IUCrData

ISSN 2414-3146

{*N*′-[(*E*)-1-(5-Chloro-2-oxidophenyl)ethylidene]-4-methoxybenzohydrazidato-κ^3O,N',O'}(1*H*-imidazole-κN^3)nickel(II)

Jian-Guo Chang*

Department of Chemistry and Chemical Engineering, Taishan University, 271021 Taian, Shandong, People's Republic of China. *Correspondence e-mail: tsucjg@163.com

Received 13 March 2022
Accepted 16 March 2022

Edited by E. R. T. Tiekink, Sunway University, Malaysia

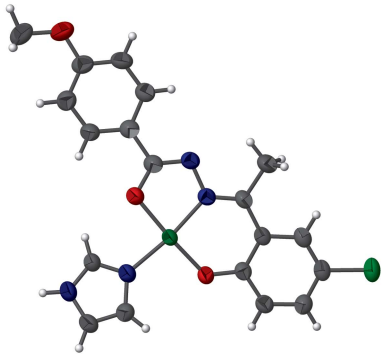
Keywords: crystal structure; acylhydrazone; hydrogen bonding; imidazole; nickel complex.

CCDC reference: 2159183

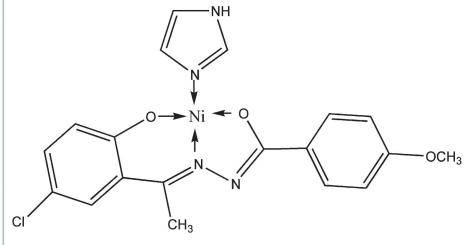
Structural data: full structural data are available from iucrdata.iucr.org

In the title complex, [Ni($C_{16}H_{13}ClN_2O_3$)($C_3H_4N_2$)], the Ni^{II} ion is coordinated by two O atoms and one N atom derived from the dianionic *N*′-[(1*E*)-1-(5-chloro-2-hydroxyphenyl)ethylidene]-4-methoxybenzohydrazide ligand and one N atom from the imidazole molecule. The N_2O_2 donor set defines an approximate square-planar geometry. The dihedral angles between the imidazole ring and the fused six-membered and methoxybenzene rings are 17.78 (14) and 13.23 (16)°, respectively; the dihedral angle between the C_6 rings is 6.63 (12)°. The most prominent feature of the molecular packing is the formation of 4_1-helical chains (along the *c* axis) mediated by imidazole-N—H···O(phenoxide) hydrogen bonding; these are linked by methyl-C—H···Cl interactions.

3D view



Chemical scheme



Structure description

Acylhydrazones, as a special kind of Schiff base, have been widely investigated because of their strong coordination ability (Singh *et al.*, 1982; Salem, 1998; Yu *et al.*, 2010) and flexible coordination modes involving the N and O donor atoms (Liu *et al.*, 2005; Chang, 2011; Zheng *et al.*, 2011). As has been widely reported in the literature, acylhydrazone complexes display various biological activities such as anti-microbial (Yang *et al.*, 2020), anti-tubercular (Peng, 2011), anti-cancer (Morgan *et al.*, 2003) and anti-oxidant (Chang *et al.*, 2015). As an extension of work into the structural characterization of aroylhydrazone complexes, the title complex, [Ni($C_{16}H_{13}ClN_2O_3$)($C_3H_4N_2$)], has been synthesized and its crystal structure determined.

The Ni^{II} ion in the title compound is coordinated by two O atoms and one N atom from the dianionic *N*′-[(1*E*)-1-(5-chloro-2-hydroxyphenyl)ethylidene]-4-methoxybenzohydra-

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.8995 (15)	Ni1—N2	1.9344 (17)
Ni1—O2	1.8820 (15)	Ni1—N3	1.9664 (18)
O1—Ni1—N2	82.18 (7)	O2—Ni1—N2	94.33 (7)
O1—Ni1—N3	90.33 (7)	O2—Ni1—N3	93.16 (7)
O2—Ni1—O1	173.63 (7)	N2—Ni1—N3	172.50 (8)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···O2^{i}	0.92 (4)	1.93 (4)	2.818 (3)	161 (3)
C8—H8*A*···Cl1^{ii}	0.96	2.86	3.700 (3)	147

Symmetry codes: (i) $-y+\frac{5}{4}, x+\frac{1}{4}, -z+\frac{5}{4}$; (ii) $-x+\frac{3}{2}, -y+1, z-\frac{1}{2}$.

zide ligand and one N atom from the imidazole molecule. In this complex, the Ni atom is located in a slightly distorted square-planar environment (Fig. 1 and Table 1). The Ni—O bond lengths are systematically shorter than the Ni—N bonds, and the maximum deviation from the ideal square-planar geometry in terms of angles is found for O1—Ni1—N2 = 82.18 (7)°. The two benzene rings, C1–C6 (*A*) and C10–C15 (*B*), and the imidazole ring (*C*) make dihedral angles of 6.63 (12)° (*A*/*B*), 17.78 (14)° (*A*/*C*) and 13.23 (16)° (*B*/*C*).

The molecular packing is consolidated by imidazole-N—H···O(phenoxide) hydrogen bonding (Table 2) along the *c* axis, which leads to a 4_1 helical chain. The chains are connected by C—H···Cl interactions (Table 2) into a three-dimensional architecture; a view of the unit-cell contents is given in Fig. 2.

Synthesis and crystallization

The Schiff base ligand, *N*′-[(1*E*)-1-(5-chloro-2-hydroxyphenyl)ethylidene]-4-methoxybenzohydrazide (0.100 mmol, 0.0319 g), 1*H*-imidazole (0.100 mmol, 0.0068 g), $Ni(NO_3)_2{\cdot}6H_2O$ (0.100 mmol, 0.0292 g), methanol (10 ml) and distilled water (5 ml) were mixed in a 50 ml flask. The mixture was stirred at room temperature for 1 h, the pH was adjusted with saturated sodium carbonate solution to about 8 followed by filtration. Red rectangular block-shaped crystals were obtained after about one month by evaporating the filtrate in air (yield 31%).

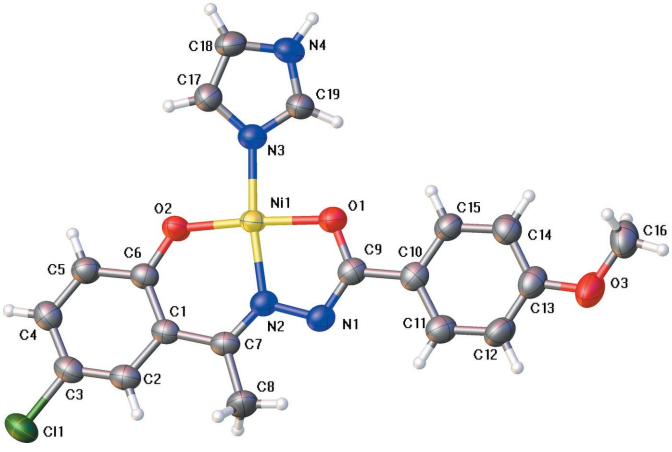


Figure 1
The molecular structure, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Ni(C_{16}H_{13}ClN_2O_3)(C_3H_4N_2)]$
M_r	443.52
Crystal system, space group	Tetragonal, $I4_1/a$
Temperature (K)	295
a, *c* (Å)	30.879 (4), 8.0750 (16)
V (Å^3)	7700 (3)
Z	16
Radiation type	Mo *Kα*
μ (mm^{-1})	1.18
Crystal size (mm)	0.35 × 0.25 × 0.16
Data collection	
Diffractometer	Bruker APEXII CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2003)
T_{min}, T_{max}	0.735, 0.860
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23938, 4924, 3431
R_{int}	0.038
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.678
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.038, 0.106, 1.00
No. of reflections	4924
No. of parameters	259
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.79, −0.21

Computer programs: *APEX2* and *SAINT* (Bruker, 2003), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

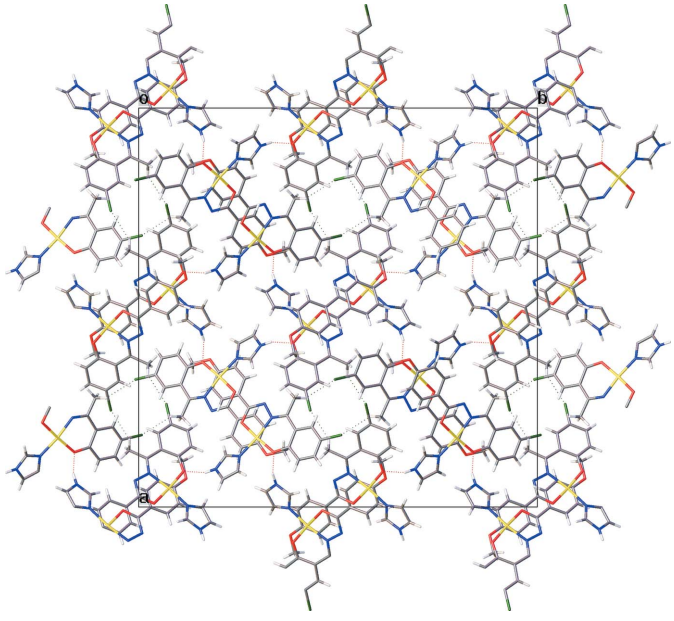


Figure 2
A view in projection down the *c* axis of the unit-cell contents.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

Funding information

The author would like to thank Taishan University for support of this work.

References

Bruker (2003). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Chang, H.-Q., Jia, L., Xu, J., Wu, W.-N., Zhu, T.-F., Chen, R.-H., Ma, T.-L., Wang, Y. & Xu, Z.-Q. (2015). *Transition Met. Chem.* **40**, 485–491.

Chang, J.-G. (2011). *Acta Cryst.* E**67**, m1886.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

Liu, M.-L., Dou, J.-M., Wang, D.-Q. & Li, D.-C. (2005). *Acta Cryst.* E**61**, m1366–m1367.

Morgan, L. R., Thangaraj, K. & Leblanc, B. (2003). *J. Med. Chem.* **46**, 4552–4563.

Peng, S.-J. (2011). *J. Chem. Crystallogr.* **41**, 280–285.

Salem, A. A. (1998). *Microchem. J.* **60**, 51–66.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Singh, R. B., Jain, P. & Singh, R. P. (1982). *Talanta*, **29**, 77–84.

Yang, J., Liu, X.-R., Yu, M.-K., Yang, W.-B., Yang, Z. & Zhao, S.-S. (2020). *Polyhedron*, **187**, 114619.

Yu, G.-M., Zhao, L., Guo, Y.-N., Xu, G.-F., Zou, L.-F., Tang, J.-K. & Li, Y.-H. (2010). *J. Mol. Struct.* **982**, 139–144.

Zheng, C.-Z., Wang, L. & Liu, J. (2011). *Acta Cryst.* E**67**, m978.

full crystallographic data

IUCrData (2022). **7**, x220295 [https://doi.org/10.1107/S2414314622002954]

{*N*′-[(*E*)-1-(5-Chloro-2-oxidophenyl)ethylidene]-4-methoxybenzohydrazidato-κ^3O,N',O'}(1*H*-imidazole-κN^3)nickel(II)

Jian-Guo Chang

{*N*′-[(*E*)-1-(5-Chloro-2-oxidophenyl)ethylidene]-4-methoxybenzohydrazidato-κ^3O,N',O'}(1*H*-imidazole-κN^3)nickel(II)

Crystal data

$[Ni(C_{16}H_{13}ClN_2O_3)(C_3H_4N_2)]$
M_r = 443.52
Tetragonal, $I4_1/a$
a = 30.879 (4) Å
c = 8.0750 (16) Å
V = 7700 (3) Å^3
Z = 16
$F(000)$ = 3648
D_x = 1.530 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5154 reflections
θ = 2.6–25.1°
μ = 1.18 mm^{-1}
T = 295 K
Block, brown
0.35 × 0.25 × 0.16 mm

Data collection

Bruker APEXII CCD area detector diffractometer
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2003)
T_{min} = 0.735, T_{max} = 0.860
23938 measured reflections
4924 independent reflections
3431 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 28.8°, θ_{min} = 1.9°
h = −28→40
k = −41→39
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.106
S = 1.00
4924 reflections
259 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0616P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Special details

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.67356 (2)	0.70309 (2)	0.69948 (3)	0.03734 (10)
Cl1	0.68036 (2)	0.49257 (2)	1.08616 (9)	0.06233 (19)
O1	0.71130 (5)	0.74129 (5)	0.5847 (2)	0.0506 (4)
O2	0.63727 (4)	0.66083 (5)	0.7940 (2)	0.0468 (4)
O3	0.86943 (7)	0.82096 (6)	0.1939 (3)	0.0818 (6)
N1	0.75900 (5)	0.68423 (6)	0.6093 (2)	0.0444 (4)
N2	0.72374 (5)	0.66565 (5)	0.6917 (2)	0.0407 (4)
N3	0.62734 (6)	0.74687 (6)	0.6931 (2)	0.0469 (4)
N4	0.59505 (7)	0.80650 (7)	0.6168 (3)	0.0573 (5)
H4	0.5865 (10)	0.8318 (11)	0.566 (4)	0.100 (11)*
C1	0.69302 (6)	0.60618 (6)	0.8443 (3)	0.0395 (5)
C2	0.70039 (8)	0.56518 (7)	0.9178 (3)	0.0468 (5)
H2	0.728018	0.553255	0.912614	0.056*
C3	0.66852 (8)	0.54265 (7)	0.9955 (3)	0.0471 (5)
C4	0.62689 (8)	0.55887 (7)	1.0092 (3)	0.0494 (5)
H4A	0.605335	0.543496	1.064097	0.059*
C5	0.61852 (7)	0.59863 (7)	0.9385 (3)	0.0478 (5)
H5	0.590670	0.609875	0.946780	0.057*
C6	0.64995 (7)	0.62290 (7)	0.8548 (3)	0.0406 (5)
C7	0.72926 (7)	0.62824 (7)	0.7636 (3)	0.0418 (5)
C8	0.77365 (8)	0.60794 (9)	0.7632 (4)	0.0637 (7)
H8A	0.772858	0.581362	0.701572	0.095*
H8B	0.782430	0.602062	0.875021	0.095*
H8C	0.793945	0.627451	0.712772	0.095*
C9	0.74864 (7)	0.72329 (7)	0.5599 (3)	0.0430 (5)
C10	0.78074 (7)	0.74904 (7)	0.4658 (3)	0.0436 (5)
C11	0.82214 (7)	0.73375 (8)	0.4304 (3)	0.0512 (6)
H11	0.830661	0.706668	0.468830	0.061*
C12	0.85065 (8)	0.75850 (8)	0.3386 (3)	0.0585 (6)
H12	0.878025	0.747719	0.313970	0.070*
C13	0.83883 (8)	0.79913 (8)	0.2832 (3)	0.0544 (6)
C14	0.79796 (8)	0.81495 (8)	0.3173 (3)	0.0531 (6)
H14	0.789633	0.842107	0.279077	0.064*
C15	0.76968 (7)	0.79008 (7)	0.4085 (3)	0.0487 (5)
H15	0.742350	0.801047	0.432655	0.058*
C16	0.85944 (10)	0.86421 (8)	0.1450 (4)	0.0709 (8)
H16A	0.836204	0.863811	0.066026	0.106*
H16B	0.884538	0.877267	0.095671	0.106*
H16C	0.850860	0.880669	0.240361	0.106*
C17	0.58978 (7)	0.75137 (7)	0.7827 (3)	0.0517 (6)
H17	0.579704	0.732134	0.862486	0.062*
C18	0.56989 (8)	0.78836 (8)	0.7357 (4)	0.0587 (6)
H18	0.543965	0.799272	0.776902	0.070*
C19	0.62897 (8)	0.78101 (7)	0.5950 (3)	0.0527 (6)
H19	0.651171	0.786450	0.519968	0.063*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.03354 (15)	0.03200 (15)	0.04649 (18)	0.00236 (10)	−0.00014 (11)	−0.00031 (11)
Cl1	0.0762 (4)	0.0409 (3)	0.0699 (4)	0.0076 (3)	−0.0036 (3)	0.0093 (3)
O1	0.0434 (8)	0.0419 (8)	0.0666 (11)	0.0041 (7)	0.0079 (7)	0.0037 (7)
O2	0.0370 (8)	0.0403 (8)	0.0633 (10)	0.0022 (6)	−0.0021 (7)	0.0089 (7)
O3	0.0736 (13)	0.0594 (11)	0.1126 (18)	−0.0087 (10)	0.0426 (12)	0.0024 (11)
N1	0.0367 (9)	0.0453 (10)	0.0512 (11)	−0.0002 (8)	−0.0009 (8)	−0.0029 (8)
N2	0.0367 (9)	0.0404 (9)	0.0451 (10)	−0.0002 (7)	−0.0013 (7)	−0.0040 (8)
N3	0.0440 (10)	0.0410 (10)	0.0557 (12)	0.0050 (8)	0.0017 (8)	0.0010 (8)
N4	0.0515 (12)	0.0400 (11)	0.0804 (16)	0.0071 (9)	0.0033 (11)	0.0071 (10)
C1	0.0424 (11)	0.0376 (11)	0.0387 (11)	0.0045 (9)	−0.0046 (9)	−0.0029 (9)
C2	0.0489 (12)	0.0433 (12)	0.0484 (13)	0.0082 (10)	−0.0056 (10)	−0.0024 (10)
C3	0.0566 (13)	0.0373 (11)	0.0473 (12)	0.0045 (10)	−0.0057 (10)	−0.0007 (9)
C4	0.0540 (13)	0.0441 (12)	0.0502 (13)	−0.0020 (10)	−0.0010 (11)	0.0026 (10)
C5	0.0412 (12)	0.0456 (12)	0.0565 (15)	0.0023 (9)	−0.0021 (10)	0.0009 (10)
C6	0.0405 (11)	0.0393 (11)	0.0420 (12)	0.0018 (9)	−0.0058 (9)	−0.0013 (9)
C7	0.0400 (11)	0.0418 (11)	0.0435 (12)	0.0069 (9)	−0.0056 (9)	−0.0027 (9)
C8	0.0442 (13)	0.0688 (16)	0.0781 (19)	0.0146 (12)	0.0061 (12)	0.0174 (14)
C9	0.0408 (11)	0.0439 (12)	0.0445 (13)	−0.0017 (9)	−0.0017 (9)	−0.0078 (9)
C10	0.0429 (12)	0.0463 (12)	0.0417 (12)	−0.0041 (9)	−0.0024 (9)	−0.0076 (9)
C11	0.0454 (12)	0.0461 (13)	0.0620 (15)	−0.0011 (10)	0.0004 (11)	−0.0066 (11)
C12	0.0408 (12)	0.0607 (15)	0.0741 (18)	0.0006 (11)	0.0106 (12)	−0.0041 (13)
C13	0.0504 (13)	0.0525 (14)	0.0602 (16)	−0.0101 (10)	0.0098 (11)	−0.0101 (11)
C14	0.0566 (14)	0.0463 (13)	0.0566 (15)	−0.0028 (11)	0.0043 (11)	−0.0021 (11)
C15	0.0422 (12)	0.0495 (13)	0.0545 (14)	0.0021 (10)	0.0060 (10)	−0.0012 (10)
C16	0.0801 (19)	0.0578 (16)	0.0749 (19)	−0.0166 (14)	0.0204 (15)	−0.0005 (14)
C17	0.0507 (13)	0.0438 (12)	0.0604 (15)	0.0005 (10)	0.0077 (11)	0.0029 (11)
C18	0.0496 (14)	0.0459 (13)	0.0805 (18)	0.0100 (11)	0.0115 (13)	−0.0003 (12)
C19	0.0485 (13)	0.0432 (12)	0.0665 (16)	0.0074 (10)	0.0089 (11)	0.0090 (11)

Geometric parameters (Å, º)

Ni1—O1	1.8995 (15)	C5—H5	0.9300
Ni1—O2	1.8820 (15)	C5—C6	1.400 (3)
Ni1—N2	1.9344 (17)	C7—C8	1.507 (3)
Ni1—N3	1.9664 (18)	C8—H8A	0.9600
Cl1—C3	1.750 (2)	C8—H8B	0.9600
O1—C9	1.296 (2)	C8—H8C	0.9600
O2—C6	1.329 (2)	C9—C10	1.481 (3)
O3—C13	1.367 (3)	C10—C11	1.392 (3)
O3—C16	1.426 (3)	C10—C15	1.392 (3)
N1—N2	1.399 (2)	C11—H11	0.9300
N1—C9	1.310 (3)	C11—C12	1.381 (3)
N2—C7	1.304 (3)	C12—H12	0.9300
N3—C17	1.374 (3)	C12—C13	1.381 (3)
N3—C19	1.320 (3)	C13—C14	1.381 (3)

N4—H4	0.92 (4)	C14—H14	0.9300
N4—C18	1.356 (3)	C14—C15	1.376 (3)
N4—C19	1.322 (3)	C15—H15	0.9300
C1—C2	1.417 (3)	C16—H16A	0.9600
C1—C6	1.429 (3)	C16—H16B	0.9600
C1—C7	1.463 (3)	C16—H16C	0.9600
C2—H2	0.9300	C17—H17	0.9300
C2—C3	1.359 (3)	C17—C18	1.351 (3)
C3—C4	1.384 (3)	C18—H18	0.9300
C4—H4A	0.9300	C19—H19	0.9300
C4—C5	1.378 (3)		

O1—Ni1—N2	82.18 (7)	C7—C8—H8B	109.5
O1—Ni1—N3	90.33 (7)	C7—C8—H8C	109.5
O2—Ni1—O1	173.63 (7)	H8A—C8—H8B	109.5
O2—Ni1—N2	94.33 (7)	H8A—C8—H8C	109.5
O2—Ni1—N3	93.16 (7)	H8B—C8—H8C	109.5
N2—Ni1—N3	172.50 (8)	O1—C9—N1	124.4 (2)
C9—O1—Ni1	110.80 (13)	O1—C9—C10	116.41 (19)
C6—O2—Ni1	125.85 (13)	N1—C9—C10	119.18 (19)
C13—O3—C16	117.3 (2)	C11—C10—C9	122.5 (2)
C9—N1—N2	109.43 (17)	C15—C10—C9	119.69 (19)
N1—N2—Ni1	113.18 (12)	C15—C10—C11	117.8 (2)
C7—N2—Ni1	128.30 (15)	C10—C11—H11	119.7
C7—N2—N1	118.25 (17)	C12—C11—C10	120.5 (2)
C17—N3—Ni1	131.96 (16)	C12—C11—H11	119.7
C19—N3—Ni1	122.48 (16)	C11—C12—H12	119.7
C19—N3—C17	105.51 (18)	C13—C12—C11	120.5 (2)
C18—N4—H4	120 (2)	C13—C12—H12	119.7
C19—N4—H4	132 (2)	O3—C13—C12	115.9 (2)
C19—N4—C18	107.6 (2)	O3—C13—C14	124.3 (2)
C2—C1—C6	116.57 (19)	C14—C13—C12	119.9 (2)
C2—C1—C7	118.67 (18)	C13—C14—H14	120.4
C6—C1—C7	124.76 (18)	C15—C14—C13	119.3 (2)
C1—C2—H2	118.8	C15—C14—H14	120.4
C3—C2—C1	122.3 (2)	C10—C15—H15	119.0
C3—C2—H2	118.8	C14—C15—C10	122.0 (2)
C2—C3—Cl1	119.64 (17)	C14—C15—H15	119.0
C2—C3—C4	121.6 (2)	O3—C16—H16A	109.5
C4—C3—Cl1	118.72 (18)	O3—C16—H16B	109.5
C3—C4—H4A	121.2	O3—C16—H16C	109.5
C5—C4—C3	117.6 (2)	H16A—C16—H16B	109.5
C5—C4—H4A	121.2	H16A—C16—H16C	109.5
C4—C5—H5	118.4	H16B—C16—H16C	109.5
C4—C5—C6	123.1 (2)	N3—C17—H17	125.6
C6—C5—H5	118.4	C18—C17—N3	108.8 (2)
O2—C6—C1	124.79 (19)	C18—C17—H17	125.6
O2—C6—C5	116.47 (18)	N4—C18—H18	126.6

C5—C6—C1	118.72 (19)	C17—C18—N4	106.7 (2)
N2—C7—C1	120.71 (18)	C17—C18—H18	126.6
N2—C7—C8	119.1 (2)	N3—C19—N4	111.4 (2)
C1—C7—C8	120.19 (19)	N3—C19—H19	124.3
C7—C8—H8A	109.5	N4—C19—H19	124.3
Ni1—O1—C9—N1	−0.8 (3)	C2—C1—C7—C8	−1.5 (3)
Ni1—O1—C9—C10	177.82 (14)	C2—C3—C4—C5	1.0 (3)
Ni1—O2—C6—C1	−6.1 (3)	C3—C4—C5—C6	0.0 (3)
Ni1—O2—C6—C5	172.09 (15)	C4—C5—C6—O2	−179.5 (2)
Ni1—N2—C7—C1	9.6 (3)	C4—C5—C6—C1	−1.2 (3)
Ni1—N2—C7—C8	−170.21 (18)	C6—C1—C2—C3	−0.4 (3)
Ni1—N3—C17—C18	177.28 (18)	C6—C1—C7—N2	−1.1 (3)
Ni1—N3—C19—N4	−177.80 (17)	C6—C1—C7—C8	178.7 (2)
Cl1—C3—C4—C5	179.21 (18)	C7—C1—C2—C3	179.8 (2)
O1—C9—C10—C11	179.9 (2)	C7—C1—C6—O2	−0.7 (3)
O1—C9—C10—C15	−0.5 (3)	C7—C1—C6—C5	−178.9 (2)
O3—C13—C14—C15	179.9 (2)	C9—N1—N2—Ni1	0.9 (2)
N1—N2—C7—C1	−176.82 (18)	C9—N1—N2—C7	−173.69 (19)
N1—N2—C7—C8	3.4 (3)	C9—C10—C11—C12	178.4 (2)
N1—C9—C10—C11	−1.4 (3)	C9—C10—C15—C14	−178.5 (2)
N1—C9—C10—C15	178.2 (2)	C10—C11—C12—C13	1.2 (4)
N2—Ni1—O1—C9	0.95 (14)	C11—C10—C15—C14	1.1 (3)
N2—Ni1—O2—C6	10.33 (18)	C11—C12—C13—O3	179.8 (2)
N2—N1—C9—O1	0.0 (3)	C11—C12—C13—C14	−1.0 (4)
N2—N1—C9—C10	−178.63 (17)	C12—C13—C14—C15	0.9 (4)
N3—Ni1—O1—C9	−179.41 (15)	C13—C14—C15—C10	−1.0 (4)
N3—Ni1—O2—C6	−170.01 (17)	C15—C10—C11—C12	−1.2 (3)
N3—C17—C18—N4	0.3 (3)	C16—O3—C13—C12	−175.6 (3)
C1—C2—C3—Cl1	−178.99 (17)	C16—O3—C13—C14	5.3 (4)
C1—C2—C3—C4	−0.8 (4)	C17—N3—C19—N4	−0.1 (3)
C2—C1—C6—O2	179.5 (2)	C18—N4—C19—N3	0.3 (3)
C2—C1—C6—C5	1.3 (3)	C19—N3—C17—C18	−0.2 (3)
C2—C1—C7—N2	178.7 (2)	C19—N4—C18—C17	−0.3 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···O2^{i}	0.92 (4)	1.93 (4)	2.818 (3)	161 (3)
C8—H8*A*···Cl1^{ii}	0.96	2.86	3.700 (3)	147

Symmetry codes: (i) −*y*+5/4, *x*+1/4, −*z*+5/4; (ii) −*x*+3/2, −*y*+1, *z*−1/2.