

Bis{2-[(*E*)-(4-fluorobenzyl)iminomethyl]-6-methoxyphenolato- κ^2N,O^1 }nickel(II)

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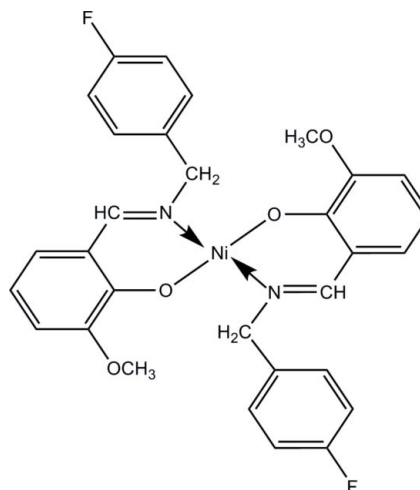
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(C-C) = 0.003$ Å; disorder in main residue; R factor = 0.047; wR factor = 0.114; data-to-parameter ratio = 17.8.

In the title compound, $[Ni(C_{15}H_{13}FNO_2)_2]$, the Ni^{II} atom is tetracoordinated by two N atoms and two O atoms from two 2-[(4-fluorobenzyl)iminomethyl]-6-methoxyphenolate ligands in a square-planar geometry. The two N atoms and two O atoms around the Ni^{II} atom are *trans* to each other, as the Ni^{II} atom lies on an inversion centre. In the fluorophenyl group, five C atoms and an F atom are disordered over two sets of positions of equal occupancy. In the crystal, the complex molecules are linked *via* intermolecular C—H...F hydrogen bonds, forming chains along [001].

Related literature

For applications of Schiff base complexes, see: Arun *et al.* (2009); Bagihalli *et al.* (2008); Yamada (1999). For a related structure, see: Mohd Tajuddin *et al.* (2010). For the synthesis of the ligand, see: Bahron *et al.* (2007).



Experimental

Crystal data

$[Ni(C_{15}H_{13}FNO_2)_2]$
 $M_r = 575.24$
Triclinic, $P\bar{1}$
 $a = 5.0110$ (2) Å
 $b = 10.9309$ (4) Å
 $c = 12.2435$ (5) Å
 $\alpha = 109.631$ (2)°
 $\beta = 99.083$ (3)°

$\gamma = 91.020$ (3)°
 $V = 621.92$ (4) Å³
 $Z = 1$
Mo $K\alpha$ radiation
 $\mu = 0.84$ mm⁻¹
 $T = 100$ K
0.49 × 0.09 × 0.03 mm

Data collection

Bruker APEXII CCD
diffractometer
Absorption correction: multi-scan
(SADABS; Bruker, 2001)
 $T_{min} = 0.685$, $T_{max} = 0.977$

14720 measured reflections
3948 independent reflections
3148 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.071$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.114$
 $S = 1.08$
3948 reflections

222 parameters
H-atom parameters constrained
 $\Delta\rho_{max} = 0.55$ e Å⁻³
 $\Delta\rho_{min} = -1.20$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C5—H5A...F1 ⁱ	0.95	2.51	3.363 (18)	150

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

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2443).

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supplementary materials

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Bis{2-[(*E*)-(4-fluorobenzyl)iminomethyl]-6-methoxyphenolato- κ^2N,O^1 }nickel(II)

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Comment

Schiff base complexes are attractive due to their simple synthesis, versatility and diverse range of applications (Yamada, 1999). Nickel(II) Schiff base complexes have been reported to possess various properties such as anti-bacterial, anti-fungal (Bagihalli *et al.*, 2008) and catalytic activities (Arun *et al.*, 2009). The title compound is bis-bidentate and related to the previously reported bis[2-(1-benzyliminoethyl)phenolato]palladium(II) (Mohd Tajuddin *et al.*, 2010), but with different metal centres and substituents on the iminoalkylphenolato and benzyl moieties.

The asymmetric unit has one half of the molecule, in which the Ni^{II} atom lies on an inversion centre (Fig. 1). The geometry around the Ni^{II} atom is square-planar, in which two N atoms and two O atoms are coplanar and *trans* to each other. The fluorophenyl group is disordered with five C atoms and an F atom over two sets of positions in an occupancy ratio of 0.50:0.50. The distances between the Ni atom and O and N atoms are 1.8298 (14) and 1.9223 (16) Å, respectively. In the crystal structure, the complex molecules are linked *via* C—H \cdots F hydrogen bonds (Table 1, Fig. 2), forming a one-dimensional chain along [0 0 1].

Experimental

The ligand 2-[(*E*)-(4-fluorobenzylimino)methyl]-6-methoxyphenol (0.519 g, 2 mmol), which was prepared according to the previously published method (Bahron *et al.*, 2007), was dissolved in ethanol (5 ml) in a round-bottomed flask. Nickel(II) acetate (0.251 g, 1 mmol) was dissolved separately in ethanol (5 ml) and added into the flask containing the ligand solution. The mixture was stirred and refluxed for 5 h, upon which a green precipitate was formed. It was isolated by gravity filtration, washed with cold ethanol and air dried at room temperature. The solid product was recrystallized from chloroform, yielding green crystals (yield: 83.9%). Melting point: 493–498 K. Analysis, calculated for C₃₀H₂₆F₂N₂NiO₄: C 62.64, H 4.56, N 4.87%; found: C 62.83, H 4.61, N 4.62%. IR (cm⁻¹): $\nu(\text{C}=\text{N})$ 1612 (s), $\nu(\text{C}-\text{O})$ 1249 (s), $\nu(\text{C}-\text{H})$ 2837 (w), $\nu(\text{C}-\text{N})$ 1340 (m), $\nu(\text{C}-\text{OCH}_3)$ 1082 (m), $\nu(\text{Ni}-\text{O})$ 648 (w), $\nu(\text{Ni}-\text{N})$ 462 (w). ¹H NMR (CDCl₃, 300 MHz, p.p.m.): δ = 6.238 (1H, s, HC=N), 6.741–7.559 (7H, m, H-aromatic), 5.695 (2H, s, CH₂), 3.703 (3H, s, OCH₃).

Refinement

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 (CH), 0.99 (CH₂) and 0.98 (CH₃) Å and with $U_{\text{iso}}(\text{H}) = 1.2(1.5 \text{ for methyl})U_{\text{eq}}(\text{C})$. Five C atoms and an F atom of the fluorophenyl group are disordered each over two sites, with a refined occupancy ratio of 0.507 (5):0.493 (5). In the final refinement, the occupancy ratio was fixed at 0.50:0.50.

Figures

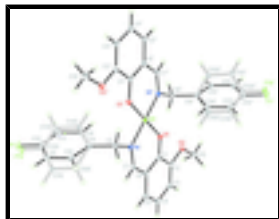


Fig. 1. The molecular structure of the title compound, showing 30% probability displacement ellipsoids. [Symmetry code: (i) $-x+1, -y+1, -z.$]

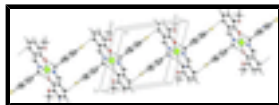


Fig. 2. The crystal packing of the title compound. Only major components of the disordered atoms are shown. Dashed lines denote hydrogen bonds.

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Crystal data

$[\text{Ni}(\text{C}_{15}\text{H}_{13}\text{FNO}_2)_2]$	$Z = 1$
$M_r = 575.24$	$F(000) = 298$
Triclinic, $P\bar{1}$	$D_x = 1.536 \text{ Mg m}^{-3}$
Hall symbol: $-P\ 1$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 5.0110 (2) \text{ \AA}$	Cell parameters from 3312 reflections
$b = 10.9309 (4) \text{ \AA}$	$\theta = 3.1\text{--}29.9^\circ$
$c = 12.2435 (5) \text{ \AA}$	$\mu = 0.84 \text{ mm}^{-1}$
$\alpha = 109.631 (2)^\circ$	$T = 100 \text{ K}$
$\beta = 99.083 (3)^\circ$	Needle, green
$\gamma = 91.020 (3)^\circ$	$0.49 \times 0.09 \times 0.03 \text{ mm}$
$V = 621.92 (4) \text{ \AA}^3$	

Data collection

Bruker APEXII CCD diffractometer	3948 independent reflections
Radiation source: fine-focus sealed tube graphite	3148 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.071$
Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 2001)	$\theta_{\text{max}} = 31.0^\circ, \theta_{\text{min}} = 1.8^\circ$
$T_{\text{min}} = 0.685, T_{\text{max}} = 0.977$	$h = -7 \rightarrow 7$
14720 measured reflections	$k = -15 \rightarrow 15$
	$l = -17 \rightarrow 16$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.047$	Hydrogen site location: inferred from neighbouring sites

$$wR(F^2) = 0.114$$

$$S = 1.08$$

3948 reflections

222 parameters

0 restraints

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2 + 0.2521P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} < 0.001$$

$$\Delta\rho_{\max} = 0.55 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -1.20 \text{ e } \text{\AA}^{-3}$$

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107) operating at 100.0 (1) K.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Ni1	0.5000	0.5000	0.0000	0.01452 (11)	
O1	0.7199 (3)	0.64851 (13)	0.03573 (12)	0.0179 (3)	
O2	1.0870 (3)	0.82320 (14)	0.03948 (13)	0.0216 (3)	
N1	0.3601 (3)	0.56402 (15)	0.14468 (14)	0.0152 (3)	
C1	0.7786 (4)	0.74804 (18)	0.13306 (17)	0.0156 (4)	
C2	0.9789 (4)	0.84687 (19)	0.13974 (18)	0.0169 (4)	
C3	1.0462 (5)	0.95465 (19)	0.24012 (19)	0.0200 (4)	
H3A	1.1799	1.0191	0.2433	0.024*	
C4	0.9191 (5)	0.9703 (2)	0.33805 (19)	0.0221 (4)	
H4A	0.9681	1.0448	0.4071	0.027*	
C5	0.7253 (5)	0.87862 (19)	0.33413 (18)	0.0204 (4)	
H5A	0.6385	0.8902	0.4001	0.024*	
C6	0.6530 (4)	0.76618 (18)	0.23190 (18)	0.0170 (4)	
C7	0.4439 (4)	0.67372 (19)	0.22852 (17)	0.0162 (4)	
H7A	0.3562	0.6949	0.2952	0.019*	
C8	0.1401 (4)	0.48995 (19)	0.17120 (17)	0.0168 (4)	
H8A	0.0373	0.4283	0.0966	0.020*	
H8B	0.0131	0.5514	0.2102	0.020*	
C9	0.2526 (4)	0.41510 (19)	0.25017 (18)	0.0177 (4)	
C15	1.2842 (5)	0.9193 (2)	0.0404 (2)	0.0233 (4)	
H15A	1.3408	0.8945	-0.0367	0.035*	
H15B	1.4419	0.9256	0.1012	0.035*	
H15C	1.2057	1.0037	0.0574	0.035*	
F1	0.549 (4)	0.2029 (11)	0.4639 (17)	0.031 (2)	0.50
C10	0.1167 (9)	0.4015 (4)	0.3345 (4)	0.0197 (8)	0.50
H10A	-0.0475	0.4425	0.3450	0.024*	0.50
C11	0.2113 (10)	0.3290 (4)	0.4062 (4)	0.0228 (8)	0.50
H11A	0.1147	0.3206	0.4644	0.027*	0.50
C12	0.449 (2)	0.2710 (7)	0.3888 (8)	0.0228 (8)	0.50
C13	0.5903 (14)	0.2752 (6)	0.3032 (6)	0.0216 (12)	0.50
H13A	0.7511	0.2312	0.2925	0.026*	0.50
C14	0.4904 (12)	0.3462 (5)	0.2325 (5)	0.0197 (10)	0.50

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H14A	0.5823	0.3489	0.1710	0.024*	0.50
F1X	0.583 (4)	0.2322 (11)	0.4752 (17)	0.0270 (16)	0.50
C10X	0.2322 (10)	0.4664 (4)	0.3718 (4)	0.0200 (8)	0.50
H10B	0.1442	0.5442	0.4006	0.024*	0.50
C11X	0.3399 (9)	0.4039 (4)	0.4485 (4)	0.0214 (7)	0.50
H11B	0.3243	0.4367	0.5294	0.026*	0.50
C12X	0.471 (2)	0.2918 (7)	0.4034 (8)	0.0214 (7)	0.50
C13X	0.4963 (13)	0.2427 (6)	0.2862 (6)	0.0201 (12)	0.50
H13B	0.5866	0.1657	0.2571	0.024*	0.50
C14X	0.3865 (11)	0.3080 (5)	0.2107 (5)	0.0164 (9)	0.50
H14B	0.4071	0.2760	0.1303	0.020*	0.50

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0169 (2)	0.01101 (16)	0.01719 (18)	-0.00043 (13)	0.00410 (14)	0.00644 (13)
O1	0.0213 (8)	0.0145 (6)	0.0180 (7)	-0.0027 (6)	0.0053 (6)	0.0050 (5)
O2	0.0236 (8)	0.0186 (7)	0.0237 (7)	-0.0048 (6)	0.0078 (6)	0.0073 (6)
N1	0.0152 (8)	0.0143 (7)	0.0171 (8)	-0.0003 (6)	0.0027 (6)	0.0069 (6)
C1	0.0165 (10)	0.0120 (8)	0.0189 (9)	0.0018 (7)	0.0009 (7)	0.0070 (7)
C2	0.0159 (10)	0.0160 (8)	0.0209 (9)	0.0020 (7)	0.0030 (8)	0.0092 (7)
C3	0.0200 (10)	0.0163 (8)	0.0247 (10)	-0.0018 (8)	0.0024 (8)	0.0091 (8)
C4	0.0268 (12)	0.0152 (9)	0.0208 (10)	-0.0034 (8)	0.0020 (9)	0.0027 (8)
C5	0.0238 (11)	0.0174 (9)	0.0191 (9)	0.0010 (8)	0.0049 (8)	0.0046 (8)
C6	0.0189 (10)	0.0141 (8)	0.0192 (9)	0.0007 (7)	0.0030 (8)	0.0073 (7)
C7	0.0179 (10)	0.0164 (8)	0.0168 (9)	0.0034 (7)	0.0044 (7)	0.0079 (7)
C8	0.0147 (9)	0.0171 (8)	0.0208 (9)	0.0007 (7)	0.0043 (8)	0.0090 (7)
C9	0.0169 (10)	0.0171 (8)	0.0203 (9)	-0.0024 (7)	0.0036 (8)	0.0083 (7)
C15	0.0204 (11)	0.0216 (9)	0.0333 (12)	-0.0020 (8)	0.0070 (9)	0.0155 (9)
F1	0.050 (6)	0.024 (4)	0.030 (4)	0.009 (4)	0.008 (3)	0.021 (4)
C10	0.020 (2)	0.0161 (18)	0.025 (2)	-0.0036 (17)	0.0072 (17)	0.0072 (16)
C11	0.032 (2)	0.0187 (16)	0.0222 (19)	0.0007 (15)	0.0068 (16)	0.0117 (14)
C12	0.032 (2)	0.0187 (16)	0.0222 (19)	0.0007 (15)	0.0068 (16)	0.0117 (14)
C13	0.024 (3)	0.018 (3)	0.023 (3)	0.006 (2)	0.005 (3)	0.008 (2)
C14	0.024 (3)	0.017 (2)	0.019 (2)	0.0003 (19)	0.006 (2)	0.0069 (18)
F1X	0.037 (4)	0.026 (5)	0.028 (3)	0.006 (4)	0.009 (3)	0.020 (4)
C10X	0.023 (2)	0.0192 (19)	0.0190 (19)	0.0064 (18)	0.0054 (17)	0.0076 (16)
C11X	0.0254 (19)	0.0235 (18)	0.0163 (17)	0.0022 (15)	0.0007 (14)	0.0096 (14)
C12X	0.0254 (19)	0.0235 (18)	0.0163 (17)	0.0022 (15)	0.0007 (14)	0.0096 (14)
C13X	0.026 (3)	0.016 (3)	0.020 (3)	0.003 (2)	0.006 (3)	0.007 (2)
C14X	0.020 (2)	0.013 (2)	0.018 (2)	0.0003 (17)	0.0049 (19)	0.0067 (17)

Geometric parameters (\AA , $^\circ$)

Ni1—O1	1.8297 (14)	C9—C10X	1.425 (5)
Ni1—N1	1.9223 (16)	C9—C14	1.428 (6)
O1—C1	1.303 (2)	C15—H15A	0.9800
O2—C2	1.367 (2)	C15—H15B	0.9800
O2—C15	1.425 (2)	C15—H15C	0.9800

N1—C7	1.299 (2)	F1—C12	1.41 (2)
N1—C8	1.495 (2)	C10—C11	1.404 (6)
C1—C6	1.409 (3)	C10—H10A	0.9500
C1—C2	1.434 (3)	C11—C12	1.371 (12)
C2—C3	1.376 (3)	C11—H11A	0.9500
C3—C4	1.407 (3)	C12—C13	1.367 (13)
C3—H3A	0.9500	C13—C14	1.390 (9)
C4—C5	1.367 (3)	C13—H13A	0.9500
C4—H4A	0.9500	C14—H14A	0.9500
C5—C6	1.420 (3)	F1X—C12X	1.32 (2)
C5—H5A	0.9500	C10X—C11X	1.388 (6)
C6—C7	1.429 (3)	C10X—H10B	0.9500
C7—H7A	0.9500	C11X—C12X	1.389 (10)
C8—C9	1.516 (3)	C11X—H11B	0.9500
C8—H8A	0.9900	C12X—C13X	1.380 (12)
C8—H8B	0.9900	C13X—C14X	1.402 (9)
C9—C14X	1.344 (5)	C13X—H13B	0.9500
C9—C10	1.369 (5)	C14X—H14B	0.9500
O1—Ni1—O1 ⁱ	180.00 (9)	C10X—C9—C14	111.5 (3)
O1—Ni1—N1	93.00 (7)	C14X—C9—C8	122.0 (3)
O1 ⁱ —Ni1—N1	87.00 (7)	C10—C9—C8	121.1 (3)
O1—Ni1—N1 ⁱ	87.00 (7)	C10X—C9—C8	118.4 (2)
O1 ⁱ —Ni1—N1 ⁱ	93.00 (6)	C14—C9—C8	121.3 (3)
N1—Ni1—N1 ⁱ	180.0	O2—C15—H15A	109.5
C1—O1—Ni1	130.38 (13)	O2—C15—H15B	109.5
C2—O2—C15	116.49 (16)	H15A—C15—H15B	109.5
C7—N1—C8	113.22 (16)	O2—C15—H15C	109.5
C7—N1—Ni1	124.50 (14)	H15A—C15—H15C	109.5
C8—N1—Ni1	122.29 (12)	H15B—C15—H15C	109.5
O1—C1—C6	123.93 (18)	C9—C10—C11	122.4 (4)
O1—C1—C2	118.37 (18)	C9—C10—H10A	118.8
C6—C1—C2	117.68 (17)	C11—C10—H10A	118.8
O2—C2—C3	125.29 (19)	C12—C11—C10	117.3 (6)
O2—C2—C1	114.03 (17)	C12—C11—H11A	121.3
C3—C2—C1	120.68 (19)	C10—C11—H11A	121.3
C2—C3—C4	120.63 (19)	C13—C12—C11	123.9 (9)
C2—C3—H3A	119.7	C13—C12—F1	118.8 (12)
C4—C3—H3A	119.7	C11—C12—F1	117.3 (12)
C5—C4—C3	120.18 (19)	C12—C13—C14	117.6 (7)
C5—C4—H4A	119.9	C12—C13—H13A	121.2
C3—C4—H4A	119.9	C14—C13—H13A	121.2
C4—C5—C6	120.33 (19)	C13—C14—C9	121.4 (5)
C4—C5—H5A	119.8	C13—C14—H14A	119.3
C6—C5—H5A	119.8	C9—C14—H14A	119.3
C1—C6—C5	120.49 (19)	C11X—C10X—C9	120.6 (3)
C1—C6—C7	120.17 (18)	C11X—C10X—H10B	119.7
C5—C6—C7	119.30 (18)	C9—C10X—H10B	119.7
N1—C7—C6	127.39 (18)	C10X—C11X—C12X	118.0 (5)

supplementary materials

N1—C7—H7A	116.3	C10X—C11X—H11B	121.0
C6—C7—H7A	116.3	C12X—C11X—H11B	121.0
N1—C8—C9	111.72 (16)	F1X—C12X—C13X	118.8 (11)
N1—C8—H8A	109.3	F1X—C12X—C11X	119.3 (10)
C9—C8—H8A	109.3	C13X—C12X—C11X	121.9 (8)
N1—C8—H8B	109.3	C12X—C13X—C14X	119.0 (7)
C9—C8—H8B	109.3	C12X—C13X—H13B	120.5
H8A—C8—H8B	107.9	C14X—C13X—H13B	120.5
C14X—C9—C10	108.2 (3)	C9—C14X—C13X	121.0 (5)
C14X—C9—C10X	119.5 (3)	C9—C14X—H14B	119.5
C10—C9—C14	117.3 (3)	C13X—C14X—H14B	119.5
N1—Ni1—O1—C1	8.77 (19)	N1—C8—C9—C10	143.9 (3)
N1 ⁱ —Ni1—O1—C1	-171.23 (19)	N1—C8—C9—C10X	102.8 (3)
O1—Ni1—N1—C7	-4.67 (18)	N1—C8—C9—C14	-42.0 (3)
O1 ⁱ —Ni1—N1—C7	175.33 (18)	C14X—C9—C10—C11	29.7 (5)
O1—Ni1—N1—C8	175.40 (15)	C10X—C9—C10—C11	-85.9 (6)
O1 ⁱ —Ni1—N1—C8	-4.60 (15)	C14—C9—C10—C11	3.4 (6)
Ni1—O1—C1—C6	-7.0 (3)	C8—C9—C10—C11	177.8 (3)
Ni1—O1—C1—C2	174.36 (14)	C9—C10—C11—C12	0.0 (7)
C15—O2—C2—C3	-0.3 (3)	C10—C11—C12—C13	-2.9 (9)
C15—O2—C2—C1	179.05 (18)	C10—C11—C12—F1	177.4 (7)
O1—C1—C2—O2	-0.1 (3)	C11—C12—C13—C14	2.1 (10)
C6—C1—C2—O2	-178.77 (18)	F1—C12—C13—C14	-178.2 (7)
O1—C1—C2—C3	179.33 (19)	C12—C13—C14—C9	1.6 (8)
C6—C1—C2—C3	0.6 (3)	C14X—C9—C14—C13	-79.1 (9)
O2—C2—C3—C4	179.04 (19)	C10—C9—C14—C13	-4.2 (6)
C1—C2—C3—C4	-0.3 (3)	C10X—C9—C14—C13	34.5 (6)
C2—C3—C4—C5	-0.4 (3)	C8—C9—C14—C13	-178.6 (4)
C3—C4—C5—C6	0.8 (3)	C14X—C9—C10X—C11X	-2.6 (6)
O1—C1—C6—C5	-178.92 (19)	C10—C9—C10X—C11X	77.3 (5)
C2—C1—C6—C5	-0.3 (3)	C14—C9—C10X—C11X	-29.9 (5)
O1—C1—C6—C7	-1.2 (3)	C8—C9—C10X—C11X	-177.9 (3)
C2—C1—C6—C7	177.37 (18)	C9—C10X—C11X—C12X	1.1 (8)
C4—C5—C6—C1	-0.4 (3)	C10X—C11X—C12X—F1X	178.0 (9)
C4—C5—C6—C7	-178.1 (2)	C10X—C11X—C12X—C13X	0.1 (10)
C8—N1—C7—C6	179.02 (19)	F1X—C12X—C13X—C14X	-177.8 (9)
Ni1—N1—C7—C6	-0.9 (3)	C11X—C12X—C13X—C14X	0.1 (11)
C1—C6—C7—N1	5.2 (3)	C10—C9—C14X—C13X	-34.3 (6)
C5—C6—C7—N1	-177.1 (2)	C10X—C9—C14X—C13X	2.8 (7)
C7—N1—C8—C9	-80.9 (2)	C14—C9—C14X—C13X	81.2 (9)
Ni1—N1—C8—C9	99.07 (17)	C8—C9—C14X—C13X	177.9 (4)
N1—C8—C9—C14X	-72.4 (3)	C12X—C13X—C14X—C9	-1.6 (9)

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

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C5—H5A \cdots F1 ⁱⁱ	0.95	2.51	3.363 (18)	150

Symmetry codes: (ii) $-x+1, -y+1, -z+1$.

Fig. 1

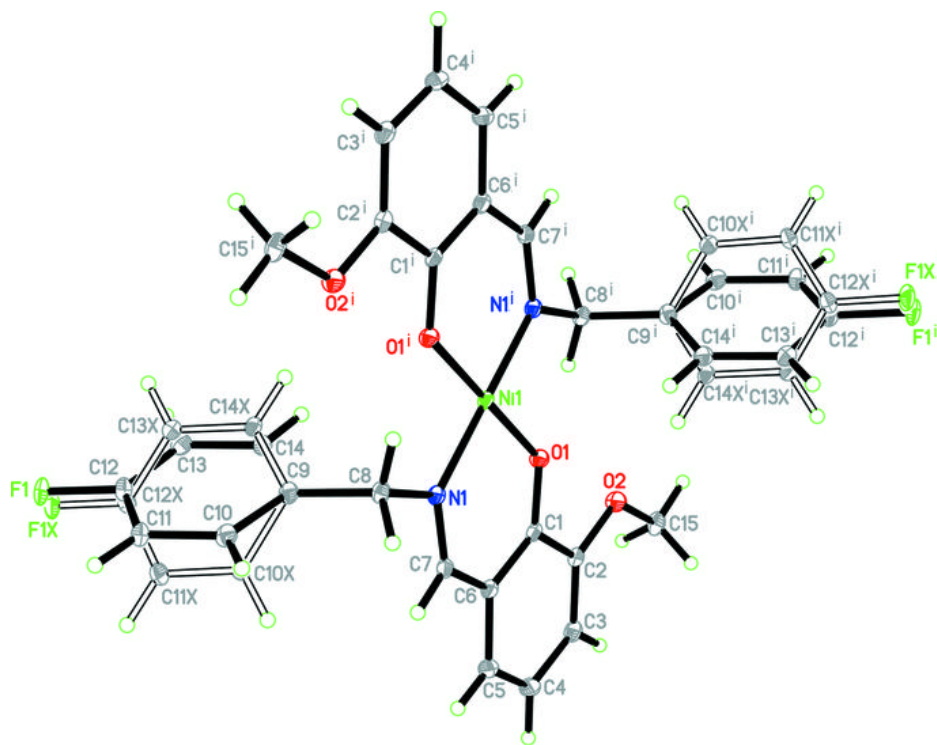


Fig. 2

