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# Bis{4-chloro-2-[(2-hydroxyethyl)iminomethyl]phenolato}nickel(II) monohydrate

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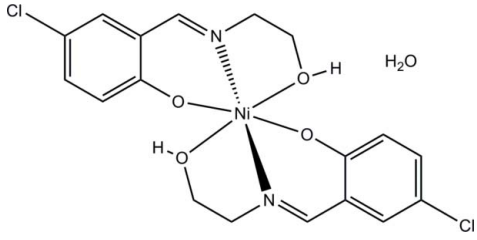
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.039; $wR$ factor = 0.076; data-to-parameter ratio = 16.3.

The title mononuclear nickel(II) complex, $[Ni(C_9H_9ClNO_2)_2]\cdot H_2O$, was obtained by the reaction of 5-chlorosalicylaldehyde, 2-aminoethanol and nickel nitrate in methanol. The Ni atom is six-coordinated by two phenolate O, two imine N and two hydroxy O atoms from two crystallographically different Schiff base ligands, forming an octahedral geometry. In the crystal, molecules are linked through intermolecular O—H···O and O—H···Cl hydrogen bonds.

## Related literature

For our investigations of urease inhibitors, see: Wang (2009); Wang & Ye (2011). For similar nickel(II) complexes, see: Arıcı *et al.* (2005); Liu *et al.* (2006); Li & Wang (2007); Ali *et al.* (2006).




## Experimental

### Crystal data

$[Ni(C_9H_9ClNO_2)_2]\cdot H_2O$
$M_r$ = 473.97
Orthorhombic, $P2_12_12_1$
$a$ = 9.846 (1) Å
$b$ = 12.646 (2) Å
$c$ = 16.006 (2) Å
$V$ = 1992.9 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.27 mm$^{-1}$
$T$ = 298 K
0.30 × 0.27 × 0.27 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.701, $T_{max}$ = 0.725
11691 measured reflections
4328 independent reflections
3147 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.048

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.076
$S$ = 1.04
4328 reflections
265 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.35 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.39 e Å$^{-3}$
Absolute structure: Flack (1983), 1855 Friedel pairs
Flack parameter: 0.015 (15)

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Ni1—N2 | 1.996 (3) | Ni1—O1 | 2.015 (2) |
| Ni1—N1 | 2.000 (3) | Ni1—O2 | 2.131 (2) |
| Ni1—O3 | 2.011 (2) | Ni1—O4 | 2.160 (3) |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O5—H5*B*···O1$^{i}$ | 0.86 (1) | 2.00 (2) | 2.846 (4) | 167 (4) |
| O4—H4···O5$^{ii}$ | 0.85 (1) | 1.97 (2) | 2.798 (4) | 165 (4) |
| O2—H2···O3$^{iii}$ | 0.85 (1) | 1.87 (2) | 2.699 (3) | 165 (4) |
| O5—H5*A*···Cl2 | 0.84 (1) | 2.73 (2) | 3.542 (4) | 163 (4) |

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2456).

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# supplementary materials

*Acta Cryst.* (2011). E**67**, m1229 [ **doi:10.1107/S1600536811031680** ]

# Bis{4-chloro-2-[(2-hydroxyethyl)iminomethyl]phenolato}nickel(II) monohydrate

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## Comment

As part of our investigations into novel urease inhibitors (Wang & Ye, 2011; Wang, 2009), we have synthesized the title compound, a new mononuclear nickel(II) complex, Fig. 1. The compound contains a mononuclear nickel(II) complex molecule and a water molecule of crystallization. The Ni atom in the complex is six-coordinated by two phenolate O, two imine N, and two hydroxy O atoms from two Schiff base ligands, forming an octahedral geometry. The *trans* angles at the Ni atom are in the range 172.5 (1)–174.1 (1)°; the other angles are close to 90°, ranging from 80.1 (1) to 94.9 (1)°, indicating a slightly distorted octahedral coordination. The Ni–O and Ni–N bond lengths (Table 1) are typical and are comparable with those observed in other similar nickel(II) complexes (Arıcı *et al.*, 2005; Liu *et al.*, 2006; Li & Wang, 2007; Ali *et al.*, 2006).

In the crystal structure of the compound, molecules are linked through intermolecular O—H···O and O—H···Cl hydrogen bonds (Table 2), to form a three-dimensional network (Fig. 2).

## Experimental

5-Chlorosalicylaldehyde (1.0 mmol, 0.157 g), 2-aminoethanol (1.0 mmol, 0.061 g), and nickel nitrate hexahydrate (0.5 mmol, 0.146 g) were dissolved in MeOH (30 ml). The mixture was stirred at room temperature for 10 min to give a clear green solution. After keeping the solution in air for a week, green block-shaped crystals were formed at the bottom of the vessel.

## Refinement

The water and hydroxy H atoms were located from a difference Fourier map and refined isotropically, with O—H and H···H distances restrained to 0.85 (1) and 1.37 (2) Å, respectively. Their isotropic displacement parameters were fixed at 0.08 Å$^2$). The remaining H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with $U_{iso}$(H) set at 1.2$U_{eq}$(C and O).

## Figures

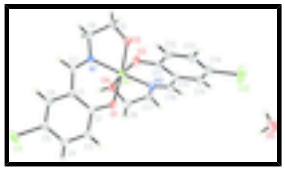

Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

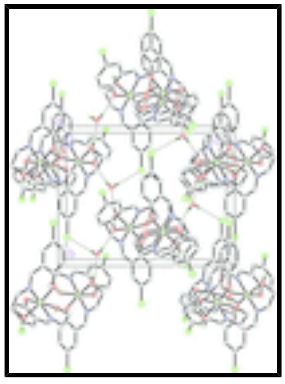

Fig. 2. The molecular packing of the title compound, viewed along the *a* axis. Intermolecular hydrogen bonds are shown as dashed lines.

**Bis{4-chloro-2-[(2-hydroxyethyl)iminomethyl]phenolato}nickel(II) monohydrate**

*Crystal data*

| | |
|---|---|
| $[Ni(C_9H_9ClNO_2)_2]\cdot H_2O$ | $D_x = 1.580$ Mg m$^{-3}$ |
| $M_r = 473.97$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Orthorhombic, $P2_12_12_1$ | Cell parameters from 2792 reflections |
| $a = 9.846$ (1) Å | $\theta = 2.4$–$24.5°$ |
| $b = 12.646$ (2) Å | $\mu = 1.27$ mm$^{-1}$ |
| $c = 16.006$ (2) Å | $T = 298$ K |
| $V = 1992.9$ (4) Å$^3$ | Block, green |
| $Z = 4$ | 0.30 × 0.27 × 0.27 mm |
| $F(000) = 976$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 4328 independent reflections |
| Radiation source: fine-focus sealed tube | 3147 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.048$ |
| ω scans | $\theta_{max} = 27.0°$, $\theta_{min} = 2.4°$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $h = -12\rightarrow12$ |
| $T_{min} = 0.701$, $T_{max} = 0.725$ | $k = -14\rightarrow16$ |
| 11691 measured reflections | $l = -20\rightarrow14$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.039$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.076$ | $w = 1/[\sigma^2(F_o^2) + (0.0206P)^2 + 0.1322P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.04$ | $(\Delta/\sigma)_{max} < 0.001$ |

| | |
|---|---|
| 4328 reflections | $\Delta\rho_{max}$ = 0.35 e Å$^{-3}$ |
| 265 parameters | $\Delta\rho_{min}$ = −0.39 e Å$^{-3}$ |
| 5 restraints | Absolute structure: Flack (1983), 1855 Friedel pairs |
| Primary atom site location: structure-invariant direct methods | Flack parameter: 0.015 (15) |

*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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Ni1 | 0.53364 (4) | 0.24034 (3) | 0.09823 (3) | 0.03031 (12) |
| Cl1 | −0.07950 (10) | −0.02347 (9) | 0.24602 (7) | 0.0569 (3) |
| Cl2 | 0.4617 (2) | 0.80769 (9) | 0.02875 (10) | 0.1053 (6) |
| N1 | 0.4422 (3) | 0.1170 (2) | 0.04386 (17) | 0.0293 (7) |
| N2 | 0.6463 (3) | 0.3534 (2) | 0.15079 (19) | 0.0331 (7) |
| O1 | 0.3912 (2) | 0.2511 (2) | 0.18821 (14) | 0.0396 (6) |
| O2 | 0.6727 (2) | 0.21542 (19) | −0.00183 (15) | 0.0351 (6) |
| H2 | 0.7545 (17) | 0.195 (3) | 0.000 (3) | 0.080* |
| O3 | 0.4326 (2) | 0.34479 (18) | 0.02676 (15) | 0.0353 (6) |
| O4 | 0.6595 (3) | 0.1451 (2) | 0.17926 (17) | 0.0427 (7) |
| H4 | 0.634 (4) | 0.0850 (18) | 0.198 (3) | 0.080* |
| O5 | 0.5861 (4) | 0.9351 (2) | 0.2104 (2) | 0.0666 (9) |
| H5A | 0.575 (5) | 0.905 (3) | 0.1640 (12) | 0.080* |
| H5B | 0.601 (4) | 0.886 (2) | 0.2461 (17) | 0.080* |
| C1 | 0.2544 (3) | 0.1029 (3) | 0.1421 (2) | 0.0285 (8) |
| C2 | 0.2870 (3) | 0.1881 (3) | 0.1969 (2) | 0.0312 (9) |
| C3 | 0.1979 (3) | 0.2045 (3) | 0.2648 (2) | 0.0369 (9) |
| H3 | 0.2154 | 0.2602 | 0.3012 | 0.044* |
| C4 | 0.0863 (4) | 0.1416 (3) | 0.2794 (2) | 0.0385 (9) |
| H4A | 0.0302 | 0.1547 | 0.3250 | 0.046* |
| C5 | 0.0581 (3) | 0.0591 (3) | 0.2259 (2) | 0.0377 (10) |
| C6 | 0.1391 (3) | 0.0405 (3) | 0.1584 (2) | 0.0353 (9) |
| H6 | 0.1177 | −0.0147 | 0.1223 | 0.042* |
| C7 | 0.3306 (3) | 0.0749 (3) | 0.0684 (2) | 0.0317 (9) |
| H7 | 0.2953 | 0.0210 | 0.0354 | 0.038* |
| C8 | 0.5114 (3) | 0.0774 (3) | −0.0304 (2) | 0.0376 (9) |
| H8A | 0.4449 | 0.0547 | −0.0714 | 0.045* |

| | | | | |
|---|---|---|---|---|
| H8B | 0.5671 | 0.0170 | −0.0157 | 0.045* |
| C9 | 0.6000 (4) | 0.1642 (3) | −0.0674 (2) | 0.0409 (10) |
| H9A | 0.6634 | 0.1339 | −0.1071 | 0.049* |
| H9B | 0.5438 | 0.2152 | −0.0966 | 0.049* |
| C10 | 0.5384 (4) | 0.5021 (3) | 0.0821 (2) | 0.0361 (9) |
| C11 | 0.4462 (3) | 0.4476 (3) | 0.0297 (2) | 0.0322 (9) |
| C12 | 0.3640 (4) | 0.5102 (3) | −0.0228 (2) | 0.0398 (10) |
| H12 | 0.3043 | 0.4765 | −0.0592 | 0.048* |
| C13 | 0.3680 (4) | 0.6183 (3) | −0.0226 (3) | 0.0486 (11) |
| H13 | 0.3114 | 0.6569 | −0.0578 | 0.058* |
| C14 | 0.4562 (6) | 0.6693 (3) | 0.0297 (3) | 0.0550 (12) |
| C15 | 0.5406 (4) | 0.6136 (3) | 0.0800 (2) | 0.0512 (11) |
| H15 | 0.6014 | 0.6498 | 0.1141 | 0.061* |
| C16 | 0.6327 (4) | 0.4522 (3) | 0.1399 (2) | 0.0395 (10) |
| H16 | 0.6877 | 0.4966 | 0.1715 | 0.047* |
| C17 | 0.7482 (4) | 0.3129 (3) | 0.2095 (3) | 0.0476 (12) |
| H17A | 0.7642 | 0.3645 | 0.2532 | 0.057* |
| H17B | 0.8331 | 0.3006 | 0.1804 | 0.057* |
| C18 | 0.6985 (4) | 0.2117 (3) | 0.2472 (3) | 0.0497 (11) |
| H18A | 0.7699 | 0.1785 | 0.2797 | 0.060* |
| H18B | 0.6215 | 0.2250 | 0.2835 | 0.060* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ni1 | 0.02362 (18) | 0.0263 (2) | 0.0410 (3) | −0.0021 (2) | −0.0013 (2) | −0.0026 (2) |
| Cl1 | 0.0378 (6) | 0.0680 (7) | 0.0648 (8) | −0.0153 (5) | 0.0081 (6) | 0.0168 (6) |
| Cl2 | 0.1734 (16) | 0.0291 (6) | 0.1135 (12) | −0.0054 (9) | −0.0607 (13) | 0.0109 (6) |
| N1 | 0.0269 (17) | 0.0244 (15) | 0.0367 (18) | 0.0013 (13) | 0.0017 (14) | −0.0003 (14) |
| N2 | 0.0255 (16) | 0.0317 (18) | 0.042 (2) | −0.0035 (14) | −0.0052 (14) | 0.0019 (15) |
| O1 | 0.0363 (12) | 0.0363 (14) | 0.0463 (15) | −0.0070 (13) | 0.0054 (11) | −0.0114 (15) |
| O2 | 0.0233 (11) | 0.0422 (16) | 0.0398 (15) | −0.0034 (11) | 0.0018 (12) | −0.0067 (12) |
| O3 | 0.0255 (14) | 0.0290 (13) | 0.0513 (17) | −0.0018 (11) | −0.0073 (12) | −0.0043 (12) |
| O4 | 0.0506 (18) | 0.0326 (15) | 0.0449 (18) | −0.0009 (14) | −0.0107 (15) | 0.0006 (14) |
| O5 | 0.079 (2) | 0.0501 (19) | 0.071 (2) | −0.0112 (18) | −0.004 (2) | 0.0169 (16) |
| C1 | 0.0223 (17) | 0.028 (2) | 0.035 (2) | −0.0022 (15) | −0.0032 (16) | 0.0050 (16) |
| C2 | 0.0274 (19) | 0.030 (2) | 0.036 (2) | −0.0001 (16) | −0.0022 (17) | 0.0039 (17) |
| C3 | 0.0323 (19) | 0.038 (2) | 0.041 (3) | 0.0041 (16) | −0.0019 (18) | −0.0024 (18) |
| C4 | 0.0312 (19) | 0.049 (2) | 0.035 (2) | 0.0061 (19) | 0.0062 (17) | 0.008 (2) |
| C5 | 0.024 (2) | 0.042 (2) | 0.047 (3) | −0.0032 (17) | −0.0015 (18) | 0.0138 (19) |
| C6 | 0.0302 (19) | 0.038 (2) | 0.037 (2) | −0.0020 (17) | −0.0038 (18) | 0.0033 (19) |
| C7 | 0.0293 (19) | 0.0265 (19) | 0.039 (2) | −0.0040 (16) | −0.0037 (17) | 0.0002 (16) |
| C8 | 0.033 (2) | 0.041 (2) | 0.039 (2) | −0.0057 (17) | 0.0062 (17) | −0.0090 (17) |
| C9 | 0.036 (2) | 0.047 (2) | 0.039 (2) | −0.0118 (18) | 0.0011 (18) | −0.0060 (19) |
| C10 | 0.0386 (19) | 0.0278 (18) | 0.042 (2) | −0.0028 (18) | −0.003 (2) | 0.0008 (16) |
| C11 | 0.026 (2) | 0.032 (2) | 0.039 (2) | −0.0033 (16) | 0.0021 (17) | −0.0031 (17) |
| C12 | 0.036 (2) | 0.037 (2) | 0.046 (3) | −0.0033 (18) | −0.0059 (18) | 0.003 (2) |
| C13 | 0.057 (3) | 0.040 (2) | 0.049 (3) | 0.005 (2) | −0.010 (2) | 0.010 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C14 | 0.086 (3) | 0.026 (2) | 0.053 (3) | −0.003 (2) | −0.006 (3) | 0.0055 (19) |
| C15 | 0.068 (3) | 0.033 (2) | 0.053 (3) | −0.009 (2) | −0.016 (3) | −0.0025 (19) |
| C16 | 0.034 (2) | 0.031 (2) | 0.054 (3) | −0.0088 (17) | −0.0082 (18) | −0.0051 (19) |
| C17 | 0.039 (2) | 0.043 (2) | 0.060 (3) | −0.006 (2) | −0.021 (2) | −0.005 (2) |
| C18 | 0.052 (2) | 0.043 (3) | 0.055 (3) | 0.0039 (19) | −0.019 (2) | 0.002 (2) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Ni1—N2 | 1.996 (3) | C4—C5 | 1.377 (5) |
| Ni1—N1 | 2.000 (3) | C4—H4A | 0.9300 |
| Ni1—O3 | 2.011 (2) | C5—C6 | 1.363 (5) |
| Ni1—O1 | 2.015 (2) | C6—H6 | 0.9300 |
| Ni1—O2 | 2.131 (2) | C7—H7 | 0.9300 |
| Ni1—O4 | 2.160 (3) | C8—C9 | 1.522 (5) |
| Cl1—C5 | 1.741 (3) | C8—H8A | 0.9700 |
| Cl2—C14 | 1.751 (4) | C8—H8B | 0.9700 |
| N1—C7 | 1.283 (4) | C9—H9A | 0.9700 |
| N1—C8 | 1.458 (4) | C9—H9B | 0.9700 |
| N2—C16 | 1.269 (4) | C10—C15 | 1.410 (5) |
| N2—C17 | 1.467 (4) | C10—C11 | 1.415 (5) |
| O1—C2 | 1.307 (4) | C10—C16 | 1.454 (5) |
| O2—C9 | 1.425 (4) | C11—C12 | 1.410 (5) |
| O2—H2 | 0.847 (10) | C12—C13 | 1.368 (5) |
| O3—C11 | 1.308 (4) | C12—H12 | 0.9300 |
| O4—C18 | 1.428 (4) | C13—C14 | 1.367 (5) |
| O4—H4 | 0.852 (10) | C13—H13 | 0.9300 |
| O5—H5B | 0.860 (10) | C14—C15 | 1.355 (5) |
| O5—H5A | 0.844 (10) | C15—H15 | 0.9300 |
| C1—C6 | 1.407 (4) | C16—H16 | 0.9300 |
| C1—C2 | 1.426 (5) | C17—C18 | 1.497 (5) |
| C1—C7 | 1.442 (5) | C17—H17A | 0.9700 |
| C2—C3 | 1.412 (5) | C17—H17B | 0.9700 |
| C3—C4 | 1.377 (5) | C18—H18A | 0.9700 |
| C3—H3 | 0.9300 | C18—H18B | 0.9700 |
| N2—Ni1—N1 | 172.89 (12) | N1—C7—C1 | 126.4 (3) |
| N2—Ni1—O3 | 92.54 (11) | N1—C7—H7 | 116.8 |
| N1—Ni1—O3 | 92.40 (10) | C1—C7—H7 | 116.8 |
| N2—Ni1—O1 | 92.13 (11) | N1—C8—C9 | 109.7 (3) |
| N1—Ni1—O1 | 92.89 (10) | N1—C8—H8A | 109.7 |
| O3—Ni1—O1 | 91.03 (10) | C9—C8—H8A | 109.7 |
| N2—Ni1—O2 | 93.76 (11) | N1—C8—H8B | 109.7 |
| N1—Ni1—O2 | 81.20 (10) | C9—C8—H8B | 109.7 |
| O3—Ni1—O2 | 89.28 (10) | H8A—C8—H8B | 108.2 |
| O1—Ni1—O2 | 174.08 (10) | O2—C9—C8 | 109.2 (3) |
| N2—Ni1—O4 | 80.06 (11) | O2—C9—H9A | 109.8 |
| N1—Ni1—O4 | 94.87 (11) | C8—C9—H9A | 109.8 |
| O3—Ni1—O4 | 172.50 (10) | O2—C9—H9B | 109.8 |
| O1—Ni1—O4 | 90.43 (10) | C8—C9—H9B | 109.8 |
| O2—Ni1—O4 | 90.02 (10) | H9A—C9—H9B | 108.3 |

| | | | |
|---|---|---|---|
| C7—N1—C8 | 120.4 (3) | C15—C10—C11 | 118.9 (3) |
| C7—N1—Ni1 | 125.2 (3) | C15—C10—C16 | 116.0 (3) |
| C8—N1—Ni1 | 114.3 (2) | C11—C10—C16 | 125.1 (3) |
| C16—N2—C17 | 120.3 (3) | O3—C11—C12 | 118.5 (3) |
| C16—N2—Ni1 | 126.0 (3) | O3—C11—C10 | 124.8 (3) |
| C17—N2—Ni1 | 113.6 (2) | C12—C11—C10 | 116.7 (3) |
| C2—O1—Ni1 | 125.6 (2) | C13—C12—C11 | 122.9 (4) |
| C9—O2—Ni1 | 107.31 (19) | C13—C12—H12 | 118.6 |
| C9—O2—H2 | 111 (3) | C11—C12—H12 | 118.6 |
| Ni1—O2—H2 | 129 (3) | C14—C13—C12 | 119.4 (4) |
| C11—O3—Ni1 | 125.6 (2) | C14—C13—H13 | 120.3 |
| C18—O4—Ni1 | 106.4 (2) | C12—C13—H13 | 120.3 |
| C18—O4—H4 | 110 (3) | C15—C14—C13 | 120.6 (4) |
| Ni1—O4—H4 | 123 (3) | C15—C14—Cl2 | 120.4 (4) |
| H5B—O5—H5A | 106 (2) | C13—C14—Cl2 | 119.0 (4) |
| C6—C1—C2 | 119.4 (3) | C14—C15—C10 | 121.6 (4) |
| C6—C1—C7 | 115.7 (3) | C14—C15—H15 | 119.2 |
| C2—C1—C7 | 124.9 (3) | C10—C15—H15 | 119.2 |
| O1—C2—C3 | 118.7 (3) | N2—C16—C10 | 125.6 (3) |
| O1—C2—C1 | 124.9 (3) | N2—C16—H16 | 117.2 |
| C3—C2—C1 | 116.4 (3) | C10—C16—H16 | 117.2 |
| C4—C3—C2 | 122.8 (3) | N2—C17—C18 | 109.5 (3) |
| C4—C3—H3 | 118.6 | N2—C17—H17A | 109.8 |
| C2—C3—H3 | 118.6 | C18—C17—H17A | 109.8 |
| C3—C4—C5 | 119.5 (4) | N2—C17—H17B | 109.8 |
| C3—C4—H4A | 120.2 | C18—C17—H17B | 109.8 |
| C5—C4—H4A | 120.2 | H17A—C17—H17B | 108.2 |
| C6—C5—C4 | 120.4 (3) | O4—C18—C17 | 106.6 (3) |
| C6—C5—Cl1 | 119.9 (3) | O4—C18—H18A | 110.4 |
| C4—C5—Cl1 | 119.8 (3) | C17—C18—H18A | 110.4 |
| C5—C6—C1 | 121.5 (3) | O4—C18—H18B | 110.4 |
| C5—C6—H6 | 119.3 | C17—C18—H18B | 110.4 |
| C1—C6—H6 | 119.3 | H18A—C18—H18B | 108.6 |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O5—H5B···O1$^{i}$ | 0.86 (1) | 2.00 (2) | 2.846 (4) | 167 (4) |
| O4—H4···O5$^{ii}$ | 0.85 (1) | 1.97 (2) | 2.798 (4) | 165 (4) |
| O2—H2···O3$^{iii}$ | 0.85 (1) | 1.87 (2) | 2.699 (3) | 165 (4) |
| O5—H5A···Cl2 | 0.84 (1) | 2.73 (2) | 3.542 (4) | 163 (4) |

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

**Fig. 1**

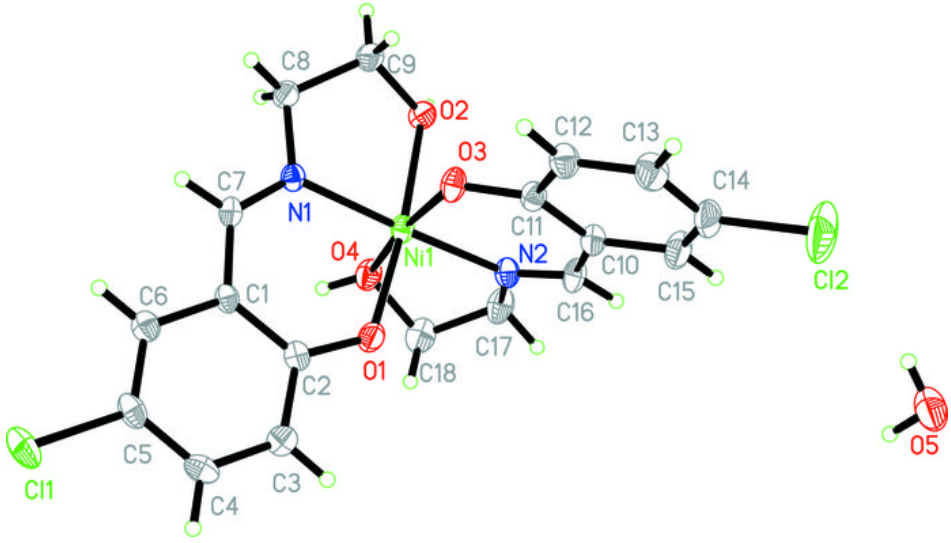
C8
C9
O2
C12
C13
O3
C7
N1
C14
C11
Ni1
N2
C10
Cl2
O4
C15
C6
C1
C16
C17
O1
C18
C2
O5
C5
C3
Cl1
C4

**Fig. 2**