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# Crystal structure of bis{2-[(*E*)-(4-methoxybenzyl)iminomethyl]phenolato- $\kappa^2N,O^1$ }nickel(II)

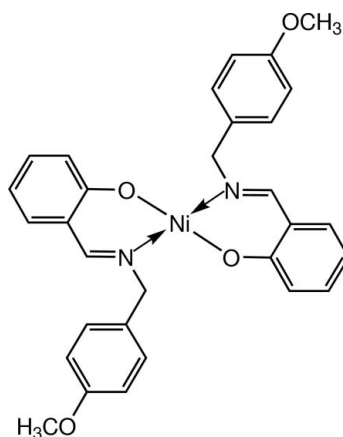
 Hadariah Bahron,<sup>a,b</sup> Amalina Mohd Tajuddin,<sup>a</sup> Wan Nazihah Wan Ibrahim,<sup>a,b</sup> Hoong-Kun Fun<sup>c,d,\*</sup>‡ and Suchada Chantrapromma<sup>e</sup>§

<sup>a</sup>Faculty of Applied Sciences, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia, <sup>b</sup>DDH CoRe, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia, <sup>c</sup>X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, <sup>d</sup>Department of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, PO Box 2457, Riyadh 11451, Saudi Arabia, and <sup>e</sup>Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkhla 90112, Thailand. \*Correspondence e-mail: hkfun@usm.my

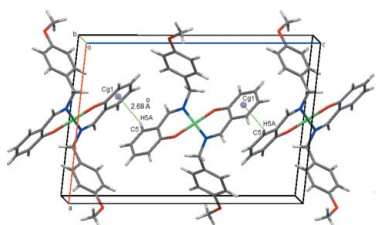
The asymmetric unit of the title compound, [Ni(C<sub>15</sub>H<sub>14</sub>NO<sub>2</sub>)<sub>2</sub>], comprises an Ni<sup>II</sup> cation, lying on an inversion centre, and a Schiff base anion that acts as a bidentate ligand. The Ni<sup>II</sup> cation is in a square-planar coordination environment binding to the imine N and phenolate O 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 1.9191 (11) and 1.8407 (9) Å, respectively. The plane of the methoxybenzene ring makes a dihedral angle of 84.92 (6)° with that of the phenolate ring. In the crystal, molecules are linked into screw chains by weak C–H···O hydrogen bonds. Additional C–H···O hydrogen bonds, together with C–H··· $\pi$  contacts, arrange the molecules into sheets parallel to the *ac* plane.

## 1. Chemical context

Schiff bases have often been used as chelating ligands in coordination chemistry as they readily form stable complexes with most transition metal ions (Kalita *et al.*, 2014; Mohamed *et al.*, 2010). Metal complexes of Schiff bases containing nitrogen and other donor atoms have received attention because of their stability, biological activity (Islam *et al.*, 2014) and potential applications in other fields, such as catalysis (Mohd Tajuddin *et al.*, 2012).



The title compound, bis{2-[(*E*)-(4-methoxybenzyl)iminomethyl]phenolato- $\kappa^2N,O^1$ }nickel(II), (I), is related to bis{2-[1-(benzylimino)ethyl]phenolato}palladium(II) (Mohd Tajuddin *et al.*, 2010) in terms of the geometry around the metal centre. However, we have extended our investigation to include a nickel compound with a Schiff base ligand that has a 4-methoxy substituent on the phenyl ring of the benzyl unit bound to the imine N atom (Fig. 1).



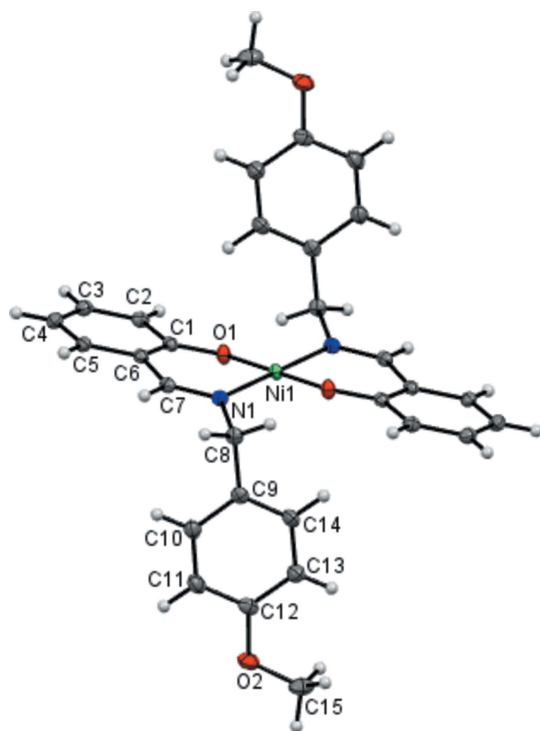


Figure 1

The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The symmetry-related Schiff base ligand is generated by the symmetry code  $(-x + 1, -y, -z + 1)$ .

## 2. Structural commentary

The asymmetric unit of (I) consists of an  $\text{Ni}^{\text{II}}$  cation that lies on an inversion centre and a Schiff base anion that functions as a bidentate ligand (Fig. 1). The  $\text{N}_2\text{O}_2$  donor set of the chelating Schiff base ligands has the N1 and O1 donor atoms mutually *trans*, in a distorted square-planar coordination geometry, with  $\text{O1-Ni1-N1} = 92.30(4)^\circ$  and  $\text{O1-Ni1-N1}^i = 87.70(4)^\circ$  [symmetry code: (i)  $-x + 1, -y, -z + 1$ ] and a maximum deviation from the  $\text{NiN}_2\text{O}_2$  least-squares plane of  $0.731(1) \text{ \AA}$  for the N1 atom. The  $\text{Ni1-N1}$  and  $\text{Ni1-O1}$  bond lengths in the  $\text{N}_2\text{O}_2$  coordination plane are  $1.9191(11)$  and  $1.8407(9) \text{ \AA}$ , respectively. These are similar to those observed

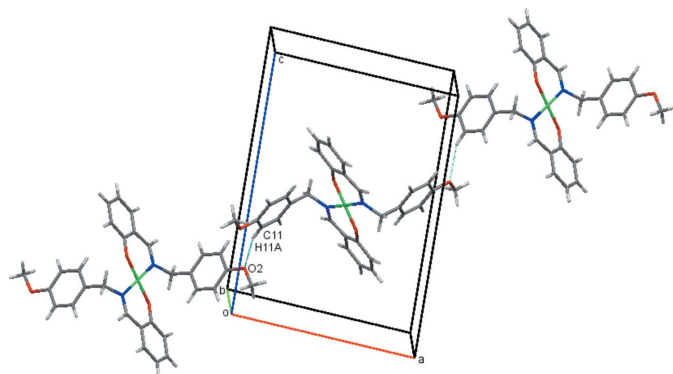


Figure 2

Screw chains of molecules of (I) linked by  $\text{C-H}\cdots\text{O}$  contacts (shown as dashed lines).

Table 1

Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ ).

Cg1 is the centroid of the C1–C6 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C11-H11A}\cdots\text{O2}^i$	0.95	2.47	3.3709 (17)	158
$\text{C14-H14A}\cdots\text{O1}^{ii}$	0.95	2.57	3.2281 (17)	126
$\text{C5-H5A}\cdots\text{Cg1}^{iii}$	0.95	2.68	3.3918 (13)	132

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

in the other closely related  $\text{Ni}^{\text{II}}$  complexes with  $\text{N}_2\text{O}_2$ -coordinating Schiff base ligands (Bahron *et al.*, 2011; Mohd Tajuddin *et al.*, 2010). Other bond lengths and angles observed in the structure are also normal. The methoxy substituent is coplanar with the ring to which it is bound, the  $\text{C15-O2-C12-C13}$  torsion angle being  $3.93(2)^\circ$ . The plane of the methoxybenzene ring (C9–C14) makes a dihedral angle of  $84.92(6)^\circ$  with that of the phenolate benzene ring (C1–C6). A weak intramolecular  $\text{C14-H14}\cdots\text{O1}$  contact is also observed that affects the overall molecular conformation.

## 3. Supramolecular features

In the crystal (Fig. 2), molecules are linked into screw chains by weak  $\text{C11-H11A}\cdots\text{O2}$  interactions (Fig. 2 and Table 1). Additional  $\text{C5-H5A}\cdots\text{Cg1}$  contacts link molecules into chains along the *c*-axis direction (Fig. 3 and Table 1) resulting in sheets parallel to the *ac* plane and stacked along the *b* axis (Fig. 4).

## 4. Database survey

A search of the Cambridge Structural Database (Version 5.35, November 2013 with 3 updates; Allen, 2002) reveals a total of 1191  $\text{Ni}^{\text{II}}$  complexes with an  $\text{NiN}_2\text{O}_2$  coordination sphere. No fewer than 333 of these had the  $\text{Ni}^{\text{II}}$  atom chelated by two 3-(iminomethyl)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

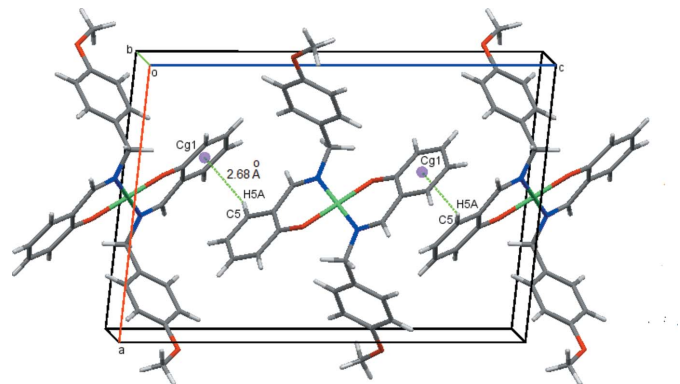
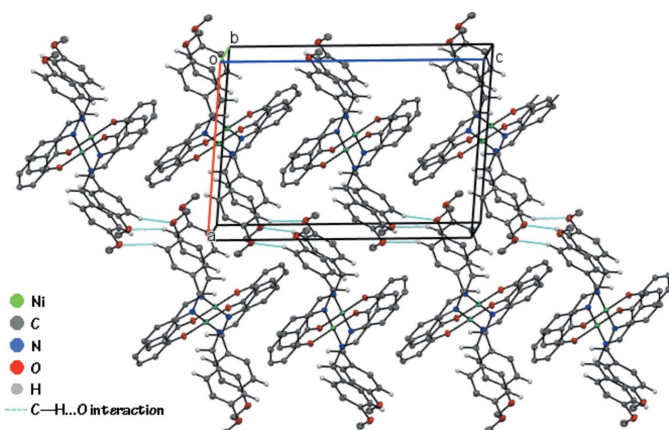


Figure 3

$\text{C-H}\cdots\pi$  contacts for (I), shown as dotted lines, with ring centroids shown as coloured spheres. Cg1 is the centroid of the C1–C6 ring.



**Figure 4**  
The packing of (I), viewed along the *b* axis, showing the stacking of sheets of Ni<sup>II</sup> complex molecules. Only H atoms involved in weak C—H...O interactions are shown for clarity.

in seven discrete structures including the closely related bis(2-[(*E*)-(4-fluorobenzyl)iminomethyl]-6-methoxyphenolato-κ<sup>2</sup>N,O<sup>1</sup>)nickel(II) (Bahron *et al.*, 2011) and bis[2-[(benzylimino)methyl]-5-methoxyphenolato]nickel(II) (Gou *et al.*, 2013)

### 5. Synthesis and crystallization

*N*-4-Methoxybenzylsalicylideneimine (5 mmol, 0.6041 g) was dissolved in ethanol (15 ml). An ethanolic solution of nickel(II) acetate tetrahydrate (2.5 mmol, 0.6216 g) was added dropwise to the former solution and the mixture heated under reflux for 4 h, producing a green solid. The solid 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 43.3%; m.p. 469–472 K). Analytical data for [Ni(C<sub>28</sub>H<sub>30</sub>N<sub>2</sub>O<sub>4</sub>)]: C 66.82, H 5.23, N 5.19%; found: C 67.03, H 5.28, N 5.15%. IR (KBr, cm<sup>-1</sup>): ν(C=N) 1605 (s), ν(C—N) 1391 (s), ν(C—O) 1325 (s), ν(Ni—O) 598 (w), ν(Ni—N) 437 (w).

### 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 C—H = 0.95 for aromatic, 0.99 for CH<sub>2</sub> and 0.98 Å for CH<sub>3</sub> hydrogens. The *U*<sub>iso</sub>(H) values were constrained to be 1.5*U*<sub>eq</sub> of the carrier atom for methyl H atoms and 1.2*U*<sub>eq</sub> for the remaining H atoms. A rotating-group model was used for the methyl groups.

### Acknowledgements

The authors would like to acknowledge the Ministry of Education of Malaysia for research grants Nos. 600-RMI/FRGS 5/3 (51/2013) and (52/2013), Universiti Teknologi

**Table 2**  
Experimental details.

Crystal data	[Ni(C <sub>15</sub> H <sub>14</sub> NO <sub>2</sub> ) <sub>2</sub> ]
Chemical formula	539.23
<i>M<sub>r</sub></i>	Monoclinic, <i>P</i> <sub>2</sub> <sub>1</sub> / <i>c</i>
Crystal system, space group	100
Temperature (K)	<i>a</i> , <i>b</i> , <i>c</i> (Å)
<i>a</i> , <i>b</i> , <i>c</i> (Å)	12.1847 (2), 5.6738 (1), 17.7620 (3)
β (°)	95.682 (1)
<i>V</i> (Å <sup>3</sup> )	1221.92 (4)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm <sup>-1</sup> )	0.84
Crystal size (mm)	0.52 × 0.30 × 0.16
Data collection	
Diffractometer	Bruker APEXII CCD area detector
Absorption correction	Multi-scan ( <i>SADABS</i> ; Bruker, 2009)
<i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>	0.670, 0.876
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	14541, 3542, 3092
<i>R</i> <sub>int</sub>	0.019
(sin θ/λ) <sub>max</sub> (Å <sup>-1</sup> )	0.703
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.028, 0.074, 1.05
No. of reflections	3542
No. of parameters	170
H-atom treatment	H-atom parameters constrained
Δρ <sub>max</sub> , Δρ <sub>min</sub> (e Å <sup>-3</sup> )	0.42, -0.32

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

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## supporting information

*Acta Cryst.* (2014). E70, 104-106 [doi:10.1107/S160053681401650X]

## Crystal structure of bis{2-[(*E*)-(4-methoxybenzyl)iminomethyl]phenolato- $\kappa^2N,O^1$ }nickel(II)

Hadariah Bahron, Amalina Mohd Tajuddin, Wan Nazihah Wan Ibrahim, Hoong-Kun Fun and Suchada Chantrapromma

### 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 *pubCIF* (Westrip, 2010).

### Bis{2-[(*E*)-(4-methoxybenzyl)iminomethyl]phenolato- $\kappa^2N,O^1$ }nickel(II)

#### Crystal data

[Ni(C<sub>15</sub>H<sub>14</sub>NO<sub>2</sub>)<sub>2</sub>]

$M_r = 539.23$

Monoclinic, *P2<sub>1</sub>/c*

Hall symbol: -P 2ybc

$a = 12.1847$  (2) Å

$b = 5.6738$  (1) Å

$c = 17.7620$  (3) Å

$\beta = 95.682$  (1)°

$V = 1221.92$  (4) Å<sup>3</sup>

$Z = 2$

$F(000) = 564$

$D_x = 1.466$  Mg m<sup>-3</sup>

Melting point = 469–472 K

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 3542 reflections

$\theta = 1.7$ – $30.0$ °

$\mu = 0.84$  mm<sup>-1</sup>

$T = 100$  K

Needle, green

$0.52 \times 0.30 \times 0.16$  mm

#### Data collection

Bruker APEXII CCD area-detector diffractometer

Radiation source: sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan (*SADABS*; Bruker, 2009)

$T_{\min} = 0.670$ ,  $T_{\max} = 0.876$

14541 measured reflections

3542 independent reflections

3092 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.019$

$\theta_{\max} = 30.0$ °,  $\theta_{\min} = 1.7$ °

$h = -17 \rightarrow 17$

$k = -7 \rightarrow 7$

$l = -24 \rightarrow 24$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.028$

$wR(F^2) = 0.074$

$S = 1.05$

3542 reflections

170 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0313P)^2 + 0.7976P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.42 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.32 \text{ e } \text{\AA}^{-3}$

### Special details

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

**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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.5000	0.0000	0.5000	0.01253 (7)
O1	0.58126 (8)	-0.03642 (16)	0.41876 (5)	0.01676 (19)
O2	-0.03916 (8)	-0.2287 (2)	0.34237 (6)	0.0272 (2)
N1	0.42000 (8)	0.2622 (2)	0.45360 (6)	0.0142 (2)
C1	0.60209 (10)	0.1191 (2)	0.36758 (6)	0.0141 (2)
C2	0.68624 (10)	0.0696 (3)	0.31981 (7)	0.0164 (2)
H2A	0.7260	-0.0744	0.3255	0.020*
C3	0.71053 (10)	0.2297 (3)	0.26525 (7)	0.0176 (2)
H3A	0.7676	0.1945	0.2343	0.021*
C4	0.65287 (11)	0.4428 (3)	0.25451 (7)	0.0182 (3)
H4A	0.6698	0.5501	0.2163	0.022*
C5	0.57101 (10)	0.4940 (2)	0.30048 (7)	0.0157 (2)
H5A	0.5315	0.6380	0.2938	0.019*
C6	0.54531 (10)	0.3354 (2)	0.35715 (6)	0.0138 (2)
C7	0.45329 (10)	0.3875 (2)	0.39913 (7)	0.0146 (2)
H7A	0.4130	0.5271	0.3857	0.018*
C8	0.31199 (10)	0.3363 (2)	0.47834 (7)	0.0163 (2)
H8A	0.2966	0.5015	0.4629	0.020*
H8B	0.3151	0.3279	0.5342	0.020*
C9	0.22048 (10)	0.1787 (2)	0.44360 (7)	0.0159 (2)
C10	0.16960 (11)	0.2254 (3)	0.37107 (7)	0.0209 (3)
H10A	0.1939	0.3559	0.3436	0.025*
C11	0.08462 (11)	0.0860 (3)	0.33834 (7)	0.0235 (3)
H11A	0.0517	0.1204	0.2888	0.028*
C12	0.04753 (10)	-0.1046 (3)	0.37812 (7)	0.0194 (3)
C13	0.09757 (11)	-0.1573 (3)	0.44988 (8)	0.0216 (3)
H13A	0.0735	-0.2887	0.4770	0.026*
C14	0.18353 (11)	-0.0150 (3)	0.48172 (8)	0.0203 (3)
H14A	0.2176	-0.0518	0.5307	0.024*
C15	-0.08444 (12)	-0.4144 (3)	0.38380 (9)	0.0274 (3)

H15A	-0.1488	-0.4812	0.3537	0.041*
H15B	-0.1069	-0.3521	0.4314	0.041*
H15C	-0.0287	-0.5376	0.3947	0.041*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ni1	0.01363 (11)	0.01119 (12)	0.01281 (10)	0.00205 (8)	0.00150 (7)	0.00034 (8)
O1	0.0207 (4)	0.0148 (5)	0.0153 (4)	0.0041 (4)	0.0044 (3)	0.0021 (3)
O2	0.0239 (5)	0.0353 (6)	0.0210 (5)	-0.0062 (5)	-0.0041 (4)	-0.0053 (4)
N1	0.0138 (4)	0.0131 (5)	0.0157 (4)	0.0010 (4)	0.0010 (3)	-0.0012 (4)
C1	0.0146 (5)	0.0148 (6)	0.0126 (5)	-0.0009 (5)	-0.0009 (4)	-0.0015 (4)
C2	0.0158 (5)	0.0168 (6)	0.0165 (5)	0.0003 (5)	0.0013 (4)	-0.0021 (5)
C3	0.0159 (5)	0.0198 (7)	0.0174 (5)	-0.0029 (5)	0.0025 (4)	-0.0026 (5)
C4	0.0187 (5)	0.0181 (6)	0.0179 (5)	-0.0039 (5)	0.0016 (4)	0.0015 (5)
C5	0.0156 (5)	0.0133 (6)	0.0176 (5)	-0.0021 (5)	-0.0007 (4)	0.0011 (5)
C6	0.0144 (5)	0.0134 (6)	0.0133 (5)	-0.0008 (4)	-0.0009 (4)	-0.0009 (4)
C7	0.0149 (5)	0.0123 (6)	0.0160 (5)	0.0010 (5)	-0.0012 (4)	-0.0009 (5)
C8	0.0159 (5)	0.0149 (6)	0.0183 (5)	0.0039 (5)	0.0029 (4)	-0.0004 (5)
C9	0.0140 (5)	0.0171 (6)	0.0167 (5)	0.0049 (5)	0.0026 (4)	-0.0008 (5)
C10	0.0201 (6)	0.0250 (7)	0.0178 (5)	0.0023 (5)	0.0027 (4)	0.0036 (5)
C11	0.0221 (6)	0.0340 (8)	0.0141 (5)	0.0021 (6)	0.0000 (4)	0.0007 (6)
C12	0.0163 (5)	0.0243 (7)	0.0174 (5)	0.0023 (5)	0.0006 (4)	-0.0057 (5)
C13	0.0212 (6)	0.0214 (7)	0.0216 (6)	-0.0012 (5)	-0.0007 (5)	0.0019 (5)
C14	0.0187 (6)	0.0227 (7)	0.0185 (6)	0.0009 (5)	-0.0030 (4)	0.0029 (5)
C15	0.0219 (6)	0.0282 (8)	0.0317 (7)	-0.0039 (6)	0.0007 (5)	-0.0100 (7)

*Geometric parameters (Å, °)*

Ni1—O1	1.8407 (9)	C6—C7	1.4374 (16)
Ni1—O1 <sup>i</sup>	1.8407 (9)	C7—H7A	0.9500
Ni1—N1	1.9191 (11)	C8—C9	1.5123 (18)
Ni1—N1 <sup>i</sup>	1.9191 (11)	C8—H8A	0.9900
O1—C1	1.3095 (15)	C8—H8B	0.9900
O2—C12	1.3717 (16)	C9—C14	1.3892 (19)
O2—C15	1.427 (2)	C9—C10	1.3986 (17)
N1—C7	1.2977 (16)	C10—C11	1.384 (2)
N1—C8	1.4887 (15)	C10—H10A	0.9500
C1—C6	1.4123 (18)	C11—C12	1.392 (2)
C1—C2	1.4221 (16)	C11—H11A	0.9500
C2—C3	1.3813 (18)	C12—C13	1.3898 (18)
C2—H2A	0.9500	C13—C14	1.3967 (19)
C3—C4	1.402 (2)	C13—H13A	0.9500
C3—H3A	0.9500	C14—H14A	0.9500
C4—C5	1.3810 (17)	C15—H15A	0.9800
C4—H4A	0.9500	C15—H15B	0.9800
C5—C6	1.4080 (17)	C15—H15C	0.9800
C5—H5A	0.9500		

O1—Ni1—O1 <sup>i</sup>	180.000 (1)	C6—C7—H7A	116.9
O1—Ni1—N1	92.30 (4)	N1—C8—C9	110.50 (10)
O1 <sup>i</sup> —Ni1—N1	87.70 (4)	N1—C8—H8A	109.5
O1—Ni1—N1 <sup>i</sup>	87.70 (4)	C9—C8—H8A	109.5
O1 <sup>i</sup> —Ni1—N1 <sup>i</sup>	92.30 (4)	N1—C8—H8B	109.5
N1—Ni1—N1 <sup>i</sup>	180.00 (6)	C9—C8—H8B	109.5
C1—O1—Ni1	128.67 (8)	H8A—C8—H8B	108.1
C12—O2—C15	117.36 (11)	C14—C9—C10	117.60 (12)
C7—N1—C8	114.59 (11)	C14—C9—C8	122.03 (11)
C7—N1—Ni1	124.19 (9)	C10—C9—C8	120.37 (12)
C8—N1—Ni1	121.22 (8)	C11—C10—C9	121.56 (13)
O1—C1—C6	123.41 (11)	C11—C10—H10A	119.2
O1—C1—C2	118.82 (12)	C9—C10—H10A	119.2
C6—C1—C2	117.77 (11)	C10—C11—C12	119.86 (12)
C3—C2—C1	120.40 (12)	C10—C11—H11A	120.1
C3—C2—H2A	119.8	C12—C11—H11A	120.1
C1—C2—H2A	119.8	O2—C12—C13	124.20 (13)
C2—C3—C4	121.55 (12)	O2—C12—C11	115.95 (12)
C2—C3—H3A	119.2	C13—C12—C11	119.84 (13)
C4—C3—H3A	119.2	C12—C13—C14	119.37 (13)
C5—C4—C3	118.84 (12)	C12—C13—H13A	120.3
C5—C4—H4A	120.6	C14—C13—H13A	120.3
C3—C4—H4A	120.6	C9—C14—C13	121.74 (12)
C4—C5—C6	120.87 (12)	C9—C14—H14A	119.1
C4—C5—H5A	119.6	C13—C14—H14A	119.1
C6—C5—H5A	119.6	O2—C15—H15A	109.5
C5—C6—C1	120.55 (11)	O2—C15—H15B	109.5
C5—C6—C7	118.67 (12)	H15A—C15—H15B	109.5
C1—C6—C7	120.51 (11)	O2—C15—H15C	109.5
N1—C7—C6	126.28 (12)	H15A—C15—H15C	109.5
N1—C7—H7A	116.9	H15B—C15—H15C	109.5
N1—Ni1—O1—C1	22.59 (11)	Ni1—N1—C7—C6	9.30 (18)
N1 <sup>i</sup> —Ni1—O1—C1	-157.41 (11)	C5—C6—C7—N1	-178.90 (12)
O1—Ni1—N1—C7	-19.81 (11)	C1—C6—C7—N1	7.05 (19)
O1—Ni1—N1—C8	159.85 (9)	C7—N1—C8—C9	99.88 (13)
O1 <sup>i</sup> —Ni1—N1—C8	-20.15 (9)	Ni1—N1—C8—C9	-79.80 (11)
Ni1—O1—C1—C6	-13.67 (17)	N1—C8—C9—C14	95.30 (14)
Ni1—O1—C1—C2	166.19 (9)	N1—C8—C9—C10	-84.93 (14)
O1—C1—C2—C3	-179.94 (11)	C14—C9—C10—C11	0.7 (2)
C6—C1—C2—C3	-0.06 (18)	C8—C9—C10—C11	-179.09 (12)
C1—C2—C3—C4	-0.79 (19)	C9—C10—C11—C12	0.5 (2)
C2—C3—C4—C5	0.89 (19)	C15—O2—C12—C13	3.9 (2)
C3—C4—C5—C6	-0.13 (19)	C15—O2—C12—C11	-175.51 (13)
C4—C5—C6—C1	-0.71 (18)	C10—C11—C12—O2	178.05 (12)
C4—C5—C6—C7	-174.76 (11)	C10—C11—C12—C13	-1.4 (2)
O1—C1—C6—C5	-179.33 (11)	O2—C12—C13—C14	-178.31 (13)

C2—C1—C6—C5	0.80 (17)	C11—C12—C13—C14	1.1 (2)
O1—C1—C6—C7	-5.40 (18)	C10—C9—C14—C13	-1.0 (2)
C2—C1—C6—C7	174.74 (11)	C8—C9—C14—C13	178.78 (12)
C8—N1—C7—C6	-170.38 (11)	C12—C13—C14—C9	0.1 (2)

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

*Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )*

*Cg1* is the centroid of the C1—C6 ring.

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C11—H11 <i>A</i> $\cdots$ O2 <sup>ii</sup>	0.95	2.47	3.3709 (17)	158
C14—H14 <i>A</i> $\cdots$ O1 <sup>i</sup>	0.95	2.57	3.2281 (17)	126
C5—H5 <i>A</i> $\cdots$ Cg1 <sup>iii</sup>	0.95	2.68	3.3918 (13)	132

Symmetry codes: (i)  $-x+1, -y, -z+1$ ; (ii)  $-x, y+1/2, -z+1/2$ ; (iii)  $-x+1, y+1/2, -z+1/2$ .