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# Diaquabis{2,4-dibromo-6-[2-(isopropylammonio)ethyliminomethyl]phenolato}nickel(II) dichloride hemihydrate

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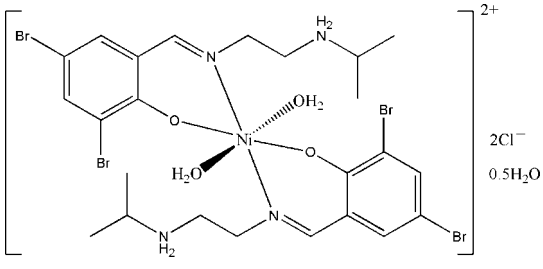
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.009 Å; disorder in solvent or counterion; $R$ factor = 0.050; $wR$ factor = 0.126; data-to-parameter ratio = 15.7.

The title complex, $[Ni(C_{12}H_{16}Br_2N_2O_2)_2(H_2O)_2]Cl_2\cdot 0.5H_2O$, consists of a centrosymmetric mononuclear nickel(II) complex cation, two symmetry-related chloride anions and a half-occupancy water molecule. The Ni atom, lying on an inversion centre, is six-coordinated by two phenol O atoms, two imine N atoms from two Schiff base ligands, and the O atoms from two water molecules, forming an octahedral geometry. Adjacent molecules are linked through intermolecular hydrogen bonds, forming chains running along the $b$ axis.

## Related literature

For related literature, see: Angulo *et al.* (2001); Dey *et al.* (2004); Diao (2007); Diao *et al.* (2007); Edison *et al.* (2004); Liu *et al.* (2006); Ramadevi *et al.* (2005); Suh *et al.* (1996); Tang (2006); Zhang (2006); Zhu *et al.* (2004).




## Experimental

### Crystal data

$[Ni(C_{12}H_{16}Br_2N_2O_2)_2(H_2O)_2]Cl_2\cdot 0.5H_2O$
$M_r$ = 902.83
Monoclinic, $P2_1/c$
$a$ = 12.685 (3) Å
$b$ = 7.0450 (14) Å
$c$ = 17.501 (4) Å
$\beta$ = 106.57 (3)°
$V$ = 1499.0 (6) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 6.20 mm$^{-1}$
$T$ = 293 (2) K
0.23 × 0.22 × 0.20 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.330, $T_{max}$ = 0.370
(expected range = 0.258–0.290)
11682 measured reflections
3094 independent reflections
1968 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.073

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.126
$S$ = 1.01
3094 reflections
197 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.70 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.76 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2$A$···Cl1$^{i}$ | 0.90 | 2.19 | 3.027 (5) | 154 |
| N2—H2$A$···O2$^{ii}$ | 0.90 | 2.60 | 3.155 (7) | 121 |
| N2—H2$B$···O1$^{ii}$ | 0.90 | 1.74 | 2.620 (6) | 166 |
| N2—H2$B$···Br1$^{ii}$ | 0.90 | 2.87 | 3.368 (5) | 117 |
| O2—H2$C$···Cl1$^{ii}$ | 0.84 (7) | 2.14 (6) | 2.977 (4) | 174 (9) |
| O2—H2$D$···Cl1$^{iii}$ | 0.85 (6) | 2.19 (4) | 2.989 (5) | 157 (9) |
| O3—H3$A$···O1$^{iv}$ | 0.85 | 2.49 | 3.316 (13) | 163.1 |

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: RZ2166).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, m2785-m2786 [ **doi:10.1107/S1600536807051513** ]

# Diaquabis{2,4-dibromo-6-[2-(isopropylammonio)ethyliminomethyl]phenolato}nickel(II) dichloride hemihydrate

**C.-B. Tang**

## Comment

Nickel(II) complexes play an important role in both bioinorganic chemistry and coordination chemistry (Suh *et al.*, 1996; Angulo *et al.*, 2001; Dey *et al.*, 2004; Edison *et al.*, 2004; Ramadevi *et al.*, 2005). Recently, the author has reported a mononuclear nickel(II) complex derived from the Schiff base ligand 2-bromo-4-chloro-6-[2-(diethylamino)ethyliminomethyl]phenol (Tang, 2006). As a further study of the structures of such complexes, the title mononuclear nickel(II) complex, derived from the Schiff base ligand 2,4-dibromo-6-[(2-isopropylaminoethylimino)methyl]phenol, is reported in this paper.

The title complex consists of a centrosymmetric mononuclear nickel(II) complex cation, two symmetry-related chloride anions, and half water molecule (Fig. 1). The Ni atom, lying on the inversion centre, is six-coordinated by two phenolic oxygen atoms, two imine N atoms from two Schiff base ligands, and by two oxygen atoms from two water molecules, forming an octahedral geometry. The coordinative bond lengths and angles are within normal ranges and comparable with the corresponding values observed in other similar nickel(II) complexes (Zhu *et al.*, 2004; Liu *et al.*, 2006; Zhang, 2006; Diao, 2007; Diao *et al.*, 2007).

In the crystal structure, ajacent molecules are linked through intermolecular N—H···O, N–H···Cl, N—H···Br and O–H···Cl hydrogen bonds, forming chains running along the *b* axis, as shown in Fig. 2.

## Experimental

3,5-Dibromo-2-hydroxybenzaldehyde (0.2 mmol, 56.0 mg) and *N*-isopropyl-1,2-diaminoethane (0.2 mmol, 20.4 mg) were dissolved in methanol (10 ml). To the mixture was added an aqueous solution (1 ml) of nickel(II) chloride hexahydrate (0.1 mmol, 23.8 mg). The final mixture was stirred at room temperature for 30 min, resulting in a green solution. The solution was allowed to stand still in air for a week, yielding green block-shaped crystals of the complex.

## Refinement

H3A, H3B, H2C and H2D were located from a difference Fourier map and refined isotropically, with O—H distances restrained to 0.85 (1) Å, and H···H distance restrained to 1.37 (2) Å. Other H atoms were constrained to ideal geometries, with C—H = 0.93–0.98 Å, N—H = 0.90 Å, and with $U_{iso}$(H) set to 1.2$U_{eq}$(C,*N*) and 1.5$U_{eq}$(methyl C). The lattice water molecule is disordered, with occupancy of 0.25.

## Figures

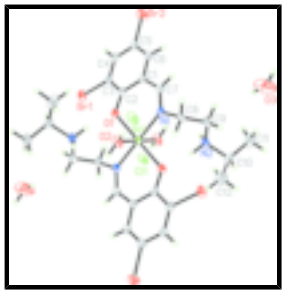

Fig. 1. The structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are at the symmetry position $1-x, 2-y, 1-z$.

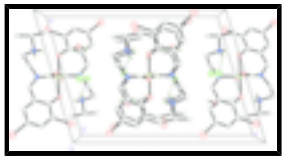

Fig. 2. Packing diagram of the title compound viewed along the *b* axis. Hydrogen atoms not involved in hydrogen bonding interactions (dashed lines) are omitted for clarity.

## Diaquabis{2,4-dibromo-6-[2- (isopropylammonio)ethyliminomethyl]phenolato}nickel(II) dichloride hemihydrate

*Crystal data*

| | |
|---|---|
| $[Ni(C_{12}H_{16}Br_2N_2O_2)_2(H_2O)_2]Cl_2·0.5H_2O$ | $F_{000}$ = 894 |
| $M_r$ = 902.83 | $D_x$ = 2.000 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 1836 reflections |
| $a$ = 12.685 (3) Å | θ = 2.4–24.9º |
| $b$ = 7.0450 (14) Å | μ = 6.20 mm$^{-1}$ |
| $c$ = 17.501 (4) Å | $T$ = 293 (2) K |
| β = 106.57 (3)º | Block, green |
| $V$ = 1499.0 (6) Å$^3$ | 0.23 × 0.22 × 0.20 mm |
| $Z$ = 2 | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 3094 independent reflections |
| Radiation source: fine-focus sealed tube | 1968 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.073 |
| $T$ = 293(2) K | $\theta_{max}$ = 26.5º |
| ω scans | $\theta_{min}$ = 1.7º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h$ = −15→15 |
| $T_{min}$ = 0.330, $T_{max}$ = 0.370 | $k$ = −8→8 |
| 11682 measured reflections | $l$ = −21→21 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.050$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.126$ | $w = 1/[\sigma^2(F_o^2) + (0.0625P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.01$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 3094 reflections | $\Delta\rho_{max} = 0.70$ e Å$^{-3}$ |
| 197 parameters | $\Delta\rho_{min} = -0.75$ e Å$^{-3}$ |
| 6 restraints | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | |

*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 $F^2 > 2$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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Ni1 | 0.5000 | 1.0000 | 0.5000 | 0.0260 (3) | |
| Br1 | 0.12695 (6) | 0.84155 (9) | 0.49949 (4) | 0.0434 (2) | |
| Br2 | 0.05294 (7) | 0.59011 (13) | 0.18878 (5) | 0.0616 (3) | |
| Cl1 | 0.48050 (17) | 0.4909 (2) | 0.63566 (10) | 0.0487 (5) | |
| O1 | 0.3353 (3) | 0.9775 (5) | 0.4683 (2) | 0.0301 (10) | |
| O2 | 0.4839 (4) | 1.2618 (5) | 0.4926 (3) | 0.0423 (12) | |
| N1 | 0.4928 (4) | 0.9890 (6) | 0.3815 (3) | 0.0273 (11) | |
| N2 | 0.6982 (4) | 0.8048 (6) | 0.4195 (3) | 0.0345 (13) | |
| H2A | 0.6499 | 0.7117 | 0.4200 | 0.041* | |
| H2B | 0.6982 | 0.8856 | 0.4593 | 0.041* | |
| C1 | 0.3097 (5) | 0.8639 (7) | 0.3374 (3) | 0.0269 (14) | |
| C2 | 0.2780 (5) | 0.8899 (8) | 0.4081 (4) | 0.0286 (14) | |
| C3 | 0.1762 (5) | 0.8157 (8) | 0.4078 (4) | 0.0320 (15) | |
| C4 | 0.1117 (5) | 0.7276 (8) | 0.3449 (4) | 0.0345 (15) | |
| H4 | 0.0440 | 0.6804 | 0.3467 | 0.041* | |
| C5 | 0.1440 (5) | 0.7056 (8) | 0.2772 (4) | 0.0356 (15) | |

| | | | | | |
|---|---|---|---|---|---|
| C6 | 0.2421 (5) | 0.7774 (9) | 0.2732 (4) | 0.0322 (15) | |
| H6 | 0.264 (5) | 0.741 (9) | 0.232 (4) | 0.040 (19)* | |
| C7 | 0.4103 (5) | 0.9311 (8) | 0.3266 (4) | 0.0317 (15) | |
| H7 | 0.4162 | 0.9326 | 0.2748 | 0.038* | |
| C8 | 0.5861 (5) | 1.0499 (8) | 0.3532 (4) | 0.0313 (15) | |
| H8A | 0.5569 | 1.1118 | 0.3020 | 0.038* | |
| H8B | 0.6274 | 1.1444 | 0.3901 | 0.038* | |
| C9 | 0.6611 (5) | 0.9057 (9) | 0.3444 (4) | 0.0361 (16) | |
| H9A | 0.7232 | 0.9623 | 0.3310 | 0.043* | |
| H9B | 0.6247 | 0.8189 | 0.3021 | 0.043* | |
| C10 | 0.8093 (6) | 0.7205 (9) | 0.4351 (4) | 0.0416 (17) | |
| H10 | 0.8615 | 0.8233 | 0.4353 | 0.050* | |
| C11 | 0.8067 (7) | 0.5971 (10) | 0.3689 (5) | 0.066 (2) | |
| H11A | 0.7412 | 0.5212 | 0.3568 | 0.099* | |
| H11B | 0.8701 | 0.5159 | 0.3826 | 0.099* | |
| H11C | 0.8071 | 0.6722 | 0.3232 | 0.099* | |
| C12 | 0.8337 (7) | 0.6441 (11) | 0.5172 (5) | 0.076 (3) | |
| H12A | 0.7781 | 0.5540 | 0.5198 | 0.114* | |
| H12B | 0.8346 | 0.7462 | 0.5537 | 0.114* | |
| H12C | 0.9042 | 0.5828 | 0.5313 | 0.114* | |
| H2C | 0.496 (8) | 1.325 (10) | 0.455 (3) | 0.114* | |
| H2D | 0.503 (8) | 1.327 (10) | 0.535 (3) | 0.114* | |
| O3 | 0.728 (2) | 0.810 (3) | 0.1714 (8) | 0.146 (14) | 0.25 |
| H3A | 0.7048 | 0.7449 | 0.1289 | 0.219* | 0.25 |
| H3B | 0.7013 | 0.7704 | 0.2079 | 0.219* | 0.25 |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ni1 | 0.0331 (7) | 0.0166 (5) | 0.0314 (6) | −0.0026 (5) | 0.0141 (5) | −0.0012 (4) |
| Br1 | 0.0462 (5) | 0.0374 (4) | 0.0562 (5) | −0.0086 (3) | 0.0300 (4) | −0.0085 (3) |
| Br2 | 0.0564 (6) | 0.0652 (6) | 0.0616 (5) | −0.0223 (4) | 0.0140 (4) | −0.0286 (4) |
| Cl1 | 0.0817 (14) | 0.0268 (8) | 0.0444 (10) | −0.0077 (9) | 0.0289 (10) | −0.0023 (7) |
| O1 | 0.033 (3) | 0.025 (2) | 0.035 (2) | −0.0034 (18) | 0.014 (2) | −0.0050 (19) |
| O2 | 0.073 (3) | 0.015 (2) | 0.047 (3) | −0.004 (2) | 0.028 (3) | 0.003 (2) |
| N1 | 0.034 (3) | 0.014 (2) | 0.038 (3) | 0.001 (2) | 0.016 (3) | −0.001 (2) |
| N2 | 0.041 (3) | 0.020 (3) | 0.047 (3) | −0.001 (2) | 0.019 (3) | −0.008 (2) |
| C1 | 0.035 (4) | 0.015 (3) | 0.030 (3) | −0.002 (2) | 0.007 (3) | 0.000 (2) |
| C2 | 0.032 (4) | 0.018 (3) | 0.039 (4) | 0.001 (3) | 0.015 (3) | 0.003 (3) |
| C3 | 0.035 (4) | 0.021 (3) | 0.043 (4) | 0.002 (3) | 0.017 (3) | 0.000 (3) |
| C4 | 0.031 (4) | 0.025 (3) | 0.049 (4) | −0.004 (3) | 0.014 (3) | 0.000 (3) |
| C5 | 0.035 (4) | 0.024 (3) | 0.048 (4) | −0.004 (3) | 0.012 (3) | −0.008 (3) |
| C6 | 0.040 (4) | 0.026 (3) | 0.033 (4) | 0.001 (3) | 0.014 (3) | 0.001 (3) |
| C7 | 0.043 (4) | 0.021 (3) | 0.033 (4) | −0.001 (3) | 0.014 (3) | 0.001 (3) |
| C8 | 0.041 (4) | 0.018 (3) | 0.041 (4) | −0.001 (3) | 0.022 (3) | 0.002 (3) |
| C9 | 0.048 (4) | 0.031 (3) | 0.036 (4) | −0.004 (3) | 0.022 (3) | −0.001 (3) |
| C10 | 0.037 (4) | 0.025 (3) | 0.062 (5) | 0.000 (3) | 0.013 (4) | −0.003 (3) |
| C11 | 0.068 (6) | 0.037 (4) | 0.099 (7) | 0.005 (4) | 0.034 (5) | −0.022 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C12 | 0.080 (7) | 0.042 (5) | 0.098 (7) | 0.028 (4) | 0.012 (6) | 0.014 (5) |
| O3 | 0.19 (4) | 0.15 (3) | 0.07 (2) | 0.00 (3) | −0.02 (2) | 0.00 (2) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Ni1—O2$^{i}$ | 1.856 (4) | C4—C5 | 1.368 (8) |
| Ni1—O2 | 1.856 (4) | C4—H4 | 0.9300 |
| Ni1—O1$^{i}$ | 2.009 (4) | C5—C6 | 1.363 (8) |
| Ni1—O1 | 2.009 (4) | C6—H6 | 0.88 (6) |
| Ni1—N1$^{i}$ | 2.052 (5) | C7—H7 | 0.9300 |
| Ni1—N1 | 2.052 (5) | C8—C9 | 1.430 (8) |
| Br1—C3 | 1.890 (6) | C8—H8A | 0.9700 |
| Br2—C5 | 1.836 (6) | C8—H8B | 0.9700 |
| O1—C2 | 1.258 (7) | C9—H9A | 0.9700 |
| O2—H2C | 0.84 (7) | C9—H9B | 0.9700 |
| O2—H2D | 0.85 (6) | C10—C11 | 1.442 (9) |
| N1—C7 | 1.269 (7) | C10—C12 | 1.482 (10) |
| N1—C8 | 1.471 (7) | C10—H10 | 0.9800 |
| N2—C9 | 1.449 (8) | C11—H11A | 0.9600 |
| N2—C10 | 1.481 (8) | C11—H11B | 0.9600 |
| N2—H2A | 0.9000 | C11—H11C | 0.9600 |
| N2—H2B | 0.9000 | C12—H12A | 0.9600 |
| C1—C6 | 1.348 (8) | C12—H12B | 0.9600 |
| C1—C2 | 1.419 (8) | C12—H12C | 0.9600 |
| C1—C7 | 1.423 (8) | O3—H3A | 0.8524 |
| C2—C3 | 1.392 (8) | O3—H3B | 0.8518 |
| C3—C4 | 1.323 (8) | | |
| O2$^{i}$—Ni1—O2 | 180.000 (1) | C6—C5—C4 | 120.3 (6) |
| O2$^{i}$—Ni1—O1$^{i}$ | 88.52 (19) | C6—C5—Br2 | 119.1 (5) |
| O2—Ni1—O1$^{i}$ | 91.48 (19) | C4—C5—Br2 | 120.5 (5) |
| O2$^{i}$—Ni1—O1 | 91.48 (19) | C1—C6—C5 | 119.9 (6) |
| O2—Ni1—O1 | 88.52 (19) | C1—C6—H6 | 123 (4) |
| O1$^{i}$—Ni1—O1 | 180.00 (7) | C5—C6—H6 | 116 (4) |
| O2$^{i}$—Ni1—N1$^{i}$ | 89.71 (18) | N1—C7—C1 | 125.7 (6) |
| O2—Ni1—N1$^{i}$ | 90.29 (18) | N1—C7—H7 | 117.1 |
| O1$^{i}$—Ni1—N1$^{i}$ | 88.57 (18) | C1—C7—H7 | 117.1 |
| O1—Ni1—N1$^{i}$ | 91.43 (18) | C9—C8—N1 | 116.9 (5) |
| O2$^{i}$—Ni1—N1 | 90.29 (18) | C9—C8—H8A | 108.1 |
| O2—Ni1—N1 | 89.71 (18) | N1—C8—H8A | 108.1 |
| O1$^{i}$—Ni1—N1 | 91.43 (18) | C9—C8—H8B | 108.1 |
| O1—Ni1—N1 | 88.57 (18) | N1—C8—H8B | 108.1 |
| N1$^{i}$—Ni1—N1 | 180.000 (1) | H8A—C8—H8B | 107.3 |
| C2—O1—Ni1 | 125.2 (4) | C8—C9—N2 | 107.8 (5) |
| Ni1—O2—H2C | 123 (6) | C8—C9—H9A | 110.2 |
| Ni1—O2—H2D | 119 (6) | N2—C9—H9A | 110.2 |
| H2C—O2—H2D | 109 (7) | C8—C9—H9B | 110.2 |

| | | | |
|---|---|---|---|
| C7—N1—C8 | 114.1 (5) | N2—C9—H9B | 110.2 |
| C7—N1—Ni1 | 124.5 (4) | H9A—C9—H9B | 108.5 |
| C8—N1—Ni1 | 121.4 (4) | C11—C10—N2 | 106.9 (6) |
| C9—N2—C10 | 114.2 (5) | C11—C10—C12 | 120.7 (6) |
| C9—N2—H2A | 108.7 | N2—C10—C12 | 104.4 (6) |
| C10—N2—H2A | 108.7 | C11—C10—H10 | 108.1 |
| C9—N2—H2B | 108.7 | N2—C10—H10 | 108.1 |
| C10—N2—H2B | 108.7 | C12—C10—H10 | 108.1 |
| H2A—N2—H2B | 107.6 | C10—C11—H11A | 109.5 |
| C6—C1—C2 | 120.9 (6) | C10—C11—H11B | 109.5 |
| C6—C1—C7 | 114.9 (5) | H11A—C11—H11B | 109.5 |
| C2—C1—C7 | 124.1 (5) | C10—C11—H11C | 109.5 |
| O1—C2—C3 | 120.1 (5) | H11A—C11—H11C | 109.5 |
| O1—C2—C1 | 123.7 (5) | H11B—C11—H11C | 109.5 |
| C3—C2—C1 | 116.2 (6) | C10—C12—H12A | 109.5 |
| C4—C3—C2 | 122.2 (6) | C10—C12—H12B | 109.5 |
| C4—C3—Br1 | 118.4 (5) | H12A—C12—H12B | 109.5 |
| C2—C3—Br1 | 119.4 (5) | C10—C12—H12C | 109.5 |
| C3—C4—C5 | 120.4 (6) | H12A—C12—H12C | 109.5 |
| C3—C4—H4 | 119.8 | H12B—C12—H12C | 109.5 |
| C5—C4—H4 | 119.8 | H3A—O3—H3B | 111.5 |

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

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2A···Cl1$^{ii}$ | 0.90 | 2.19 | 3.027 (5) | 154 |
| N2—H2A···O2$^{i}$ | 0.90 | 2.60 | 3.155 (7) | 121 |
| N2—H2B···O1$^{i}$ | 0.90 | 1.74 | 2.620 (6) | 166 |
| N2—H2B···Br1$^{i}$ | 0.90 | 2.87 | 3.368 (5) | 117 |
| O2—H2C···Cl1$^{i}$ | 0.84 (7) | 2.14 (6) | 2.977 (4) | 174 (9) |
| O2—H2D···Cl1$^{iii}$ | 0.85 (6) | 2.19 (4) | 2.989 (5) | 157 (9) |
| O3—H3A···O1$^{iv}$ | 0.85 | 2.49 | 3.316 (13) | 163.1 |

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

**Fig. 1**

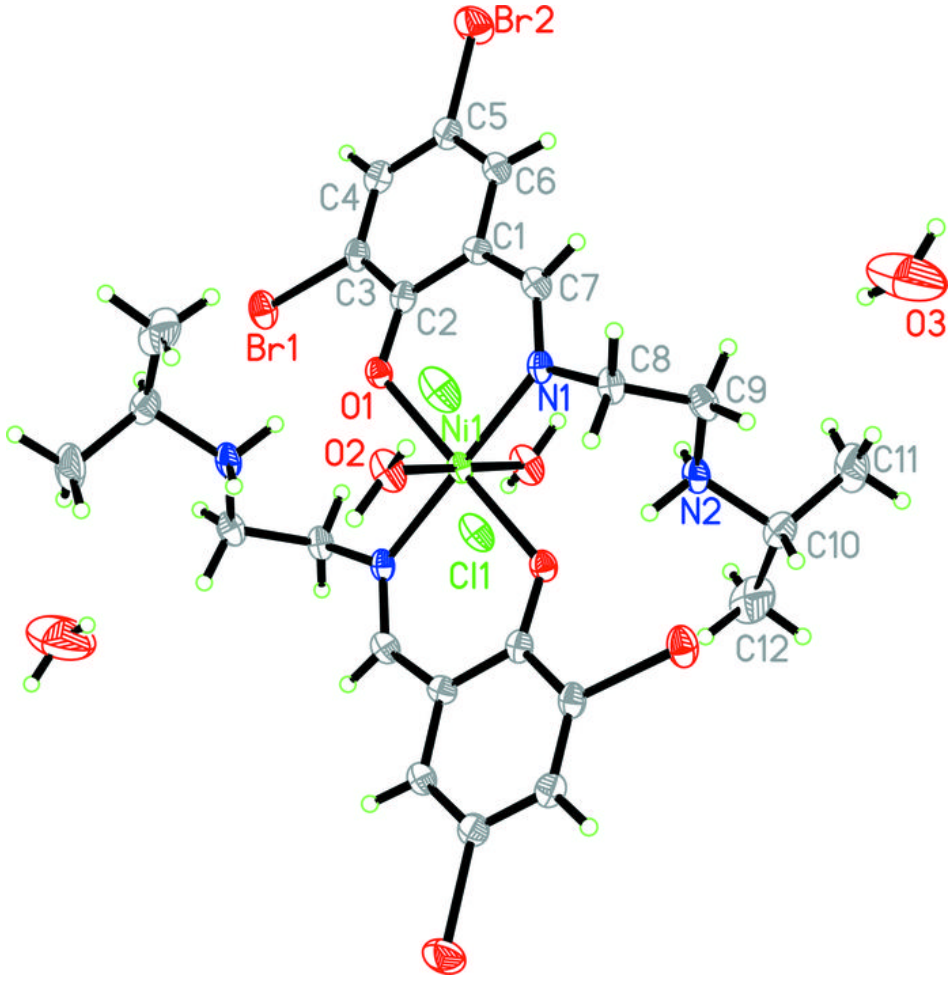

**Fig. 2**