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Bis{4-chloro-2-[1-(2,4,6-trimethylphenylimino)ethyl]phenolato}nickel(II)

Wen-Chou Hung and Chu-Chieh Lin*

Department of Chemistry, National Chung Hsing University, Taichung 402, Taiwan
Correspondence e-mail: cchlin@mail.nchu.edu.tw

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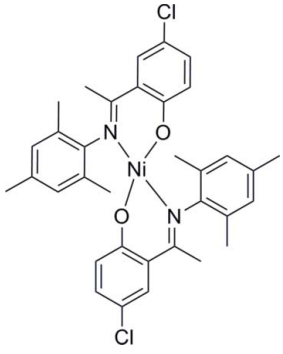
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.058; wR factor = 0.160; data-to-parameter ratio = 15.9.

The Ni^{II} atom in the title complex, $[Ni(C_{17}H_{17}ClNO)_2]$, is tetracoordinated by two N atoms and two O atoms from two bidentate salicylideneiminate ligands, forming a square-planar environment. The asymmetric unit consists of two half-molecules; in each molecule the Ni atom lies on a centre of symmetry.

Related literature

For information on applications of nickel-based catalysts in the polymerization of olefins, see: Bauers & Mecking (2001*a*,*b*); Chang *et al.* (2004); Dennett *et al.* (2004); Diamanti *et al.* (2003); Hu *et al.* (2005); Lee *et al.* (2001); Sun *et al.* (2003); Wang *et al.* (1998); Younkin *et al.* (2000); Zhang *et al.* (2003).



Experimental

Crystal data

$[Ni(C_{17}H_{17}ClNO)_2]$
M_r = 632.24
Triclinic, $P\overline{1}$
a = 11.1181 (16) Å
b = 11.2882 (16) Å
c = 12.4119 (17) Å
α = 84.730 (3)°
β = 88.689 (3)°
γ = 79.574 (3)°
V = 1525.5 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.85 mm^{-1}
T = 298 (2) K
0.30 × 0.20 × 0.02 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.583, T_{max} = 0.983
8811 measured reflections
5935 independent reflections
3446 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.160
S = 1.01
5935 reflections
373 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.65 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.829 (3)	Ni2—O2	1.809 (3)
Ni1—N1	1.910 (3)	Ni2—N2	1.915 (3)
O1^{i}—Ni1—N1	88.41 (13)	O2^{ii}—Ni2—N2	88.73 (13)
O1—Ni1—N1	91.59 (13)	O2—Ni2—N2	91.27 (13)

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); 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: GK2118).

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Bis{4-chloro-2-[1-(2,4,6-trimethylphenylimino)ethyl]phenolato}nickel(II)

Wen-Chou Hung and Chu-Chieh Lin

S1. Comment

Polymerization of olefins with nickel based catalysts has attracted intensive attention recently because they can catalyze not only the polymerization of olefins but also co-polymerization of ethylene with olefins containing functional groups (Zhang *et al.*, 2003; Diamanti *et al.*, 2003; Sun *et al.*, 2003; Dennett *et al.*, 2004). Single-component nickel salicylaldimine complexes have shown great activity toward polymerization of ethylene with very low number of branches in the absence of cocatalysts at low temperatures and pressures (Younkin *et al.*, 2000). Most recently, several examples of nickel-salicylideneimines type catalysts used for olefin polymerization in the presence or absence of cocatalysts are reported (Wang *et al.*, 1998; Bauers & Mecking, 2001*a*,b; Hu *et al.*, 2005; Lee *et al.*, 2001). We report herein the synthesis and crystal structure of a nickel salicylideneimine complex (I), a potential catalyst for olefin polymerization.

The solid structure of (I) reveals a monomeric centrosymmetric Ni^{II} complex (Fig. 1) in which the geometry around Ni^{II} atom is an ideal square-palnar. The metal atom is coordinated by two bidentate ligands with the two oxygen and two nitrogen atoms positioned *trans.* The NiN_2O_2 units are coplanar and the Ni–N and Ni–O bond distances are similar to those reported for salicylaldimine nickel(II) complexes (Chang *et al.*, 2004). The dihedral angles between the mesityl substituent and the benzene ring are 54.99 (0.16) and 63.70 (0.15) Å in the two symmetry independent molecules.

S2. Experimental

The ligand, 4-chloro-2-[1-(2,4,6-trimethylphenylimino)ethyl]phenol was prepared by the reaction of 5-chloro-2-hydroxy-acetophenone (50 mmol) with 2,4,6-trimethylaniline (50 mmol) in refluxed 1-butanol (50 ml) for 2 day. The mixture, which was evaporated to dryness, afforded yellow liquid. The residue was purified by column chromatography (silica gel, ethyl acetate/hexane=1:12) and the desired fraction was collected. The volatile materials were removed under vacuum to give a yellow oil. The title complex was synthesized by the following procedures. Nickel(II) bromide (2 mmol) was refluxed in THF for 2 days and and solution was evaporeted to dryness. A mixture of 4-chloro-2-[1-(2,4,6-trimethyl-phenylimino)-ethyl]-phenol (2 mmol) and triethyl amine (2 mmol) in toluene (20 ml) was added. The resulting mixture was refluxed for 3 h while the solution color changed from yellow to green slowly. The mixture was filtered through celite and the filtrate was allowed to stand at room temperature for 2 days, yielding green crystals.

S3. Refinement

All non-H atoms were initially located in a difference Fourier map. The methyl H atoms were then constrained to an ideal geometry with C—H distances of 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C), but each group was allowed to rotate freely about its C—C bond. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances in the range 0.95–1.00 Å and U_{iso}(H) =1.2U_{eq}(C).

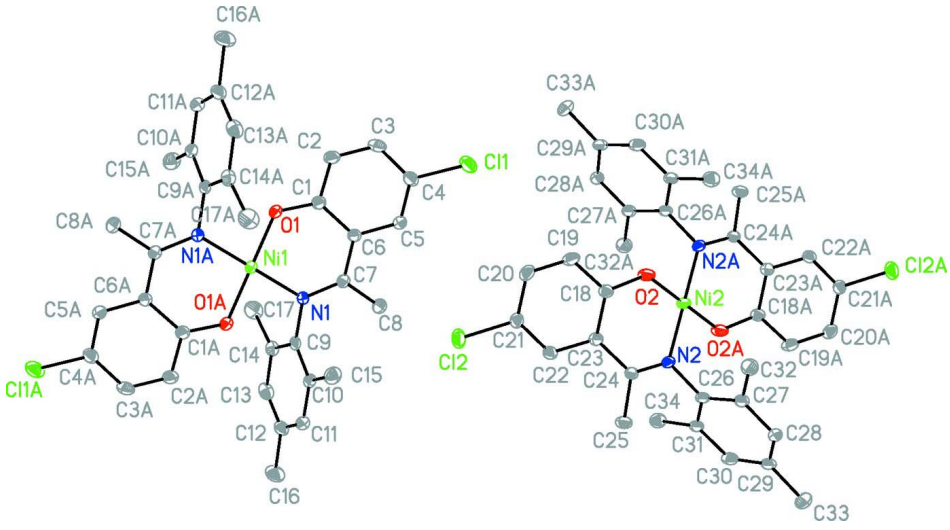

Figure 1

A view of the molecular structure of (I) with displacement ellipsoids shown at the 20% probability level. Hydrogen atoms have been removed for clarity. The atoms designated with the A letter have been genereted by symmetry operations: (i) -*x*, -*y* + 1, -*z* (for the molecule with Ni1) (II) -*x* + 1, -*y* - 1, -*z* - 1 (for the molecule with the Ni2 atom).

Bis{4-chloro-2-[1-(2,4,6-trimethylphenylimino)ethyl]phenolato}nickel(II)

Crystal data

$[Ni(C_{17}H_{17}ClNO)_2]$
$M_r = 632.24$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 11.1181\ (16)$ Å
$b = 11.2882\ (16)$ Å
$c = 12.4119\ (17)$ Å
$\alpha = 84.730\ (3)°$
$\beta = 88.689\ (3)°$
$\gamma = 79.574\ (3)°$
$V = 1525.5\ (4)$ Å^3
$Z = 2$
$F(000) = 660$
$D_x = 1.376$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2140 reflections
$\theta = 2.5–25.5°$
$\mu = 0.85$ mm^{-1}
$T = 298$ K
Parallelpiped, green
0.30 × 0.20 × 0.02 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.583$, $T_{max} = 0.983$
8811 measured reflections
5935 independent reflections
3446 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.8°$
$h = -13\rightarrow13$
$k = -13\rightarrow7$
$l = -15\rightarrow13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.160$
$S = 1.01$
5935 reflections
373 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

$w = 1/[\sigma^2(F_o^2) + (0.065P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.69$ e Å^{-3}
$\Delta\rho_{min} = -0.65$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.0000	0.5000	0.0000	0.0384 (2)
Ni2	0.5000	−0.5000	0.5000	0.0375 (2)
Cl1	0.50884 (12)	0.14354 (16)	0.25696 (12)	0.0778 (5)
Cl2	0.08634 (13)	0.04318 (11)	0.36364 (12)	0.0655 (4)
O1	0.1654 (3)	0.4851 (3)	−0.0199 (3)	0.0500 (8)
O2	0.4906 (3)	−0.3400 (3)	0.5115 (3)	0.0535 (9)
N1	0.0102 (3)	0.3286 (3)	0.0098 (3)	0.0363 (8)
N2	0.3306 (3)	−0.4898 (3)	0.5373 (3)	0.0355 (8)
C1	0.2400 (4)	0.4049 (4)	0.0402 (4)	0.0418 (11)
C2	0.3525 (4)	0.4330 (4)	0.0702 (4)	0.0512 (12)
H2A	0.3716	0.5078	0.0459	0.061*
C3	0.4343 (4)	0.3531 (5)	0.1343 (4)	0.0518 (12)
H3A	0.5073	0.3743	0.1539	0.062*
C4	0.4081 (4)	0.2413 (5)	0.1697 (4)	0.0475 (12)
C5	0.3030 (4)	0.2071 (4)	0.1394 (3)	0.0428 (11)
H5A	0.2881	0.1304	0.1627	0.051*
C6	0.2174 (4)	0.2863 (4)	0.0737 (3)	0.0375 (10)
C7	0.1066 (4)	0.2486 (4)	0.0392 (3)	0.0380 (10)
C8	0.1094 (4)	0.1150 (4)	0.0370 (4)	0.0541 (13)
H8A	0.0314	0.1018	0.0139	0.081*
H8B	0.1267	0.0753	0.1082	0.081*
H8C	0.1718	0.0826	−0.0124	0.081*
C9	−0.0976 (4)	0.2846 (3)	−0.0210 (3)	0.0366 (10)
C10	−0.1735 (4)	0.2435 (4)	0.0600 (4)	0.0407 (10)
C11	−0.2745 (4)	0.1995 (4)	0.0290 (4)	0.0498 (12)
H11A	−0.3239	0.1693	0.0822	0.060*
C12	−0.3044 (4)	0.1988 (4)	−0.0783 (4)	0.0511 (12)
C13	−0.2316 (4)	0.2455 (4)	−0.1562 (4)	0.0525 (13)
H13A	−0.2520	0.2475	−0.2286	0.063*
C14	−0.1271 (4)	0.2902 (4)	−0.1292 (4)	0.0442 (11)

C15	−0.1473 (5)	0.2481 (5)	0.1777 (4)	0.0600 (14)
H15A	−0.2085	0.2161	0.2212	0.090*
H15B	−0.1484	0.3304	0.1921	0.090*
H15C	−0.0682	0.2008	0.1950	0.090*
C16	−0.4160 (5)	0.1486 (5)	−0.1097 (5)	0.0808 (19)
H16A	−0.4559	0.1205	−0.0454	0.121*
H16B	−0.3905	0.0826	−0.1535	0.121*
H16C	−0.4717	0.2111	−0.1498	0.121*
C17	−0.0524 (5)	0.3460 (6)	−0.2156 (4)	0.0708 (16)
H17A	0.0150	0.3714	−0.1829	0.106*
H17B	−0.1026	0.4147	−0.2534	0.106*
H17C	−0.0219	0.2876	−0.2657	0.106*
C18	0.3957 (4)	−0.2564 (4)	0.4826 (4)	0.0399 (10)
C19	0.4156 (4)	−0.1386 (4)	0.4493 (4)	0.0513 (13)
H19A	0.4945	−0.1223	0.4511	0.062*
C20	0.3232 (4)	−0.0483 (4)	0.4147 (4)	0.0495 (12)
H20A	0.3391	0.0280	0.3911	0.059*
C21	0.2044 (4)	−0.0712 (4)	0.4150 (4)	0.0418 (11)
C22	0.1790 (4)	−0.1808 (4)	0.4511 (3)	0.0396 (10)
H22A	0.0985	−0.1930	0.4525	0.047*
C23	0.2736 (4)	−0.2772 (4)	0.4870 (3)	0.0360 (10)
C24	0.2467 (4)	−0.3940 (4)	0.5284 (3)	0.0341 (9)
C25	0.1171 (4)	−0.3974 (4)	0.5654 (4)	0.0467 (11)
H25A	0.1101	−0.4787	0.5912	0.070*
H25B	0.0624	−0.3702	0.5058	0.070*
H25C	0.0962	−0.3455	0.6226	0.070*
C26	0.2960 (3)	−0.6019 (4)	0.5848 (3)	0.0361 (10)
C27	0.3202 (4)	−0.6367 (4)	0.6934 (4)	0.0401 (10)
C28	0.2888 (4)	−0.7457 (4)	0.7373 (4)	0.0494 (12)
H28A	0.3047	−0.7705	0.8099	0.059*
C29	0.2351 (4)	−0.8172 (4)	0.6762 (4)	0.0462 (11)
C30	0.2135 (4)	−0.7802 (4)	0.5685 (4)	0.0466 (12)
H30A	0.1776	−0.8285	0.5267	0.056*
C31	0.2436 (4)	−0.6728 (4)	0.5197 (3)	0.0384 (10)
C32	0.3804 (5)	−0.5604 (5)	0.7617 (4)	0.0590 (14)
H32A	0.3959	−0.4897	0.7183	0.089*
H32B	0.4563	−0.6065	0.7892	0.089*
H32C	0.3274	−0.5363	0.8209	0.089*
C33	0.1986 (5)	−0.9327 (5)	0.7254 (5)	0.0765 (18)
H33A	0.2199	−0.9449	0.8006	0.115*
H33B	0.2407	−0.9995	0.6886	0.115*
H33C	0.1119	−0.9273	0.7182	0.115*
C34	0.2249 (4)	−0.6390 (5)	0.4010 (4)	0.0523 (12)
H34A	0.2501	−0.5629	0.3815	0.078*
H34B	0.1399	−0.6323	0.3842	0.078*
H34C	0.2726	−0.7001	0.3611	0.078*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0347 (4)	0.0269 (4)	0.0531 (5)	−0.0055 (3)	−0.0023 (4)	0.0007 (4)
Ni2	0.0260 (4)	0.0300 (4)	0.0571 (5)	−0.0074 (3)	0.0046 (4)	−0.0031 (4)
Cl1	0.0442 (7)	0.1086 (12)	0.0753 (9)	−0.0167 (8)	−0.0177 (6)	0.0308 (9)
Cl2	0.0684 (9)	0.0410 (7)	0.0836 (10)	−0.0032 (6)	−0.0288 (7)	0.0064 (7)
O1	0.0359 (17)	0.0294 (16)	0.083 (2)	−0.0067 (14)	0.0013 (16)	0.0076 (16)
O2	0.0278 (16)	0.0321 (17)	0.101 (3)	−0.0062 (14)	0.0074 (16)	−0.0083 (18)
N1	0.0326 (19)	0.0323 (19)	0.043 (2)	−0.0059 (16)	−0.0053 (16)	0.0036 (16)
N2	0.0331 (19)	0.0270 (18)	0.048 (2)	−0.0102 (16)	0.0018 (16)	−0.0001 (16)
C1	0.036 (2)	0.036 (2)	0.053 (3)	−0.006 (2)	0.004 (2)	−0.006 (2)
C2	0.040 (3)	0.040 (3)	0.078 (4)	−0.014 (2)	0.002 (2)	−0.010 (3)
C3	0.035 (3)	0.061 (3)	0.065 (3)	−0.017 (2)	−0.004 (2)	−0.017 (3)
C4	0.038 (3)	0.057 (3)	0.046 (3)	−0.007 (2)	−0.005 (2)	−0.001 (2)
C5	0.040 (2)	0.041 (3)	0.048 (3)	−0.013 (2)	−0.004 (2)	0.006 (2)
C6	0.034 (2)	0.034 (2)	0.045 (3)	−0.0071 (19)	0.0012 (19)	−0.004 (2)
C7	0.039 (2)	0.030 (2)	0.045 (3)	−0.007 (2)	0.000 (2)	−0.004 (2)
C8	0.050 (3)	0.031 (2)	0.081 (4)	−0.008 (2)	−0.007 (3)	−0.004 (3)
C9	0.036 (2)	0.022 (2)	0.051 (3)	−0.0017 (18)	−0.010 (2)	−0.0029 (19)
C10	0.042 (3)	0.032 (2)	0.048 (3)	−0.009 (2)	−0.008 (2)	0.003 (2)
C11	0.042 (3)	0.038 (3)	0.069 (3)	−0.011 (2)	−0.003 (2)	0.003 (2)
C12	0.039 (3)	0.041 (3)	0.074 (4)	−0.005 (2)	−0.014 (3)	−0.011 (3)
C13	0.053 (3)	0.053 (3)	0.051 (3)	−0.001 (2)	−0.014 (2)	−0.016 (3)
C14	0.047 (3)	0.040 (3)	0.044 (3)	−0.003 (2)	−0.004 (2)	−0.005 (2)
C15	0.068 (4)	0.065 (4)	0.047 (3)	−0.019 (3)	−0.002 (3)	0.004 (3)
C16	0.057 (3)	0.075 (4)	0.118 (5)	−0.022 (3)	−0.029 (3)	−0.021 (4)
C17	0.066 (4)	0.096 (5)	0.049 (3)	−0.013 (3)	0.003 (3)	0.001 (3)
C18	0.035 (2)	0.032 (2)	0.055 (3)	−0.008 (2)	0.001 (2)	−0.009 (2)
C19	0.042 (3)	0.037 (3)	0.077 (4)	−0.015 (2)	0.013 (3)	−0.007 (3)
C20	0.055 (3)	0.029 (2)	0.064 (3)	−0.009 (2)	0.008 (2)	−0.001 (2)
C21	0.047 (3)	0.030 (2)	0.048 (3)	−0.007 (2)	−0.008 (2)	−0.003 (2)
C22	0.035 (2)	0.038 (2)	0.047 (3)	−0.010 (2)	−0.005 (2)	−0.005 (2)
C23	0.033 (2)	0.033 (2)	0.042 (2)	−0.0062 (19)	0.0027 (19)	−0.008 (2)
C24	0.029 (2)	0.032 (2)	0.042 (2)	−0.0063 (18)	0.0006 (18)	−0.0037 (19)
C25	0.030 (2)	0.045 (3)	0.066 (3)	−0.010 (2)	0.008 (2)	−0.008 (2)
C26	0.027 (2)	0.034 (2)	0.049 (3)	−0.0109 (18)	0.0014 (19)	−0.004 (2)
C27	0.033 (2)	0.040 (3)	0.049 (3)	−0.011 (2)	−0.001 (2)	−0.004 (2)
C28	0.039 (3)	0.058 (3)	0.050 (3)	−0.017 (2)	−0.003 (2)	0.017 (2)
C29	0.031 (2)	0.042 (3)	0.068 (3)	−0.015 (2)	−0.001 (2)	0.000 (2)
C30	0.035 (2)	0.038 (3)	0.070 (3)	−0.014 (2)	0.003 (2)	−0.014 (2)
C31	0.028 (2)	0.038 (2)	0.051 (3)	−0.0104 (19)	0.0019 (19)	−0.005 (2)
C32	0.062 (3)	0.065 (3)	0.055 (3)	−0.025 (3)	−0.014 (3)	−0.001 (3)
C33	0.069 (4)	0.046 (3)	0.114 (5)	−0.024 (3)	−0.008 (3)	0.023 (3)
C34	0.053 (3)	0.057 (3)	0.050 (3)	−0.017 (2)	−0.001 (2)	−0.009 (3)

Geometric parameters (Å, º)

Ni1—O1^{i}	1.829 (3)	C15—H15B	0.9600
Ni1—O1	1.829 (3)	C15—H15C	0.9600
Ni1—N1	1.910 (3)	C16—H16A	0.9600
Ni1—N1^{i}	1.910 (3)	C16—H16B	0.9600
Ni2—O2^{ii}	1.809 (3)	C16—H16C	0.9600
Ni2—O2	1.809 (3)	C17—H17A	0.9600
Ni2—N2^{ii}	1.915 (3)	C17—H17B	0.9600
Ni2—N2	1.915 (3)	C17—H17C	0.9600
Cl1—C4	1.742 (5)	C18—C19	1.411 (6)
Cl2—C21	1.752 (4)	C18—C23	1.418 (5)
O1—C1	1.303 (5)	C19—C20	1.356 (6)
O2—C18	1.313 (5)	C19—H19A	0.9300
N1—C7	1.306 (5)	C20—C21	1.391 (6)
N1—C9	1.450 (5)	C20—H20A	0.9300
N2—C24	1.293 (5)	C21—C22	1.353 (6)
N2—C26	1.458 (5)	C22—C23	1.416 (6)
C1—C2	1.410 (6)	C22—H22A	0.9300
C1—C6	1.429 (6)	C23—C24	1.451 (5)
C2—C3	1.370 (7)	C24—C25	1.508 (5)
C2—H2A	0.9300	C25—H25A	0.9600
C3—C4	1.377 (6)	C25—H25B	0.9600
C3—H3A	0.9300	C25—H25C	0.9600
C4—C5	1.366 (6)	C26—C27	1.387 (6)
C5—C6	1.402 (6)	C26—C31	1.393 (6)
C5—H5A	0.9300	C27—C28	1.398 (6)
C6—C7	1.460 (6)	C27—C32	1.509 (6)
C7—C8	1.506 (6)	C28—C29	1.375 (6)
C8—H8A	0.9600	C28—H28A	0.9300
C8—H8B	0.9600	C29—C30	1.377 (6)
C8—H8C	0.9600	C29—C33	1.506 (6)
C9—C14	1.383 (6)	C30—C31	1.397 (6)
C9—C10	1.399 (6)	C30—H30A	0.9300
C10—C11	1.383 (6)	C31—C34	1.498 (6)
C10—C15	1.503 (6)	C32—H32A	0.9600
C11—C12	1.381 (7)	C32—H32B	0.9600
C11—H11A	0.9300	C32—H32C	0.9600
C12—C13	1.376 (7)	C33—H33A	0.9600
C12—C16	1.526 (6)	C33—H33B	0.9600
C13—C14	1.406 (6)	C33—H33C	0.9600
C13—H13A	0.9300	C34—H34A	0.9600
C14—C17	1.504 (7)	C34—H34B	0.9600
C15—H15A	0.9600	C34—H34C	0.9600
O1^{i}—Ni1—O1	180.0 (2)	H16A—C16—H16B	109.5
O1^{i}—Ni1—N1	88.41 (13)	C12—C16—H16C	109.5
O1—Ni1—N1	91.59 (13)	H16A—C16—H16C	109.5

O1^{i}—Ni1—N1^{i}	91.59 (13)	H16B—C16—H16C	109.5
O1—Ni1—N1^{i}	88.41 (13)	C14—C17—H17A	109.5
N1—Ni1—N1^{i}	180.0	C14—C17—H17B	109.5
O2^{ii}—Ni2—O2	180.0	H17A—C17—H17B	109.5
O2^{ii}—Ni2—N2^{ii}	91.27 (13)	C14—C17—H17C	109.5
O2—Ni2—N2^{ii}	88.73 (13)	H17A—C17—H17C	109.5
O2^{ii}—Ni2—N2	88.73 (13)	H17B—C17—H17C	109.5
O2—Ni2—N2	91.27 (13)	O2—C18—C19	118.4 (4)
N2^{ii}—Ni2—N2	180.00 (5)	O2—C18—C23	123.5 (4)
C1—O1—Ni1	120.3 (3)	C19—C18—C23	118.0 (4)
C18—O2—Ni2	124.6 (3)	C20—C19—C18	122.1 (4)
C7—N1—C9	117.7 (3)	C20—C19—H19A	119.0
C7—N1—Ni1	125.5 (3)	C18—C19—H19A	119.0
C9—N1—Ni1	116.7 (2)	C19—C20—C21	119.2 (4)
C24—N2—C26	117.7 (3)	C19—C20—H20A	120.4
C24—N2—Ni2	126.8 (3)	C21—C20—H20A	120.4
C26—N2—Ni2	115.4 (3)	C22—C21—C20	121.3 (4)
O1—C1—C2	119.0 (4)	C22—C21—Cl2	119.6 (4)
O1—C1—C6	123.6 (4)	C20—C21—Cl2	119.1 (3)
C2—C1—C6	117.3 (4)	C21—C22—C23	120.8 (4)
C3—C2—C1	121.8 (4)	C21—C22—H22A	119.6
C3—C2—H2A	119.1	C23—C22—H22A	119.6
C1—C2—H2A	119.1	C22—C23—C18	118.4 (4)
C2—C3—C4	119.8 (4)	C22—C23—C24	121.1 (4)
C2—C3—H3A	120.1	C18—C23—C24	120.5 (4)
C4—C3—H3A	120.1	N2—C24—C23	121.7 (4)
C5—C4—C3	121.0 (4)	N2—C24—C25	121.4 (4)
C5—C4—Cl1	119.6 (4)	C23—C24—C25	116.8 (4)
C3—C4—Cl1	119.4 (4)	C24—C25—H25A	109.5
C4—C5—C6	120.8 (4)	C24—C25—H25B	109.5
C4—C5—H5A	119.6	H25A—C25—H25B	109.5
C6—C5—H5A	119.6	C24—C25—H25C	109.5
C5—C6—C1	119.2 (4)	H25A—C25—H25C	109.5
C5—C6—C7	120.7 (4)	H25B—C25—H25C	109.5
C1—C6—C7	120.1 (4)	C27—C26—C31	121.9 (4)
N1—C7—C6	120.7 (4)	C27—C26—N2	118.6 (4)
N1—C7—C8	121.9 (4)	C31—C26—N2	119.5 (4)
C6—C7—C8	117.4 (4)	C26—C27—C28	118.0 (4)
C7—C8—H8A	109.5	C26—C27—C32	121.1 (4)
C7—C8—H8B	109.5	C28—C27—C32	121.0 (4)
H8A—C8—H8B	109.5	C29—C28—C27	121.9 (4)
C7—C8—H8C	109.5	C29—C28—H28A	119.0
H8A—C8—H8C	109.5	C27—C28—H28A	119.0
H8B—C8—H8C	109.5	C28—C29—C30	118.5 (4)
C14—C9—C10	121.3 (4)	C28—C29—C33	121.3 (5)
C14—C9—N1	119.6 (4)	C30—C29—C33	120.2 (4)
C10—C9—N1	119.0 (4)	C29—C30—C31	122.3 (4)
C11—C10—C9	118.1 (4)	C29—C30—H30A	118.8

C11—C10—C15	120.7 (4)	C31—C30—H30A	118.8
C9—C10—C15	121.2 (4)	C26—C31—C30	117.4 (4)
C12—C11—C10	122.3 (5)	C26—C31—C34	121.8 (4)
C12—C11—H11A	118.9	C30—C31—C34	120.7 (4)
C10—C11—H11A	118.9	C27—C32—H32A	109.5
C13—C12—C11	118.3 (4)	C27—C32—H32B	109.5
C13—C12—C16	120.9 (5)	H32A—C32—H32B	109.5
C11—C12—C16	120.9 (5)	C27—C32—H32C	109.5
C12—C13—C14	121.8 (4)	H32A—C32—H32C	109.5
C12—C13—H13A	119.1	H32B—C32—H32C	109.5
C14—C13—H13A	119.1	C29—C33—H33A	109.5
C9—C14—C13	118.0 (4)	C29—C33—H33B	109.5
C9—C14—C17	121.2 (4)	H33A—C33—H33B	109.5
C13—C14—C17	120.7 (4)	C29—C33—H33C	109.5
C10—C15—H15A	109.5	H33A—C33—H33C	109.5
C10—C15—H15B	109.5	H33B—C33—H33C	109.5
H15A—C15—H15B	109.5	C31—C34—H34A	109.5
C10—C15—H15C	109.5	C31—C34—H34B	109.5
H15A—C15—H15C	109.5	H34A—C34—H34B	109.5
H15B—C15—H15C	109.5	C31—C34—H34C	109.5
C12—C16—H16A	109.5	H34A—C34—H34C	109.5
C12—C16—H16B	109.5	H34B—C34—H34C	109.5

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