. & Diao, Y.-P. (2007). *Acta Cryst.* E**63**, m2291.
Marganian, C. A., Vazir, H., Baidya, N., Olmstead, M. M. & Mascharak, P. K. (1995). *J. Am. Chem. Soc.* **117**, 1584–1594.
Ren, S., Wang, R., Komatsu, K., Bonaz-Krause, P., Zyrianov, Y., McKenna, C. E., Csipke, C., Tokes, Z. A. & Lien, E. J. (2002). *J. Med. Chem.* **45**, 410–419.
Usman, A., Fun, H.-K., Karmakar, T. K., Ghosh, B. K. & Chandra, S. K. (2003). *Acta Cryst.* E**59**, m387–m389.
Van Hecke, K., Nockemann, P., Binnemans, K. & Van Meervelt, L. (2007). *Acta Cryst.* E**63**, m569–m571.

 doi:10.1107/S1600536807043103

supplementary materials

Acta Cryst. (2007). E**63**, m2495 [**doi:10.1107/S1600536807043103**]

Azido{1-[(2-diethylaminoethylimino-κ^2N,N')methyl]naphthalen-2-olato-κO}nickel(II)

Y.-P. Diao, S.-S. Huang, B.-J. Zhang 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, Huang *et al.*, 2007; Diao, Shu *et al.*, 2007; Diao, 2007*a*,b; Li, Huang *et al.*, 2007). In order to further develop the coordination chemistry of such nickel complexes, the author 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 an azido 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), *N*,*N*-diethylethane-1,2-diamine (0.1 mmol, 11.6 mg), sodium azide (0.1 mmol, 6.5 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 $U_{iso}(H) = 1.2U_{eq}(C)$ and $1.5U_{eq}$(methyl C).

Figures

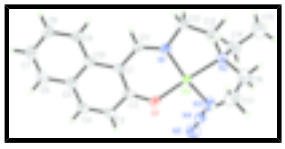


Fig. 1. The structure of the complex with 30% probability level.

Azido{1-[(2-diethylaminoethylimino-κ^2*N*,*N*')methyl]\ naphthalen-2-olato-κ*O*}nickel(II)

Crystal data

$[Ni(C_{17}H_{21}N_2O)(N_3)]$ $F_{000} = 1552$

M_r = 370.10	D_x = 1.460 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 1780 reflections
a = 7.220 (2) Å	θ = 2.3–24.9º
b = 13.873 (2) Å	μ = 1.17 mm^{-1}
c = 33.630 (5) Å	*T* = 293 (2) K
V = 3368.5 (12) Å^3	Block, red
Z = 8	0.21 × 0.17 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer	4062 independent reflections
Radiation source: fine-focus sealed tube	2839 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.057
T = 293(2) K	θ_{max} = 28.3º
ω scans	θ_{min} = 1.2º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	*h* = −9→9
T_{min} = 0.792, T_{max} = 0.826	*k* = −18→18
27240 measured reflections	*l* = −43→43

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.055	H-atom parameters constrained
$wR(F^2)$ = 0.152	$w = 1/[\sigma^2(F_o^2) + (0.0662P)^2 + 3.967P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
4062 reflections	$\Delta\rho_{max}$ = 0.94 e Å^{-3}
219 parameters	$\Delta\rho_{min}$ = −0.46 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	0.10100 (7)	0.01095 (3)	0.117402 (13)	0.04055 (17)
N1	0.1712 (4)	0.11724 (19)	0.15022 (8)	0.0424 (7)
N2	0.1712 (5)	0.1004 (2)	0.07048 (9)	0.0487 (7)
N3	−0.0160 (7)	−0.0798 (3)	0.08122 (10)	0.0784 (13)
N4	−0.1139 (5)	−0.1430 (2)	0.09152 (10)	0.0558 (8)
N5	−0.2081 (7)	−0.2050 (3)	0.09994 (13)	0.0875 (13)
O1	0.0936 (4)	−0.07559 (17)	0.16059 (7)	0.0481 (6)
C1	0.1457 (4)	0.0368 (2)	0.21414 (10)	0.0373 (7)
C2	0.1026 (4)	−0.0545 (2)	0.19821 (10)	0.0392 (7)
C3	0.0660 (5)	−0.1322 (3)	0.22519 (12)	0.0479 (9)
H3	0.0359	−0.1926	0.2151	0.058*
C4	0.0744 (5)	−0.1194 (3)	0.26479 (12)	0.0521 (10)
H4	0.0497	−0.1715	0.2813	0.063*
C5	0.1195 (5)	−0.0292 (3)	0.28224 (11)	0.0456 (8)
C6	0.1306 (6)	−0.0175 (3)	0.32361 (12)	0.0586 (11)
H6	0.1093	−0.0702	0.3401	0.070*
C7	0.1721 (6)	0.0696 (3)	0.34026 (12)	0.0631 (12)
H7	0.1806	0.0760	0.3677	0.076*
C8	0.2015 (6)	0.1485 (3)	0.31570 (11)	0.0576 (10)
H8	0.2274	0.2083	0.3269	0.069*
C9	0.1929 (5)	0.1393 (3)	0.27510 (10)	0.0468 (8)
H9	0.2141	0.1932	0.2593	0.056*
C10	0.1527 (4)	0.0502 (2)	0.25674 (10)	0.0393 (7)
C11	0.1831 (5)	0.1166 (2)	0.18845 (10)	0.0416 (8)
H11	0.2198	0.1738	0.2006	0.050*
C12	0.2103 (8)	0.2060 (3)	0.12847 (12)	0.0678 (13)
H12A	0.3084	0.2415	0.1416	0.081*
H12B	0.1006	0.2463	0.1277	0.081*
C13	0.2670 (9)	0.1810 (4)	0.08795 (12)	0.096 (2)
H13A	0.2484	0.2369	0.0711	0.115*
H13B	0.3985	0.1669	0.0881	0.115*
C14	−0.0127 (8)	0.1295 (4)	0.05226 (16)	0.0866 (15)
H14A	−0.0756	0.0716	0.0433	0.104*
H14B	−0.0886	0.1583	0.0729	0.104*
C15	−0.0020 (11)	0.1982 (5)	0.01826 (17)	0.120 (2)
H15A	0.0504	0.2580	0.0272	0.180*
H15B	−0.1241	0.2095	0.0080	0.180*
H15C	0.0746	0.1713	−0.0023	0.180*
C16	0.2778 (10)	0.0477 (4)	0.03984 (16)	0.103 (2)
H16A	0.3318	0.0940	0.0216	0.123*
H16B	0.1935	0.0073	0.0248	0.123*
C17	0.4310 (8)	−0.0148 (4)	0.05682 (19)	0.0935 (18)
H17A	0.5317	0.0253	0.0654	0.140*
H17B	0.4741	−0.0586	0.0367	0.140*
H17C	0.3842	−0.0508	0.0791	0.140*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0491 (3)	0.0340 (2)	0.0385 (3)	−0.00497 (18)	0.0024 (2)	−0.00653 (17)
N1	0.0514 (17)	0.0356 (14)	0.0403 (15)	−0.0052 (13)	0.0045 (13)	−0.0020 (12)
N2	0.063 (2)	0.0446 (17)	0.0389 (15)	0.0036 (15)	0.0034 (14)	−0.0018 (13)
N3	0.120 (4)	0.069 (2)	0.0454 (19)	−0.043 (3)	0.000 (2)	−0.0101 (17)
N4	0.068 (2)	0.0485 (19)	0.0505 (19)	−0.0078 (18)	−0.0106 (16)	−0.0050 (15)
N5	0.100 (3)	0.071 (3)	0.092 (3)	−0.037 (3)	−0.012 (3)	0.000 (2)
O1	0.0604 (16)	0.0374 (13)	0.0465 (14)	−0.0046 (11)	0.0002 (12)	−0.0067 (10)
C1	0.0311 (16)	0.0357 (16)	0.0451 (18)	0.0043 (13)	−0.0009 (13)	−0.0002 (14)
C2	0.0328 (17)	0.0363 (17)	0.0485 (19)	0.0024 (14)	0.0016 (14)	0.0004 (14)
C3	0.043 (2)	0.0355 (18)	0.065 (2)	−0.0026 (15)	0.0022 (17)	0.0066 (16)
C4	0.046 (2)	0.047 (2)	0.063 (2)	0.0017 (16)	0.0053 (18)	0.0171 (18)
C5	0.0351 (19)	0.054 (2)	0.047 (2)	0.0109 (15)	0.0023 (15)	0.0055 (16)
C6	0.053 (2)	0.073 (3)	0.050 (2)	0.013 (2)	0.0040 (18)	0.018 (2)
C7	0.059 (3)	0.089 (3)	0.041 (2)	0.020 (2)	0.0017 (18)	0.001 (2)
C8	0.061 (3)	0.065 (3)	0.047 (2)	0.006 (2)	0.0017 (19)	−0.0099 (19)
C9	0.051 (2)	0.047 (2)	0.0424 (19)	0.0056 (17)	0.0020 (16)	−0.0038 (15)
C10	0.0299 (16)	0.0438 (17)	0.0441 (19)	0.0068 (14)	0.0009 (14)	−0.0003 (15)
C11	0.044 (2)	0.0346 (17)	0.0460 (19)	−0.0003 (14)	0.0041 (15)	−0.0058 (14)
C12	0.114 (4)	0.039 (2)	0.050 (2)	−0.011 (2)	0.011 (2)	0.0002 (17)
C13	0.156 (5)	0.083 (3)	0.050 (3)	−0.071 (4)	−0.006 (3)	0.007 (2)
C14	0.101 (4)	0.074 (3)	0.084 (4)	−0.001 (3)	−0.019 (3)	0.006 (3)
C15	0.162 (7)	0.118 (5)	0.080 (4)	0.017 (5)	−0.037 (4)	0.012 (4)
C16	0.134 (6)	0.094 (4)	0.080 (4)	0.011 (4)	0.045 (4)	0.006 (3)
C17	0.094 (4)	0.093 (4)	0.094 (4)	0.028 (3)	0.023 (3)	−0.004 (3)

Geometric parameters (Å, °)

Ni1—O1	1.885 (2)	C7—C8	1.387 (6)
Ni1—N1	1.910 (3)	C7—H7	0.9300
Ni1—N3	1.944 (3)	C8—C9	1.373 (5)
Ni1—N2	2.071 (3)	C8—H8	0.9300
N1—C11	1.289 (4)	C9—C10	1.412 (5)
N1—C12	1.459 (5)	C9—H9	0.9300
N2—C13	1.440 (5)	C11—H11	0.9300
N2—C16	1.479 (6)	C12—C13	1.465 (6)
N2—C14	1.517 (6)	C12—H12A	0.9700
N3—N4	1.179 (5)	C12—H12B	0.9700
N4—N5	1.132 (5)	C13—H13A	0.9700
O1—C2	1.300 (4)	C13—H13B	0.9700
C1—C2	1.410 (5)	C14—C15	1.490 (7)
C1—C11	1.430 (5)	C14—H14A	0.9700
C1—C10	1.446 (5)	C14—H14B	0.9700
C2—C3	1.433 (5)	C15—H15A	0.9600
C3—C4	1.345 (5)	C15—H15B	0.9600
C3—H3	0.9300	C15—H15C	0.9600

C4—C5	1.420 (5)	C16—C17	1.518 (8)
C4—H4	0.9300	C16—H16A	0.9700
C5—C6	1.403 (6)	C16—H16B	0.9700
C5—C10	1.417 (5)	C17—H17A	0.9600
C6—C7	1.365 (6)	C17—H17B	0.9600
C6—H6	0.9300	C17—H17C	0.9600
O1—Ni1—N1	93.10 (11)	C10—C9—H9	119.2
O1—Ni1—N3	93.28 (13)	C9—C10—C5	116.8 (3)
N1—Ni1—N3	167.63 (17)	C9—C10—C1	123.6 (3)
O1—Ni1—N2	167.40 (12)	C5—C10—C1	119.6 (3)
N1—Ni1—N2	84.99 (12)	N1—C11—C1	126.5 (3)
N3—Ni1—N2	91.01 (14)	N1—C11—H11	116.7
C11—N1—C12	119.5 (3)	C1—C11—H11	116.7
C11—N1—Ni1	126.1 (2)	N1—C12—C13	108.7 (3)
C12—N1—Ni1	114.4 (2)	N1—C12—H12A	109.9
C13—N2—C16	114.7 (4)	C13—C12—H12A	109.9
C13—N2—C14	112.3 (4)	N1—C12—H12B	109.9
C16—N2—C14	107.8 (4)	C13—C12—H12B	109.9
C13—N2—Ni1	105.8 (2)	H12A—C12—H12B	108.3
C16—N2—Ni1	111.2 (3)	N2—C13—C12	115.4 (4)
C14—N2—Ni1	104.7 (3)	N2—C13—H13A	108.4
N4—N3—Ni1	124.0 (3)	C12—C13—H13A	108.4
N5—N4—N3	177.4 (4)	N2—C13—H13B	108.4
C2—O1—Ni1	127.2 (2)	C12—C13—H13B	108.4
C2—C1—C11	120.5 (3)	H13A—C13—H13B	107.5
C2—C1—C10	120.0 (3)	C15—C14—N2	115.7 (5)
C11—C1—C10	119.5 (3)	C15—C14—H14A	108.3
O1—C2—C1	125.7 (3)	N2—C14—H14A	108.3
O1—C2—C3	115.9 (3)	C15—C14—H14B	108.3
C1—C2—C3	118.4 (3)	N2—C14—H14B	108.3
C4—C3—C2	121.3 (3)	H14A—C14—H14B	107.4
C4—C3—H3	119.3	C14—C15—H15A	109.5
C2—C3—H3	119.3	C14—C15—H15B	109.5
C3—C4—C5	122.4 (3)	H15A—C15—H15B	109.5
C3—C4—H4	118.8	C14—C15—H15C	109.5
C5—C4—H4	118.8	H15A—C15—H15C	109.5
C6—C5—C10	120.0 (4)	H15B—C15—H15C	109.5
C6—C5—C4	121.7 (4)	N2—C16—C17	113.6 (5)
C10—C5—C4	118.3 (3)	N2—C16—H16A	108.9
C7—C6—C5	121.5 (4)	C17—C16—H16A	108.9
C7—C6—H6	119.3	N2—C16—H16B	108.9
C5—C6—H6	119.3	C17—C16—H16B	108.9
C6—C7—C8	119.2 (4)	H16A—C16—H16B	107.7
C6—C7—H7	120.4	C16—C17—H17A	109.5
C8—C7—H7	120.4	C16—C17—H17B	109.5
C9—C8—C7	120.8 (4)	H17A—C17—H17B	109.5
C9—C8—H8	119.6	C16—C17—H17C	109.5
C7—C8—H8	119.6	H17A—C17—H17C	109.5
C8—C9—C10	121.7 (4)	H17B—C17—H17C	109.5

C8—C9—H9	119.2

Fig. 1