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Bis[2,4-dibromo-6-(cyclopropylimino-methyl)phenolato]nickel(II)

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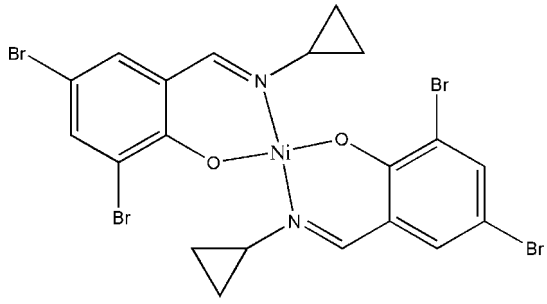
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.036; wR factor = 0.084; data-to-parameter ratio = 17.8.

The title compound, $[Ni(C_{10}H_8Br_2NO)_2]$, is a mononuclear nickel(II) complex. The Ni^{II} atom, located on an inversion centre, exhibits a square-planar coordination geometry. The metal atom is bonded to two phenolate O atoms and two imine N atoms from two Schiff base ligands.

Related literature

For related literature on Schiff base complexes, see: Chaturvedi (1977); Archer & Wang (1990); Costamagna *et al.* (1992); Yamada (1999); Li & Wang (2007); Wang & Li (2007*a*,*b*).



Experimental

Crystal data

$[Ni(C_{10}H_8Br_2NO)_2]$
M_r = 694.70
Monoclinic, $P2_1/c$
a = 8.0170 (16) Å
b = 9.2420 (18) Å
c = 14.088 (3) Å
β = 94.62 (3)°
V = 1040.4 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 8.63 mm^{-1}
T = 298 (2) K
0.23 × 0.20 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.152, T_{max} = 0.241
8738 measured reflections
2362 independent reflections
1801 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.084
S = 1.02
2362 reflections
133 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.844 (3)	Ni1—N1	1.931 (3)
O1—Ni1—O1^{i}	180.0	O1—Ni1—N1	92.33 (12)
O1—Ni1—N1^{i}	87.67 (12)		

Symmetry code: (i) $-x+1, -y, -z+1$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2080).

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supplementary materials

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Bis[2,4-dibromo-6-(cyclopropyliminomethyl)phenolato]nickel(II)

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Comment

Schiff base complexes have been of great interest for a long time (Chaturvedi, 1977; Archer & Wang, 1990; Costamagna *et al.*, 1992; Yamada, 1999). These complexes play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures. Recently, we have reported a few transition metal complexes (Wang & Li, 2007*a*,b; Li & Wang, 2007*a*). As an extension of the work on the structural investigation of these complexes, the title nickel(II) complex is reported here.

The title complex is a centrosymmetric mononuclear nickel(II) complex. The Ni^{II} atom, lying on the inversion centre, is four-coordinated and shows a square planar coordination geometry. It is bonded to two phenolate O and two imine N atoms from two Schiff base ligands. The Ni–O and Ni–N bond lengths are comparable to the corresponding values observed in other Schiff base nickel(II) complexes.

Experimental

3,5-Dibromosalicylaldehyde (0.2 mmol, 56.4 mg) and cyclopropylamine (0.2 mmol, 11.5 mg) were dissolved in a methanol solution (20 ml). The mixture was stirred at room temperature for 30 min, giving a clear yellow solution. To this solution was added a methanol solution (5 ml) of $Ni(NO_3)_2{\cdot}6H_2O$ (0.1 mmol, 29.1 mg) with stirring. The resulting mixture was stirred for a further 30 min at room temperature, giving a clear red solution. After allowing the solution to stand in air for a week, red block-shaped crystals were formed.

Refinement

H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C–H = 0.93–0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

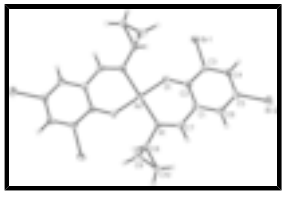

Fig. 1. Molecular structure of (I) at 30% probability level.

Bis(2,4-dibromo-6-cyclopropyliminomethylphenolato)nickel(II)

Crystal data

$[Ni(C_{10}H_8Br_2NO)_2]$	F_{000} = 668
M_r = 694.70	D_x = 2.217 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 8.0170 (16) Å	Cell parameters from 1834 reflections
b = 9.2420 (18) Å	θ = 2.5–25.3º
c = 14.088 (3) Å	μ = 8.63 mm^{-1}
β = 94.62 (3)º	T = 298 (2) K
V = 1040.4 (4) Å^3	Block, red
Z = 2	0.23 × 0.20 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer	2362 independent reflections
Radiation source: fine-focus sealed tube	1801 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.041
T = 298(2) K	θ_{max} = 27.5º
ω scan	θ_{min} = 2.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −10→10
T_{min} = 0.152, T_{max} = 0.241	k = −12→11
8738 measured reflections	l = −18→17

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.036	H-atom parameters constrained
$wR(F^2)$ = 0.084	$w = 1/[\sigma^2(F_o^2) + (0.0393P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max} < 0.001$
2362 reflections	$\Delta\rho_{max}$ = 0.51 e Å^{-3}
133 parameters	$\Delta\rho_{min}$ = −0.56 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	0.5000	0.0000	0.5000	0.02886 (18)
Br1	0.91324 (5)	−0.02357 (5)	0.26991 (3)	0.04253 (15)
Br2	1.30178 (6)	0.38800 (5)	0.48338 (3)	0.05101 (16)
O1	0.6838 (3)	0.0172 (3)	0.43016 (19)	0.0342 (6)
N1	0.6038 (4)	0.1142 (3)	0.6033 (2)	0.0283 (7)
C1	0.8438 (5)	0.1940 (4)	0.5221 (3)	0.0298 (8)
C2	0.8144 (5)	0.0988 (4)	0.4431 (3)	0.0292 (8)
C3	0.9399 (5)	0.0995 (4)	0.3777 (3)	0.0294 (8)
C4	1.0802 (5)	0.1830 (4)	0.3890 (3)	0.0327 (9)
H4	1.1601	0.1782	0.3448	0.039*
C5	1.1037 (5)	0.2754 (4)	0.4667 (3)	0.0335 (9)
C6	0.9869 (5)	0.2807 (4)	0.5324 (3)	0.0357 (9)
H6	1.0030	0.3426	0.5844	0.043*
C7	0.7349 (5)	0.1926 (4)	0.5975 (3)	0.0323 (9)
H7	0.7619	0.2553	0.6481	0.039*
C8	0.5247 (5)	0.1218 (4)	0.6926 (3)	0.0327 (9)
H8	0.4104	0.1602	0.6872	0.039*
C9	0.5548 (6)	0.0033 (5)	0.7635 (3)	0.0435 (11)
H9A	0.6342	−0.0716	0.7498	0.052*
H9B	0.4606	−0.0298	0.7968	0.052*
C10	0.6219 (5)	0.1516 (5)	0.7862 (3)	0.0431 (11)
H10A	0.7417	0.1664	0.7860	0.052*
H10B	0.5680	0.2082	0.8330	0.052*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0286 (4)	0.0337 (4)	0.0244 (4)	−0.0010 (3)	0.0028 (3)	−0.0023 (3)
Br1	0.0411 (3)	0.0576 (3)	0.0295 (2)	0.0009 (2)	0.00693 (18)	−0.00779 (19)
Br2	0.0382 (3)	0.0608 (3)	0.0544 (3)	−0.0152 (2)	0.0063 (2)	0.0010 (2)
O1	0.0311 (15)	0.0441 (17)	0.0282 (15)	−0.0076 (13)	0.0066 (12)	−0.0065 (12)
N1	0.0308 (18)	0.0289 (17)	0.0258 (16)	−0.0011 (14)	0.0059 (13)	−0.0026 (13)
C1	0.031 (2)	0.029 (2)	0.030 (2)	0.0037 (17)	0.0048 (16)	0.0030 (16)
C2	0.031 (2)	0.033 (2)	0.0234 (19)	0.0064 (17)	0.0015 (15)	0.0053 (16)
C3	0.032 (2)	0.035 (2)	0.0219 (19)	0.0047 (17)	0.0021 (15)	−0.0017 (15)
C4	0.026 (2)	0.043 (2)	0.030 (2)	0.0045 (18)	0.0067 (16)	0.0054 (17)
C5	0.028 (2)	0.035 (2)	0.037 (2)	−0.0020 (17)	0.0028 (17)	0.0078 (18)

C6	0.039 (2)	0.038 (2)	0.030 (2)	−0.0029 (19)	0.0013 (17)	−0.0016 (17)
C7	0.037 (2)	0.034 (2)	0.0257 (19)	0.0017 (18)	0.0021 (16)	−0.0052 (16)
C8	0.035 (2)	0.039 (2)	0.025 (2)	−0.0066 (18)	0.0084 (17)	−0.0064 (16)
C9	0.048 (3)	0.050 (3)	0.033 (2)	0.002 (2)	0.012 (2)	−0.0020 (19)
C10	0.042 (3)	0.057 (3)	0.032 (2)	−0.011 (2)	0.0080 (19)	−0.009 (2)

Geometric parameters (Å, °)

Ni1—O1	1.844 (3)	C4—C5	1.389 (5)
Ni1—O1^{i}	1.844 (3)	C4—H4	0.9300
Ni1—N1^{i}	1.931 (3)	C5—C6	1.370 (5)
Ni1—N1	1.931 (3)	C6—H6	0.9300
Br1—C3	1.896 (4)	C7—H7	0.9300
Br2—C5	1.898 (4)	C8—C9	1.489 (6)
O1—C2	1.291 (4)	C8—C10	1.502 (5)
N1—C7	1.284 (5)	C8—H8	0.9800
N1—C8	1.456 (5)	C9—C10	1.498 (6)
C1—C6	1.398 (5)	C9—H9A	0.9700
C1—C2	1.423 (5)	C9—H9B	0.9700
C1—C7	1.429 (5)	C10—H10A	0.9700
C2—C3	1.418 (5)	C10—H10B	0.9700
C3—C4	1.363 (5)		
O1—Ni1—O1^{i}	180.0	C5—C6—C1	120.6 (4)
O1—Ni1—N1^{i}	87.67 (12)	C5—C6—H6	119.7
O1^{i}—Ni1—N1^{i}	92.33 (12)	C1—C6—H6	119.7
O1—Ni1—N1	92.33 (12)	N1—C7—C1	127.2 (3)
O1^{i}—Ni1—N1	87.67 (12)	N1—C7—H7	116.4
N1^{i}—Ni1—N1	180.0	C1—C7—H7	116.4
C2—O1—Ni1	130.5 (2)	N1—C8—C9	119.1 (3)
C7—N1—C8	116.3 (3)	N1—C8—C10	122.4 (3)
C7—N1—Ni1	124.5 (3)	C9—C8—C10	60.1 (3)
C8—N1—Ni1	119.1 (2)	N1—C8—H8	114.8
C6—C1—C2	121.3 (4)	C9—C8—H8	114.8
C6—C1—C7	118.2 (4)	C10—C8—H8	114.8
C2—C1—C7	120.2 (3)	C8—C9—C10	60.4 (3)
O1—C2—C3	121.4 (3)	C8—C9—H9A	117.7
O1—C2—C1	123.6 (3)	C10—C9—H9A	117.7
C3—C2—C1	115.1 (3)	C8—C9—H9B	117.7
C4—C3—C2	123.3 (3)	C10—C9—H9B	117.7
C4—C3—Br1	118.2 (3)	H9A—C9—H9B	114.9
C2—C3—Br1	118.5 (3)	C9—C10—C8	59.5 (3)
C3—C4—C5	119.9 (3)	C9—C10—H10A	117.8
C3—C4—H4	120.1	C8—C10—H10A	117.8
C5—C4—H4	120.1	C9—C10—H10B	117.8
C6—C5—C4	119.9 (4)	C8—C10—H10B	117.8
C6—C5—Br2	120.5 (3)	H10A—C10—H10B	115.0
C4—C5—Br2	119.6 (3)		

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1.

Fig. 1