research communications

Crystal structure of bis{2-[(E)-(4-fluorobenzyl)-iminomethyl]phenolato-κ^2N,O}nickel(II)

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The asymmetric unit of the title complex, [Ni(C₁₄H₁₁FNO)₂], contains one-half of the molecule with the Ni^{II} cation lying on an inversion centre coordinated by a bidentate Schiff base anion. The cationic Ni^{II} center is in a distorted square-planar coordination environment chelated by the imine N and phenolate O donor atoms of the two Schiff base ligands. The N and O donor atoms of the two ligands are mutually *trans* with Ni—N and Ni—O bond lengths of 1.9242 (10) and 1.8336 (9) Å, respectively. The fluorophenyl ring is almost orthogonal to the coordination plane and makes a dihedral angle of 82.98 (7)° with the phenolate ring. In the crystal, molecules are linked into screw chains by weak C—H⋯F hydrogen bonds. Additional C—H⋯π contacts arrange the molecules into sheets parallel to the *ac* plane.

1. Chemical context

Schiff base ligands are well-known and important compounds because of their wide range of biological activities and uses in industrial systems (Feng *et al.*, 2013; Kumar *et al.*, 2010; Liu *et al.*, 2005) as well as being versatile ligands for transition metals. Transition metal complexes with Schiff base ligands, especially those of Pd^{II} and Ni^{II}, have been shown to display a variety of structural features and, in some cases, exhibit interesting reactivity. In particular they can be photo-luminescent (Guo *et al.*, 2013a) and are used as catalysts for many organic reactions such as Heck and Suzuki cross-coupling reactions (Kumari *et al.*, 2012; Teo *et al.*, 2011).
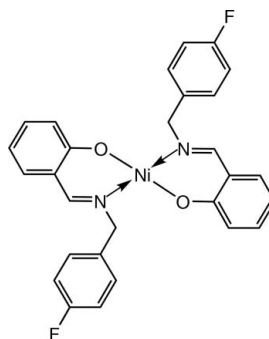
In our previous studies, we reported the syntheses and crystal structures of two related Schiff base complexes, bis{2-[(E)-(4-fluorobenzyl)iminomethyl]-6-methoxypheno-lato-κ^2N,O^1}nickel(II) (Bahron *et al.*, 2011) and bis{2-[(E)-(4-methoxybenzyl)iminomethyl]phenolato-κ^2N,O^1}nickel(II) (Bahron *et al.*, 2014). In this article, we report the successful
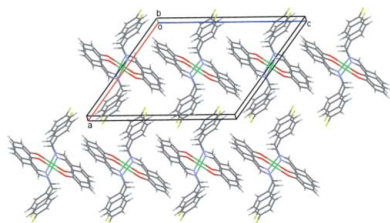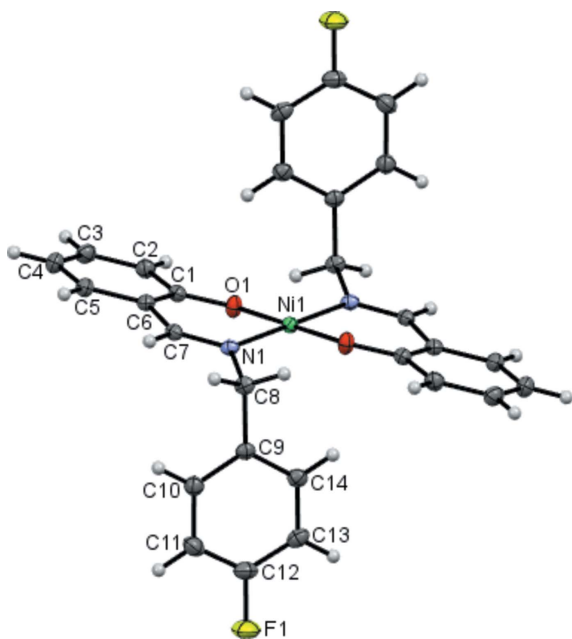
Figure 1
The molecular structure of (1), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The labelled atoms are related to the unlabelled atoms of the Schiff base ligands by the symmetry code: $1 - x, -y, 1 - z$.

synthesis of another Schiff base–Ni^{II} complex, [Ni(C$_{14}$H$_{11}$FNO)$_2$] (1), and its characterization by spectroscopy and elemental analysis. Crystal structure determination confirms the binding mode of the [(4-fluorobenzyl)iminomethyl]phenolate ligand to the Ni^{II} cation (Fig. 1). The title complex was also tested for antibacterial activity, and found to be only weakly active.

2. Structural commentary

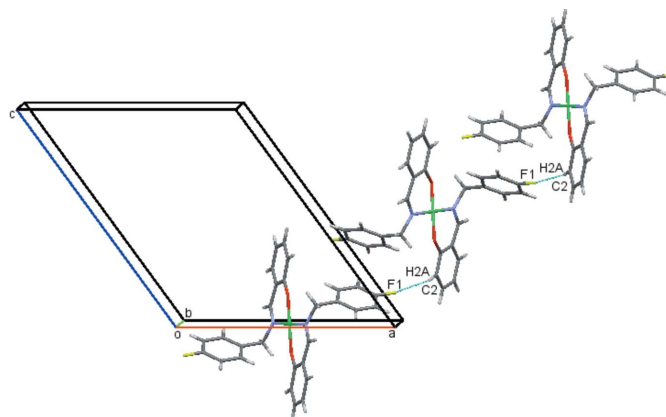The asymmetric unit of (1) contains one-half of the molecule with the Ni^{II} cation lying on an inversion centre and the Schiff base anion acting as an *N,O*-bidentate chelate ligand (Fig. 1). The cation binds to the N and the O atoms of two symmetry-related Schiff base ligand such that the N and O atoms are mutually *trans*. The N$_2$O$_2$ donor sets of the two chelating Schiff base ligands in the equatorial plane around Ni1 adopt a slightly distorted square planar coordination geometry with the angles O1—Ni1—N1 = 92.56 (4)° and O1—Ni1—N1^i =

Table 1
Hydrogen-bond geometry (Å, °).

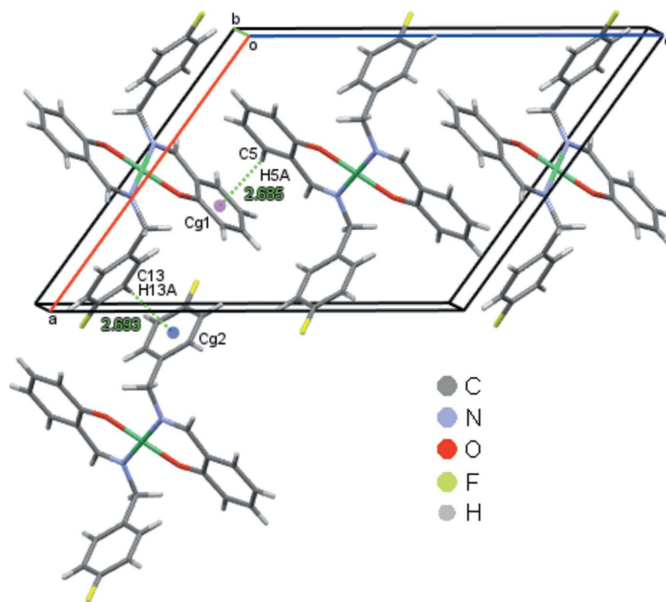*Cg*1 and *Cg*2 are the centroids of the C1–C6 and C9–C14 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8A···O1^i	0.99	2.19	2.7300 (18)	113
C14—H14A···O1^i	0.95	2.52	3.212 (2)	130
C2—H2A···F1^{ii}	0.95	2.65	3.5312 (19)	155
C5—H5A···*Cg*1^{iii}	0.95	2.69	3.4010 (18)	133
C13—H13A···*Cg*2^{iv}	0.95	2.69	3.4252 (13)	134

Symmetry codes: (i) $-x + 1, -y, -z + 1$; (ii) $x - 1, -y - \frac{1}{2}, z - \frac{1}{2}$; (iii) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$; (iv) $-x + 2, y - \frac{1}{2}, -z + \frac{3}{2}$.

Figure 2
Screw chains of molecules of (1) linked by C—H···F contacts drawn as dashed lines.

87.44 (4)° [symmetry code: (i) $1 - x, -y, 1 - z$]. As expected under inversion symmetry, the *trans* angles (N11—Ni1—N1^i and O1—Ni1—O1^i) are found to be linear. The Ni1—N1 and Ni1—O1 distances in the N$_2$O$_2$ coordination plane are 1.9242 (10) Å and 1.8336 (9) Å, respectively. These compare well with those observed in the two other closely related Ni^{II} complexes with N$_2$O$_2$ coordinating Schiff base ligands (Bahron *et al.*, 2011; 2014). The Ni1/O1/C1/C6/C7/N1 ring adopts an envelope conformation with the Ni1 atom displaced by 0.3885 (5) Å from the O1/C1/C6/C7/N1 plane, with the puckering parameters $Q = 0.2429$ (10) Å, $\theta = 65.3$ (3) and $\varphi = 4.0$ (3)°. Other bond lengths and angles observed in the structure are also normal. The fluorophenyl ring (C9–C14) makes a dihedral angle of 82.98 (7)° with the phenolate ring (C1–C6).

Figure 3
C—H···π contacts for (1) drawn as dotted lines with ring centroids shown as coloured spheres. *Cg*1 and *Cg*2 are the centroids of the C1–C6 and C9–C14 rings, respectively.
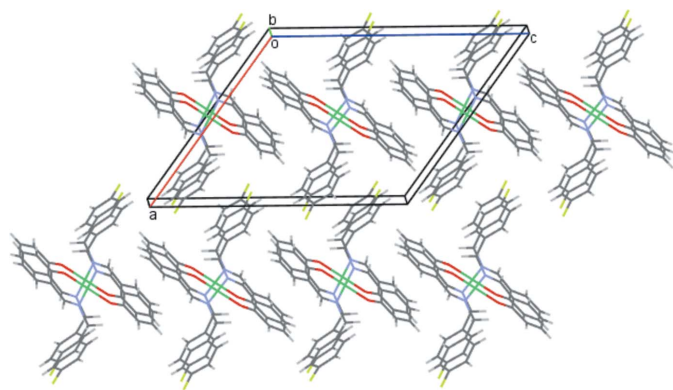
Figure 4
The packing of (1) viewed along the *b* axis showing molecular sheets of the Ni^{II} complex.

3. Supramolecular features

In the crystal packing, the molecules are linked into screw chains by weak C2—H2A···F1 interactions (Fig. 2, Table 1). C—H···π interactions involving both the fluorophenyl and the phenolate rings, C5—H5A···Cg1 and C13—H13A···Cg2, connect the molecules into chains along the *c*-axis direction (Fig. 3, Table 1). They also contribute to the formation of sheets parallel to the *ac* plane, which are further stacked along the *b* axis as shown in Fig. 4.

4. Database survey

A search of the Cambridge Database (Version 5.35, November 2013 with 3 updates) revealed a total of 1191 Ni^{II} complexes with an NiN$_2$O$_2$ coordination sphere. No fewer than 333 of these had the Ni atom chelated by two 3-(imino-methyl)phenolate residues. No corresponding structures with a benzyl or substituted benzyl unit bound to the imino N atom were found. However extending the search to allow additional substitution on the phenolate ring resulted in eight discrete structures including the two closely related structures mentioned previously (Bahron *et al.*, 2011, 2014), and several other related complexes (see, for example Guo *et al.* 2013*a*,*b*; Senol *et al.* 2011; Chen *et al.* 2010).

5. Synthesis and crystallization

An ethanolic solution of 4-fluorobenzylamine (4 mmol, 0.5010 g) was added to salicylaldehyde (4 mmol, 0.4970 g), dissolved in absolute ethanol (2 ml), forming a bright-yellow solution. The mixture was heated under reflux for an hour to produce the ligand, (*E*)-2-[(4-fluorobenzylimino)methyl]-phenol. Nickel(II) acetate tetrahydrate (2 mmol, 0.4983 g) was dissolved separately in absolute ethanol (10 ml) and added to a flask containing the cooled ligand solution. The mixture was stirred and refluxed for 3 h upon which a dark-green solid formed. This was filtered off, washed with ice-cold ethanol and air-dried at room temperature. The solid product was recrystallized from chloroform, yielding green crystals. Yield 68.6%; m.p. 471–473 K. Analytical data for C$_{28}$H$_{22}$F$_2$N$_2$O$_2$Ni: C, 65.28;

Table 2
Experimental details.

Crystal data	
Chemical formula	[Ni(C$_{14}$H$_{11}$FNO)$_2$]
M_r	515.17
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	13.8611 (3), 5.83340 (1), 16.9942 (3)
β (°)	125.998 (1)
V (Å^3)	1111.70 (4)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.92
Crystal size (mm)	0.47 × 0.19 × 0.11
Data collection	
Diffractometer	Bruker APEXII CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.674, 0.906
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13419, 3235, 2896
R_{int}	0.024
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.703
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.028, 0.072, 1.05
No. of reflections	3235
No. of parameters	160
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.45, −0.49

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXTL* (Sheldrick, 2008), *PLATON* (Spek, 2009), *Mercury* (Macrae *et al.*, 2006) and *publCIF* (Westrip, 2010).

H, 4.30; N, 5.44. Found: C, 65.87; H, 4.39; N, 5.55. IR (KBr, cm^{-1}): ν(C=N) 1612 (*s*), ν(C—N) 1390 (*w*), ν(C—O) 1221 (*s*), ν(Ni—N) 597 (*w*), ν(Ni—O) 451 (*w*). The infrared spectra of the title complex revealed a strong band of 1612 cm^{-1} in the spectrum assignable to C=N stretching frequency upon complexation (Nair *et al.*, 2012). The appearance of new bands at 451 and 597 cm^{-1} in the spectrum of the title complex attributable to Ni—O and Ni—N vibrations, respectively, supports the suggestion above of the participation of the N atom of the imine group and O atom of the phenolic group of the ligand in the complexation with Ni^{II} cation (Ouf *et al.*, 2010). Accordingly, it can be deduced that the ligand binds to the Ni^{II} cation in an *N,O*-bidentate fashion in 2:1 ratio.

An antibacterial activity investigation of the title complex against *B. subtilis*, *S. aureus* and *E. coli* showed very mild or no inhibition with clear inhibition diameters of 7–8 mm at the highest concentration of 50 μM. The negative control of a 9:1 mixture of DMSO:acetone and the positive control of 30 U of chloramphenicol showed inhibition diameters of 6 mm and 20 mm, respectively.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were positioned geometrically and allowed to ride on their parent atoms, with d(C—H) = 0.95 Å for aromatic and 0.99 Å for CH$_2$ hydrogen

atoms. The U_{iso} values were constrained to be $1.2U_{eq}$ of the carrier atoms.

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supporting information

Crystal structure of bis{2-[(*E*)-(4-fluorobenzyl)iminomethyl]phenolato-$\kappa^2 N,O$}nickel(II)

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Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *APEX2* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008), *PLATON* (Spek, 2009), *Mercury* (Macrae *et al.*, 2006) and *publCIF* (Westrip, 2010).

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

Crystal data

[Ni(C$_{14}$H$_{11}$FNO)$_2$]	$F(000) = 532$
$M_r = 515.17$	$D_x = 1.539$ Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point = 471–476 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 13.8611$ (3) Å	Cell parameters from 3235 reflections
$b = 5.83340$ (1) Å	$\theta = 1.8$–30.0°
$c = 16.9942$ (3) Å	$\mu = 0.92$ mm^{-1}
$\beta = 125.998$ (1)°	$T = 100$ K
$V = 1111.70$ (4) Å^3	Plate, green
$Z = 2$	0.47 × 0.19 × 0.11 mm

Data collection

Bruker APEXII CCD area detector diffractometer	13419 measured reflections
Radiation source: sealed tube	3235 independent reflections
Graphite monochromator	2896 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.024$
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)	$\theta_{max} = 30.0°$, $\theta_{min} = 1.8°$
$T_{min} = 0.674$, $T_{max} = 0.906$	$h = -19{\rightarrow}19$
	$k = -8{\rightarrow}8$
	$l = -23{\rightarrow}23$

Refinement

Refinement on F^2	0 restraints
Least-squares matrix: full	Primary atom site location: structure-invariant direct methods
$R[F^2 > 2\sigma(F^2)] = 0.028$	
$wR(F^2) = 0.072$	Secondary atom site location: difference Fourier map
$S = 1.05$	
3235 reflections	Hydrogen site location: inferred from neighbouring sites
160 parameters	

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0322P)^2 + 0.7123P]$

   where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.45$ e Å^{-3}

$\Delta\rho_{min} = -0.49$ e Å^{-3}

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 > 2sigma(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	0.01062 (7)
F1	1.07321 (8)	−0.19874 (17)	0.63754 (7)	0.0297 (2)
N1	0.58764 (8)	0.26207 (18)	0.50481 (7)	0.01200 (19)
O1	0.41017 (8)	−0.01507 (15)	0.36693 (7)	0.01520 (18)
C1	0.38843 (10)	0.1456 (2)	0.30461 (9)	0.0133 (2)
C2	0.29659 (11)	0.1091 (2)	0.20455 (9)	0.0160 (2)
H2A	0.2528	−0.0303	0.1840	0.019*
C3	0.27066 (11)	0.2756 (2)	0.13703 (9)	0.0174 (2)
H3A	0.2085	0.2490	0.0704	0.021*
C4	0.33373 (12)	0.4832 (2)	0.16425 (10)	0.0175 (2)
H4A	0.3147	0.5959	0.1168	0.021*
C5	0.42385 (11)	0.5206 (2)	0.26118 (9)	0.0151 (2)
H5A	0.4676	0.6600	0.2804	0.018*
C6	0.45190 (10)	0.3546 (2)	0.33205 (8)	0.0125 (2)
C7	0.55207 (10)	0.3936 (2)	0.43090 (9)	0.0125 (2)
H7A	0.5968	0.5294	0.4434	0.015*
C8	0.70465 (10)	0.3283 (2)	0.59589 (9)	0.0134 (2)
H8A	0.7024	0.3042	0.6524	0.016*
H8B	0.7198	0.4930	0.5933	0.016*
C9	0.80423 (10)	0.1869 (2)	0.60823 (8)	0.0133 (2)
C10	0.86635 (11)	0.2669 (2)	0.57233 (9)	0.0166 (2)
H10A	0.8456	0.4110	0.5402	0.020*
C11	0.95823 (11)	0.1396 (3)	0.58258 (10)	0.0202 (3)
H11A	1.0010	0.1957	0.5588	0.024*
C12	0.98511 (11)	−0.0701 (3)	0.62825 (10)	0.0196 (3)
C13	0.92625 (11)	−0.1569 (2)	0.66508 (9)	0.0174 (2)
H13A	0.9471	−0.3019	0.6965	0.021*
C14	0.83553 (11)	−0.0255 (2)	0.65471 (9)	0.0152 (2)
H14A	0.7942	−0.0816	0.6798	0.018*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.01005 (10)	0.01029 (11)	0.01063 (11)	−0.00089 (7)	0.00557 (8)	0.00019 (7)
F1	0.0240 (4)	0.0360 (5)	0.0340 (5)	0.0125 (4)	0.0197 (4)	0.0035 (4)
N1	0.0105 (4)	0.0115 (5)	0.0129 (4)	−0.0003 (3)	0.0063 (4)	−0.0010 (4)
O1	0.0168 (4)	0.0142 (4)	0.0122 (4)	−0.0036 (3)	0.0072 (3)	0.0005 (3)
C1	0.0123 (5)	0.0149 (5)	0.0138 (5)	0.0010 (4)	0.0084 (4)	0.0009 (4)
C2	0.0141 (5)	0.0177 (6)	0.0148 (5)	−0.0015 (4)	0.0077 (5)	−0.0003 (4)
C3	0.0141 (5)	0.0218 (6)	0.0136 (5)	0.0016 (4)	0.0066 (4)	0.0010 (5)
C4	0.0176 (6)	0.0188 (6)	0.0157 (6)	0.0029 (4)	0.0096 (5)	0.0049 (5)
C5	0.0153 (5)	0.0144 (6)	0.0167 (6)	0.0012 (4)	0.0100 (5)	0.0022 (4)
C6	0.0115 (5)	0.0133 (5)	0.0135 (5)	0.0014 (4)	0.0077 (4)	0.0010 (4)
C7	0.0122 (5)	0.0115 (5)	0.0158 (5)	−0.0002 (4)	0.0093 (4)	−0.0005 (4)
C8	0.0119 (5)	0.0116 (5)	0.0140 (5)	−0.0017 (4)	0.0062 (4)	−0.0020 (4)
C9	0.0103 (5)	0.0149 (5)	0.0114 (5)	−0.0012 (4)	0.0045 (4)	−0.0015 (4)
C10	0.0154 (5)	0.0179 (6)	0.0156 (5)	−0.0010 (4)	0.0086 (5)	0.0007 (4)
C11	0.0174 (6)	0.0271 (7)	0.0192 (6)	−0.0004 (5)	0.0126 (5)	−0.0003 (5)
C12	0.0139 (5)	0.0249 (7)	0.0182 (6)	0.0039 (5)	0.0085 (5)	−0.0020 (5)
C13	0.0139 (5)	0.0162 (6)	0.0161 (6)	0.0013 (4)	0.0054 (5)	−0.0002 (4)
C14	0.0123 (5)	0.0152 (6)	0.0155 (5)	−0.0018 (4)	0.0068 (4)	−0.0008 (4)

Geometric parameters (Å, º)

Ni1—O1^i	1.8336 (9)	C5—H5A	0.9500
Ni1—O1	1.8336 (9)	C6—C7	1.4351 (16)
Ni1—N1^i	1.9242 (10)	C7—H7A	0.9500
Ni1—N1	1.9242 (10)	C8—C9	1.5133 (16)
F1—C12	1.3613 (15)	C8—H8A	0.9900
N1—C7	1.2967 (16)	C8—H8B	0.9900
N1—C8	1.4915 (15)	C9—C14	1.3943 (17)
O1—C1	1.3097 (15)	C9—C10	1.3960 (17)
C1—C6	1.4130 (17)	C10—C11	1.3937 (18)
C1—C2	1.4187 (17)	C10—H10A	0.9500
C2—C3	1.3801 (18)	C11—C12	1.378 (2)
C2—H2A	0.9500	C11—H11A	0.9500
C3—C4	1.4031 (19)	C12—C13	1.3834 (19)
C3—H3A	0.9500	C13—C14	1.3926 (17)
C4—C5	1.3794 (18)	C13—H13A	0.9500
C4—H4A	0.9500	C14—H14A	0.9500
C5—C6	1.4100 (17)		
O1^i—Ni1—O1	180.0	N1—C7—C6	126.56 (11)
O1^i—Ni1—N1^i	92.56 (4)	N1—C7—H7A	116.7
O1—Ni1—N1^i	87.44 (4)	C6—C7—H7A	116.7
O1^i—Ni1—N1	87.44 (4)	N1—C8—C9	110.45 (9)
O1—Ni1—N1	92.56 (4)	N1—C8—H8A	109.6
N1^i—Ni1—N1	180.00 (6)	C9—C8—H8A	109.6

C7—N1—C8	114.48 (10)	N1—C8—H8B	109.6
C7—N1—Ni1	123.90 (8)	C9—C8—H8B	109.6
C8—N1—Ni1	121.62 (8)	H8A—C8—H8B	108.1
C1—O1—Ni1	129.03 (8)	C14—C9—C10	118.57 (11)
O1—C1—C6	123.23 (11)	C14—C9—C8	121.18 (11)
O1—C1—C2	118.67 (11)	C10—C9—C8	120.25 (11)
C6—C1—C2	118.10 (11)	C11—C10—C9	121.36 (12)
C3—C2—C1	120.18 (12)	C11—C10—H10A	119.3
C3—C2—H2A	119.9	C9—C10—H10A	119.3
C1—C2—H2A	119.9	C12—C11—C10	117.89 (12)
C2—C3—C4	121.73 (12)	C12—C11—H11A	121.1
C2—C3—H3A	119.1	C10—C11—H11A	121.1
C4—C3—H3A	119.1	F1—C12—C11	118.81 (12)
C5—C4—C3	118.79 (12)	F1—C12—C13	118.24 (13)
C5—C4—H4A	120.6	C11—C12—C13	122.95 (12)
C3—C4—H4A	120.6	C12—C13—C14	118.04 (12)
C4—C5—C6	120.87 (12)	C12—C13—H13A	121.0
C4—C5—H5A	119.6	C14—C13—H13A	121.0
C6—C5—H5A	119.6	C13—C14—C9	121.18 (12)
C5—C6—C1	120.33 (11)	C13—C14—H14A	119.4
C5—C6—C7	118.85 (11)	C9—C14—H14A	119.4
C1—C6—C7	120.62 (11)		
O1^i—Ni1—N1—C7	−161.69 (10)	C8—N1—C7—C6	171.36 (11)
O1—Ni1—N1—C7	18.31 (10)	Ni1—N1—C7—C6	−8.09 (17)
O1^i—Ni1—N1—C8	18.90 (9)	C5—C6—C7—N1	177.97 (11)
O1—Ni1—N1—C8	−161.10 (9)	C1—C6—C7—N1	−7.20 (18)
N1^i—Ni1—O1—C1	158.63 (10)	C7—N1—C8—C9	−97.31 (12)
N1—Ni1—O1—C1	−21.37 (10)	Ni1—N1—C8—C9	82.15 (11)
Ni1—O1—C1—C6	12.98 (17)	N1—C8—C9—C14	−87.37 (13)
Ni1—O1—C1—C2	−166.89 (9)	N1—C8—C9—C10	92.19 (13)
O1—C1—C2—C3	179.45 (11)	C14—C9—C10—C11	−0.29 (18)
C6—C1—C2—C3	−0.42 (17)	C8—C9—C10—C11	−179.86 (12)
C1—C2—C3—C4	0.48 (19)	C9—C10—C11—C12	0.9 (2)
C2—C3—C4—C5	−0.03 (19)	C10—C11—C12—F1	178.90 (12)
C3—C4—C5—C6	−0.47 (19)	C10—C11—C12—C13	−0.9 (2)
C4—C5—C6—C1	0.52 (18)	F1—C12—C13—C14	−179.49 (11)
C4—C5—C6—C7	175.37 (11)	C11—C12—C13—C14	0.3 (2)
O1—C1—C6—C5	−179.94 (11)	C12—C13—C14—C9	0.31 (19)
C2—C1—C6—C5	−0.07 (17)	C10—C9—C14—C13	−0.32 (18)
O1—C1—C6—C7	5.30 (18)	C8—C9—C14—C13	179.25 (11)
C2—C1—C6—C7	−174.83 (11)		

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

Hydrogen-bond geometry (Å, º)

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and C9–C14 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*A*···O1[i]	0.99	2.19	2.7300 (18)	113
C14—H14*A*···O1[i]	0.95	2.52	3.212 (2)	130
C2—H2*A*···F1[ii]	0.95	2.65	3.5312 (19)	155
C5—H5*A*···*Cg*1[iii]	0.95	2.69	3.4010 (18)	133
C13—H13*A*···*Cg*2[iv]	0.95	2.69	3.4252 (13)	134

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) *x*−1, −*y*−1/2, *z*−1/2; (iii) −*x*+1, *y*+1/2, −*z*+1/2; (iv) −*x*+2, *y*−1/2, −*z*+3/2.