In the title complex, \([\text{Ni}(\text{C}_{16}\text{H}_{13}\text{ClN}_{2}\text{O}_{3})(\text{C}_{3}\text{H}_{4}\text{N}_{2})]\), the Ni\(^{II}\) ion is coordinated by two O atoms and one N atom derived from the dianionic \(N'-(1E)-1-(5\text{-chloro-2-hydroxyphenyl})\text{ethylidene}-4\text{-methoxybenzohydrazide}\) ligand and one N atom from the imidazole molecule. The N\(_2\)O\(_2\) 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)\(^\circ\), respectively; the dihedral angle between the \(C_6\) rings is 6.63 (12)\(^\circ\). 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.

Structure description

Acylhydrazones, as a special kind of Schiff base, have been widely investigated because of their strong coordination ability (Singh \textit{et al.}, 1982; Salem, 1998; Yu \textit{et al.}, 2010) and flexible coordination modes involving the N and O donor atoms (Liu \textit{et al.}, 2005; Chang, 2011; Zheng \textit{et al.}, 2011). As has been widely reported in the literature, acylhydrazone complexes display various biological activities such as anti-microbial (Yang \textit{et al.}, 2020), anti-tubercular (Peng, 2011), anti-cancer (Morgan \textit{et al.}, 2003) and anti-oxidant (Chang \textit{et al.}, 2015). As an extension of work into the structural characterization of aroylhydrazone complexes, the title complex, \([\text{Ni}(\text{C}_{16}\text{H}_{13}\text{ClN}_{2}\text{O}_{3})(\text{C}_{3}\text{H}_{4}\text{N}_{2})]\), 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 \(N'-(1E)-1-(5\text{-chloro-2-hydroxyphenyl})\text{ethylidene}-4\text{-methoxybenzohydrazide}\) ligand and one N atom from the imidazole molecule.
Jian-Guo Chang / C15
IUCrData (2022). 7, x220295

Table 1
Selected geometric parameters (Å, °).

| Bond | Distance (Å) | Angle (°) |
|------|--------------|-----------|
| 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···O2i | 0.92 (4) | 1.93 (4) | 2.818 (3) | 161 (3) |
| C8—H8···Cl1ii | 0.96 | 2.86 | 3.700 (3) | 147 |

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

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

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

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 41 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’-[(1E)-1-(5-chloro-2-hydroxyphenyl)ethyldene]-4-methoxybenzohydrazide (0.100 mmol, 0.0319 g), 1H-imidazole (0.100 mmol, 0.0068 g), Ni(NO3)2·6H2O (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%).
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., 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. E67, m1886.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, A. H. (2009). J. Appl. Cryst. 42, 339–341.
Liu, M.-L., Dou, J.-M., Wang, D.-Q. & Li, D.-C. (2005). Acta Cryst. E61, 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. (2015a). Acta Cryst. A71, 3–8.
Sheldrick, G. M. (2015b). Acta Cryst. C71, 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. E67, m978.
IUCrData (2022). 7, x220295  [https://doi.org/10.1107/S2414314622002954]

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

Jian-Guo Chang

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

Crystal data

\[\text{Ni(C}_16\text{H}_{13}\text{ClN}_2\text{O}_3)(\text{C}_3\text{H}_4\text{N}_2)\]

Mr = 443.52

Tetragonal, \(I\ 4_1/a\)

\(a = 30.879 (4) \text{ Å}\)

\(c = 8.0750 (16) \text{ Å}\)

\(V = 7700 (3) \text{ Å}^3\)

\(Z = 16\)

\(F(000) = 3648\)

Data collection

Bruker APEXII CCD area detector diffractometer

Graphite monochromator

phi and \(\omega\) scans

Absorption correction: multi-scan

(SADABS; Bruker, 2003)

\(T_{\text{min}} = 0.735, T_{\text{max}} = 0.860\)

23938 measured reflections

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 independent 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

\(w = 1/\left[\sigma^2(F_o^2) + (0.0616P)^2\right]\)

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

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

\(\Delta\rho_{\text{max}} = 0.79\ \text{e} \text{ Å}^{-3}\)

\(\Delta\rho_{\text{min}} = -0.20\ \text{e} \text{ Å}^{-3}\)

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         | Uiso* or Ueq |
|-----|-----------|-----------|-----------|-------------|
| 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  | 0.59050 (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)

|       | U¹¹  | U¹²  | U¹³  | U²²  | U²³  | U³³  |
|-------|------|------|------|------|------|------|
| Ni1   | 0.03354 (15) | 0.03200 (15) | 0.04649 (18) | 0.00236 (10) | −0.00014 (11) | −0.000031 (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) | 0.037 (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 (10) | −0.0046 (9) | 0.0007 (9) |
| C2    | 0.0489 (12) | 0.0433 (12) | 0.0484 (13) | 0.0082 (10) | −0.0056 (10) | 0.0022 (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) | 0.0002 (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, °)

|       | Ni1—O1  | 1.8995 (15) | C5—H5      | 0.9300 |
|-------|---------|-------------|------------|--------|
| Ni1—O2 | 1.8820 (15) | 1.400 (3) | C5—C6      | 1.507 (3) |
| Ni1—N2 | 1.9344 (17) | 0.9600 |
| Ni1—N3 | 1.9664 (18) | 0.9600 |
| C11—C3 | 1.750 (2) | 0.9600 |
| O1—C9 | 1.296 (2) | 0.9600 |
| O2—C6 | 1.329 (2) | 1.481 (3) |
| O3—C13 | 1.367 (3) | 1.392 (3) |
| O3—C16 | 1.426 (3) | 1.392 (3) |
| N1—N2 | 1.399 (2) | 0.9300 |
| N1—C9 | 1.310 (3) | 1.381 (3) |
| N2—C7 | 1.304 (3) | 0.9300 |
| N3—C17 | 1.374 (3) | 1.381 (3) |
| N3—C19 | 1.320 (3) | 1.381 (3) |
| Bond          | Distance (Å) | Bond          | Distance (Å) |
|---------------|--------------|---------------|--------------|
| 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—C11     | 119.64 (17)  | C14—C15—H15   | 119.0        |
| C2—C3—C4      | 121.6 (2)    | O3—C16—H16A   | 109.5        |
| C4—C3—C11     | 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

N1i—O1—C9—N1 −0.8 (3) C2—C1—C7—C8 −1.5 (3)
N1i—O1—C9—C10 177.82 (14) C2—C3—C4—C5 1.0 (3)
N1i—O2—C6—C1 −6.1 (3) C3—C4—C5—C6 0.0 (3)
N1i—O2—C6—C5 172.09 (15) C4—C5—C6—O2 −179.5 (2)
N1i—N2—C7—C1 9.6 (3) C4—C5—C6—C1 −1.2 (3)
N1i—N2—C7—C8 −170.21 (18) C6—C1—C2—C3 −0.4 (3)
N1i—N3—C17—C18 177.28 (18) C6—C1—C7—N2 −1.1 (3)
N1i—N3—C19—N4 −177.80 (17) C6—C1—C7—C8 178.7 (2)
N1—N2—C7—C1 −176.82 (18) C9—N1—N2—Ni1 −173.69 (19)
N1—N2—C7—C8 3.4 (3) C9—N1—N2—C7 0.9 (3)
N1—C9—C10—C11 −1.4 (3) C9—N1—N2—C7 −173.69 (19)
N1—C9—C10—C15 178.2 (2) C9—N1—N2—Ni1 178.4 (2)
N2—N1i—O1—C9 0.95 (14) C9—C10—C11—C12 178.4 (2)
N2—Ni1—O2—C6 10.33 (18) C9—C10—C11—C12 178.4 (2)
N2—N1—C9—O1 0.0 (3) C10—C11—C12—C13 12.4 (4)
N2—N1—C9—C10 −178.63 (17) C10—C11—C12—C13 −1.0 (4)
N3—N1i—O1—C9 −179.41 (15) C11—C10—C11—C12 −1.0 (4)
N3—Ni1—O2—C6 −170.01 (17) C11—C10—C11—C12 1.1 (3)
N3—C17—C18—N4 0.3 (3) C11—C10—C11—C12 1.1 (3)
C1—C2—C3—C11 −178.99 (17) C16—O3—C13—C12 −175.6 (3)
C1—C2—C3—C4 −0.8 (4) C16—O3—C13—C12 5.3 (4)
C2—C1—C6—O2 179.5 (2) C17—N3—C19—N4 −0.1 (3)
C2—C1—C6—C5 1.3 (3) C18—N4—C19—N3 0.3 (3)
C2—C1—C7—N2 178.7 (2) C19—N3—C17—C18 −0.2 (3)

Hydrogen-bond geometry (Å, °)

| D—H···A    | D···A | H···A | D···A | D—H···A |
|------------|-------|-------|-------|--------|
| N4—H4···O2i | 0.92 (4) | 1.93 (4) | 2.818 (3) | 161 (3) |
| C8—H8A···C11ii | 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.