

C10A	0.1969 (4)	0.2853 (2)	0.13686 (13)	0.0508 (6)
C11A	0.2325 (3)	0.3410 (2)	0.08395 (13)	0.0474 (5)
C12A	0.2670 (4)	0.2979 (2)	0.00840 (13)	0.0500 (6)
C13A	0.2684 (3)	0.2058 (2)	-0.01183 (13)	0.0474 (5)
C14A	0.2343 (3)	0.1507 (2)	0.04111 (12)	0.0450 (5)
C15A	0.2346 (3)	0.0532 (2)	0.02316 (14)	0.0484 (5)
C16A	0.2683 (4)	0.0018 (2)	-0.04342 (14)	0.0502 (6)
C17A	0.2714 (3)	-0.0947 (2)	-0.05712 (12)	0.0438 (5)
C18A	0.3172 (4)	-0.1407 (2)	-0.12901 (14)	0.0519 (6)
C19A	0.3195 (4)	-0.2309 (2)	-0.14436 (14)	0.0528 (6)
C20A	0.2346 (4)	-0.2376 (2)	-0.02067 (14)	0.0543 (6)
C21A	0.2298 (4)	-0.1480 (2)	-0.00238 (14)	0.0521 (6)
C22A	0.2578 (7)	0.4893 (3)	0.0511 (2)	0.0779 (10)
C23A	0.2434 (7)	0.4809 (3)	0.1864 (2)	0.0784 (10)
C24A	0.2762 (6)	-0.3789 (2)	-0.1088 (2)	0.0718 (8)
N5B	0.1694 (3)	0.40742 (13)	0.61611 (11)	0.0531 (5)
N6B	0.3070 (3)	-0.29303 (13)	0.43527 (11)	0.0456 (4)
C9B	0.2612 (3)	0.1888 (2)	0.64186 (12)	0.0438 (5)
C10B	0.2402 (3)	0.2780 (2)	0.65959 (12)	0.0453 (5)
C11B	0.1963 (3)	0.31897 (15)	0.60023 (12)	0.0405 (5)
C12B	0.1766 (3)	0.2652 (2)	0.52332 (12)	0.0419 (5)
C13B	0.1969 (3)	0.1766 (2)	0.50690 (12)	0.0422 (5)
C14B	0.2389 (3)	0.13488 (15)	0.56573 (12)	0.0394 (5)
C15B	0.2602 (3)	0.0403 (2)	0.55064 (12)	0.0416 (5)
C16B	0.2395 (3)	-0.0195 (2)	0.48172 (13)	0.0421 (5)
C17B	0.2638 (3)	-0.11269 (15)	0.46800 (12)	0.0391 (4)
C18B	0.2369 (3)	-0.1682 (2)	0.39248 (12)	0.0466 (5)
C19B	0.2591 (4)	-0.2563 (2)	0.37714 (14)	0.0509 (6)
C20B	0.3333 (3)	-0.2416 (2)	0.50888 (14)	0.0507 (6)
C21B	0.3116 (4)	-0.1540 (2)	0.52662 (13)	0.0487 (6)
C22B	0.1659 (5)	0.4539 (2)	0.5536 (2)	0.0570 (7)
C23B	0.2061 (6)	0.4648 (2)	0.6948 (2)	0.0652 (8)
C24B	0.3320 (5)	-0.3885 (2)	0.4166 (2)	0.0620 (7)

Table 2. Selected geometric parameters (Å, °)

Anion			
Ni—S4	2.1658 (7)	N2—C4	1.143 (3)
Ni—S1	2.1766 (7)	N3—C7	1.146 (3)
Ni—S2	2.1787 (7)	N4—C8	1.150 (3)
Ni—S3	2.1805 (7)	C1—C2	1.355 (3)
S1—C1	1.732 (2)	C1—C3	1.429 (3)
S2—C2	1.735 (2)	C2—C4	1.424 (3)
S3—C5	1.730 (2)	C5—C6	1.357 (3)
S4—C6	1.728 (2)	C5—C7	1.428 (3)
N1—C3	1.140 (3)	C6—C8	1.432 (3)
S4—Ni—S1	177.48 (2)	S4—Ni—S3	92.22 (3)
S4—Ni—S2	86.92 (3)	S1—Ni—S3	88.64 (3)
S1—Ni—S2	92.31 (3)	S2—Ni—S3	177.64 (2)

	Cation A	Cation B
N5—C11	1.370 (3)	1.377 (3)
N5—C22	1.440 (4)	1.450 (3)
N5—C23	1.442 (4)	1.450 (3)
N6—C19	1.344 (3)	1.352 (3)
N6—C20	1.351 (3)	1.343 (3)
N6—C24	1.473 (4)	1.477 (3)
C9—C10	1.369 (3)	1.374 (3)
C9—C14	1.393 (3)	1.394 (3)
C10—C11	1.405 (3)	1.404 (3)
C11—C12	1.407 (3)	1.406 (3)
C12—C13	1.376 (3)	1.363 (3)
C13—C14	1.399 (3)	1.399 (3)
C14—C15	1.455 (3)	1.454 (3)
C15—C16	1.322 (3)	1.329 (3)
C16—C17	1.447 (3)	1.443 (3)
C17—C18	1.398 (3)	1.393 (3)
C17—C21	1.411 (3)	1.405 (3)
C18—C19	1.349 (4)	1.359 (3)
C20—C21	1.346 (4)	1.351 (3)

Data collection: XSCANS (Siemens, 1994). Cell refinement: XSCANS. Data reduction: XSCANS. Program(s) used to solve structure: *SHELXTL/PC* (Sheldrick, 1990) by direct methods. Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *SHELXTL/PC*. Software used to prepare material for publication: *SHELXL93*. Geometrical calculations: *PARST* (Nardelli, 1983).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: MU1233). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Bis(*N*-benzyl-2-hydroxy-1-naphthaldiminato)nickel(II)

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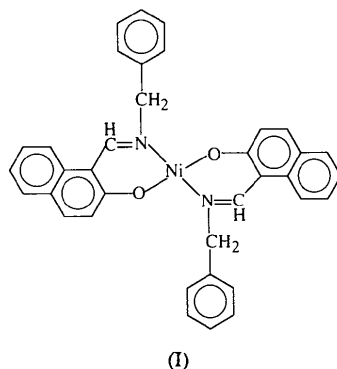
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Abstract

The crystal structure of the title compound, bis-[1-(benzyliminomethyl)-2-naphtholato-*N,O*]nickel(II), [Ni(C₁₈H₁₄NO)₂], has been determined. Two bidentate Schiff base ligands coordinate to the Ni atom in a square-planar arrangement.

Schiff base metal complexes have been used extensively in the field of coordination chemistry, *e.g.* copper(II) and nickel(II) complexes. The electron delocalization to produce resonance structures of square-planar nickel(II) and copper(II) metal complexes with ligands derived from salicylaldehyde and naphthaldehyde has been examined previously (Fernández-G. *et al.*, 1987, and references therein). Maggio, Pizzino & Romano (1974) reported that copper(II) and nickel(II) ions react with tridentate anionic Schiff bases to form dimerized square-planar complexes. The same authors also reported that *N*-(2-hydroxyphenyl)salicylaldimine reacts with the nickel(II) ion to give a pseudo-octahedral complex by polymerization. The present paper reports the structure of the Schiff base nickel complex (I).



2.110 (7) Å, respectively, which are significantly longer than those of square-planar coordination.

The bond length N(1)—C(11) is typical for a C=N double bond and the sum of the bond angles at the N(1) atom [360.0 (4)°] reflects the sp^2 hybridization.

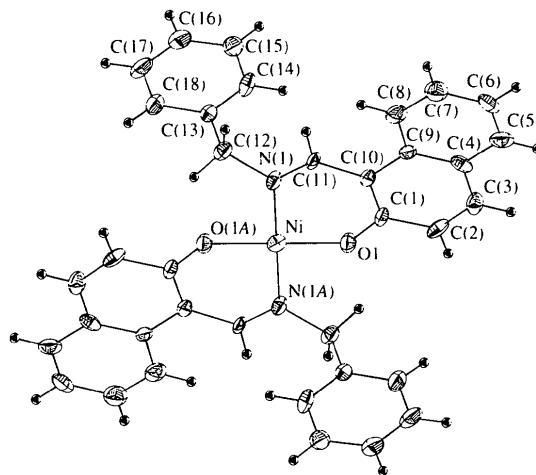


Fig. 1. Molecular structure of the title compound (*ORTEP*; Johnson, 1976). Displacement ellipsoids are plotted at the 50% probability level.

The title compound was obtained from the condensation of *N*-benzyl-2-hydroxynaphthalimine and $(\text{CH}_3\text{COO})_2\text{Ni}\cdot 4\text{H}_2\text{O}$, prepared by standard procedures (Vogel, 1966).

$$[\text{Ni}(\text{C}_{18}\text{H}_{14}\text{NO})_2]$$

$M_r = 578.7$
 Monoclinic
 $C2/c$
 $a = 20.756(1) \text{ \AA}$
 $b = 6.160(1) \text{ \AA}$
 $c = 21.475(1) \text{ \AA}$
 $\beta = 97.32(1)^\circ$
 $V = 2723.2(5) \text{ \AA}^3$
 $Z = 4$
 $D_x = 1.41 \text{ Mg m}^{-3}$

Mo K α radiation
 $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 25
 reflections
 $\theta = 2-9^\circ$
 $\mu = 0.696 \text{ mm}^{-1}$
 $T = 293 (2) \text{ K}$
 Prismatic
 $0.21 \times 0.08 \times 0.06 \text{ mm}$
 Dark red

CAD-4 diffractometer

ω / 2θ scans
 Absorption correction:
 ψ scan (Kopfmann &
 Huber, 1968; North,
 Phillips & Mathews,
 1968)
 $T_{\min} = 0.81$, $T_{\max} = 0.99$
 1607 measured reflections
 1178 independent reflections

689 observed reflections
 $[I > 2\sigma(I)]$
 $R_{\text{int}} = 0.03$
 $\theta_{\text{max}} = 21.94^\circ$
 $h = 0 \rightarrow 21$
 $k = 0 \rightarrow 6$
 $l = -22 \rightarrow 22$
 3 standard reflections
 frequency: 120 min
 intensity decay: 4.4%

Refinement

Refinement on F^2 $R[F^2 > 2\sigma(F^2)] = 0.045$ $wR(F^2) = 0.075$ $S = 1.18$

689 reflections

187 parameters

H atoms riding with fixed

 $U_{\text{iso}} = 1.6 \times U_{\text{eq}}$ of the
carrier atom $w = 1/[\sigma^2(F_o^2) + (0.0267P)^2]$ where $P = [\max(F_o^2, 0)$
 $+ 2F_c^2]/3$ $(\Delta/\sigma)_{\text{max}} = 0.04$ $\Delta\rho_{\text{max}} = 0.2 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\text{min}} = -0.2 \text{ e } \text{\AA}^{-3}$

Extinction correction: none

Atomic scattering factors

from *International Tables*for *Crystallography* (1992,

Vol. C, Tables 4.2.6.8 and

6.1.1.4)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters ($\text{\AA}^2$)
$$U_{\text{eq}} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j.$$

	x	y	z	U_{eq}
Ni	3/4	1/4	1/2	0.037 (1)
O(1)	0.7393 (2)	0.5018 (6)	0.4570 (1)	0.043 (1)
N(1)	0.8229 (2)	0.1724 (6)	0.4583 (2)	0.033 (1)
C(1)	0.7633 (3)	0.5653 (9)	0.4069 (2)	0.033 (2)
C(2)	0.7409 (2)	0.7719 (11)	0.3804 (2)	0.042 (2)
C(3)	0.7633 (3)	0.8508 (9)	0.3289 (2)	0.044 (2)
C(4)	0.8100 (2)	0.7378 (11)	0.2982 (2)	0.038 (2)
C(5)	0.8305 (2)	0.8226 (9)	0.2432 (3)	0.050 (2)
C(6)	0.8728 (3)	0.7106 (11)	0.2119 (2)	0.050 (2)
C(7)	0.8952 (3)	0.5103 (10)	0.2340 (3)	0.054 (2)
C(8)	0.8760 (3)	0.4257 (10)	0.2880 (2)	0.047 (2)
C(9)	0.8320 (2)	0.5368 (9)	0.3222 (2)	0.031 (2)
C(10)	0.8098 (2)	0.4536 (9)	0.3784 (2)	0.032 (2)
C(11)	0.8383 (2)	0.2665 (11)	0.4094 (2)	0.034 (2)
C(12)	0.8654 (3)	-0.0117 (9)	0.4817 (2)	0.038 (2)
C(13)	0.9148 (2)	0.0479 (9)	0.5372 (2)	0.031 (2)
C(14)	0.9447 (3)	0.2474 (12)	0.5425 (2)	0.046 (2)
C(15)	0.9950 (3)	0.2948 (10)	0.5926 (3)	0.049 (2)
C(16)	1.0119 (3)	0.1360 (11)	0.6365 (3)	0.061 (2)
C(17)	0.9823 (3)	-0.0612 (12)	0.6320 (3)	0.059 (2)
C(18)	0.9346 (3)	-0.1097 (10)	0.5820 (3)	0.048 (2)

Table 2. Selected geometric parameters ($\text{\AA}$, $^\circ$)

Ni—O(1)	1.805 (3)	C(6)—C(7)	1.381 (8)
Ni—N(1)	1.915 (4)	C(7)—C(8)	1.376 (7)
O(1)—C(1)	1.301 (6)	C(8)—C(9)	1.419 (7)
N(1)—C(11)	1.275 (6)	C(9)—C(10)	1.441 (7)
N(1)—C(12)	1.484 (6)	C(10)—C(11)	1.422 (7)
C(1)—C(10)	1.388 (7)	C(12)—C(13)	1.516 (6)
C(1)—C(2)	1.446 (8)	C(13)—C(18)	1.392 (7)
C(2)—C(3)	1.343 (7)	C(13)—C(14)	1.374 (8)
C(3)—C(4)	1.423 (7)	C(14)—C(15)	1.432 (7)
C(4)—C(5)	1.405 (7)	C(15)—C(16)	1.373 (8)
C(4)—C(9)	1.395 (8)	C(16)—C(17)	1.359 (9)
C(5)—C(6)	1.360 (7)	C(17)—C(18)	1.397 (7)
O(1)—Ni—N(1)	91.6 (2)	O(1)—C(1)—C(2)	116.9 (5)
O(1)—Ni—O(1A')	180.0 (2)	C(2)—C(1)—C(10)	118.0 (5)
O(1)—Ni—N(1A')	88.4 (2)	C(4)—C(9)—C(8)	116.0 (5)
Ni—O(1)—C(1)	130.3 (3)	C(1)—C(10)—C(11)	117.9 (4)
C(11)—N(1)—C(12)	115.2 (4)	N(1)—C(11)—C(10)	128.3 (5)
Ni—N(1)—C(11)	124.6 (4)	N(1)—C(12)—C(13)	113.3 (4)
Ni—N(1)—C(12)	120.2 (3)	C(12)—C(13)—C(18)	119.0 (5)
O(1)—C(1)—C(10)	125.1 (5)		

Symmetry code: (i) $\frac{3}{2} - x, \frac{1}{2} - y, 1 - z$.Table 3. Bond lengths ($\text{\AA}$) of some nickel(II) complexes

Complex	Ni—N(1)	Ni—N(2)	Ni—O	C—O	C=N
(a)	1.848 (4)	1.947 (4)	1.817 (1)	1.315 (2)	1.292 (5)
(b)	1.849 (3)	1.955 (4)	1.831 (3)	1.322 (5)	1.303 (5)
(c)	1.916 (4)	—	1.829 (2)	1.321 (3)	1.300 (2)
(d)	1.912 (3)	—	1.832 (2)	1.305 (4)	1.297 (4)
(e)	1.941 (3)	—	1.828 (3)	1.332 (5)	1.279 (6)

(f)	1.854 (4)	1.970 (4)	1.828 (4)	1.335 (8)	1.263 (5)
(g)	1.898 (4)	1.936 (5)	1.848 (8)	1.322 (2)	1.285 (4)
(h)	1.915 (4)	—	1.805 (3)	1.301 (6)	1.275 (6)

Complex: (a) {1-[(2-Hydroxyphenyl)iminomethyl]naphthalen-2-olato-*O,O',N*}piperidinenickel(II) (Elerman, Paulus & Fuess, 1991); (b) (diethylamino){1-[(2-hydroxyphenyl)iminomethyl]naphthalen-2-olato-*O,O',N*}nickel(II) (Elerman, Fuess & Paulus, 1992); (c) bis{*N*-(1,3-dioxolan-2-yl)methyl}salicylaldiminato}nickel(II) (Fernández-G. *et al.*, 1987); (d) bis{*N*-(1,3-dioxolan-2-yl)methyl}-2-hydroxy-1-naphthaldiminato}nickel(II) (Fernández-G. *et al.*, 1987); (e) bis[*N*-(1,3-dioxolan-2-yl)-3-hydroxy-1-naphthaldiminato]nickel(II) (Fernández-G. *et al.*, 1987); (f) [N-(2-hydroxyphenyl)salicylaldiminato]amminenickel(II) (Elerman, Svoboda & Fuess, 1992); (g) [N-(2-hydroxyphenyl)salicylaldiminato](diethylamine)nickel(II) (Elerman, Paulus & Svoboda, 1992); (h) bis(*N*-benzyl-2-hydroxy-1-naphthaldiminato)nickel(II) (present work).

The structure was solved by direct phase determination. All non-H atoms were refined anisotropically by full-matrix least-squares methods. All atoms except the Ni atom, which is at a special position, were refined without any constraints. Values of distances and angles in the rings show no significant differences from those of an ideal benzene ring.

Data collection: *SDP-Plus* (Frenz, 1985). Cell refinement: *SDP-Plus*. Data reduction: *SDP-Plus*. Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993).

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Lists of structure factors, torsion angles, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: KA1135). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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