

(2-[[2-(2-Aminoethylamino)ethyl]imino-methyl]phenolato)nickel(II) chloride dihydrate

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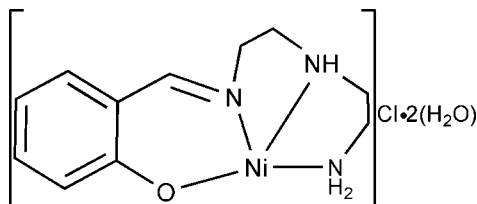
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.011$ Å; R factor = 0.079; wR factor = 0.152; data-to-parameter ratio = 13.3.

In the title complex, $[\text{Ni}(\text{C}_{11}\text{H}_{16}\text{N}_3\text{O})]\text{Cl}\cdot 2\text{H}_2\text{O}$, the Ni^{II} ion is coordinated within a distorted square-planar environment. In the crystal, intermolecular $\text{N}-\text{H}\cdots\text{Cl}$, $\text{N}-\text{H}\cdots\text{O}$, $\text{O}-\text{H}\cdots\text{O}$, $\text{O}-\text{H}\cdots\text{Cl}$ and weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds link the components into a two-dimensional network parallel to (001).

Related literature

For related structures, see: Chen & Wang (2006); Cusmano Priolo *et al.* (1983); Kratochvíl *et al.* (1989, 1991); Liu *et al.* (2004); Loub *et al.* (1989, 1990); Podlahová *et al.* (1988); Rotondo *et al.* (1983); Zhang *et al.* (2006); Zhu *et al.* (2004).



Experimental

Crystal data

 $[\text{Ni}(\text{C}_{11}\text{H}_{16}\text{N}_3\text{O})]\text{Cl}\cdot 2\text{H}_2\text{O}$
 $M_r = 336.46$

 Monoclinic, $P2_1/n$
 $a = 7.1062$ (16) Å

 $b = 11.6685$ (19) Å

 $c = 17.677$ (2) Å

 $\beta = 96.699$ (3)°

 $V = 1455.8$ (4) Å³
 $Z = 4$

 Mo $K\alpha$ radiation

 $\mu = 1.52$ mm⁻¹
 $T = 298$ K

 $0.20 \times 0.06 \times 0.04$ mm

Data collection

Bruker SMART APEX I CCD area-detector diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

 $T_{\text{min}} = 0.783$, $T_{\text{max}} = 0.863$

13581 measured reflections

2565 independent reflections

 1860 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.099$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.079$
 $wR(F^2) = 0.152$
 $S = 1.16$

2565 reflections

193 parameters

10 restraints

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.41$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.67$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N2}-\text{H2A}\cdots\text{Cl1}^{\text{i}}$	0.87 (2)	2.55 (4)	3.325 (6)	149 (6)
$\text{N3}-\text{H3A}\cdots\text{Cl1}$	0.84 (4)	2.60 (3)	3.397 (6)	160 (5)
$\text{N3}-\text{H3B}\cdots\text{O3}^{\text{ii}}$	0.85 (2)	2.09 (3)	2.914 (8)	162 (6)
$\text{O2}-\text{H2B}\cdots\text{Cl1}$	0.83 (2)	2.27 (5)	3.091 (5)	176 (9)
$\text{O2}-\text{H2C}\cdots\text{O1}$	0.82 (6)	1.99 (6)	2.797 (6)	172 (8)
$\text{O3}-\text{H3C}\cdots\text{O2}$	0.82 (2)	1.93 (2)	2.750 (8)	175 (9)
$\text{O3}-\text{H3D}\cdots\text{Cl1}^{\text{iii}}$	0.81 (7)	2.36 (7)	3.166 (6)	172 (9)
$\text{C25}-\text{H25B}\cdots\text{O2}^{\text{i}}$	0.97	2.56	3.464 (9)	154

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

Data collection: SMART (Bruker, 2001); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; 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: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5172).

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supplementary materials

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(2- $\{2$ -(2-Aminoethylamino)ethyliminomethyl}phenolato)nickel(II) chloride dihydrate

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Comment

The Schiff base ligand 2-((2-(2-aminoethylamino)ethylimino)methyl)phenol has often been used in the synthesis of metal-organic complexes (Chen & Wang, 2006, Cusmano Priolo *et al.*, 1983, Kratochvíl *et al.*, 1989, Kratochvíl *et al.*, 1991, Loub *et al.*, 1990, Loub *et al.*, 1989, Podlahová *et al.*, 1988, Rotondo *et al.*, 1983, Zhang *et al.*, 2006, Zhu *et al.*, 2004, Liu *et al.*, 2004). In this paper, we report the title mononuclear metal complex (I).

In (I), the asymmetric unit consists of a coordination cation, one uncoordinated Cl⁻ anion and two solvent water molecules (Fig.1). The Ni^{II} ion is in a distorted square-planar coordination environment with atom Ni1 atom 0.058 Å from the plane formed by N1/N2/N3/O1. The Ni—N/O bond lengths are comparable to previously published analogs (Loub *et al.*, 1989, Podlahová *et al.*, 1988).

The crystal structure is stabilized by intermolecular hydrogen bonds (Table 1), forming a two-dimensional network parallel to the (001) plane (Fig.2).

Experimental

NiCl₂·6(H₂O) (1 mmol, 238 mg), salicylaldehyde (1 mmol, 122 mg) and diethylenetriamine (1 mmol, 103 mg) were dissolved in a mixture of ethanol and acetonitrile (50 ml, 1:1 v/v), resulting in a light-green solution. When diethyl ether was slowly diffused into this solution for one week, pale-yellow blocks suitable for X-ray diffraction were formed at the bottom of the vessel.

Refinement

All the H atoms bonded to carbon atoms were located at their geometrical positions with C—H = 0.97 Å (methylene) and 0.93 Å (aromatic), $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms bonded to imine N and water O atoms were located on the difference Fourier maps and then refined with the constraints of N—H = 0.86 (2) Å, O—H = 0.82 (2) Å, H—H = 1.35 (2) Å and the $U_{iso}(H)$ values were set 1.2 times of $U_{eq}(N)$ or 1.5 times of $U_{eq}(O)$ of their carrier atoms.

Figures

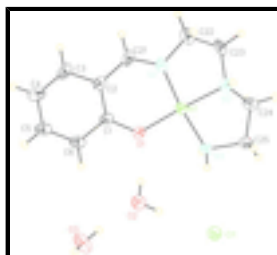


Fig. 1. Molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

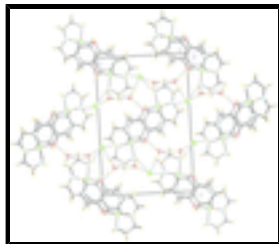


Fig. 2. Part of the crystal structure of (I), showing the formation of the two-dimensional network parallel to the (001) plane. Hydrogen bonds are shown as dashed lines.

(2-[2-(2-Aminoethylamino)ethyl]iminomethyl]phenolato)nickel(II) chloride dihydrate

Crystal data

[Ni(C₁₁H₁₆N₃O)]Cl·2H₂O

M_r = 336.46

Monoclinic, *P*2₁/*n*

Hall symbol: -*P* 2₁*y**n*

a = 7.1062 (16) Å

b = 11.6685 (19) Å

c = 17.677 (2) Å

β = 96.699 (3)°

V = 1455.8 (4) Å³

Z = 4

F(000) = 704

D_x = 1.535 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 1489 reflections

θ = 1.7–19.5°

μ = 1.52 mm⁻¹

T = 298 K

Needle, yellow

0.20 × 0.06 × 0.04 mm

Data collection

Bruker SMART APEX I CCD area-detector diffractometer

2565 independent reflections

Radiation source: fine focus sealed Siemens Mo tube graphite

1860 reflections with *I* > 2σ(*I*)

0.3° wide ω exposures scans

R_{int} = 0.099

θ_{max} = 25.0°, θ_{min} = 2.1°

Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)

h = -8→8

T_{min} = 0.783, *T_{max}* = 0.863

k = -13→13

13581 measured reflections

l = -21→21

Refinement

Refinement on *F*²

Primary atom site location: structure-invariant direct methods

Least-squares matrix: full

Secondary atom site location: difference Fourier map

R [*F*² > 2σ(*F*²)] = 0.079

Hydrogen site location: inferred from neighbouring sites

wR(*F*²) = 0.152

H atoms treated by a mixture of independent and constrained refinement

S = 1.16

w = 1/[σ²(*F_o*²) + (0.0551*P*)²]

where *P* = (*F_o*² + 2*F_c*²)/3

2565 reflections

(Δ/σ)_{max} < 0.001

193 parameters

Δρ_{max} = 0.41 e Å⁻³

10 restraints

$$\Delta\rho_{\min} = -0.67 \text{ e } \text{\AA}^{-3}$$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.63623 (11)	0.34513 (7)	0.37464 (5)	0.0333 (3)
C1	0.7236 (9)	0.5502 (6)	0.4572 (4)	0.0358 (17)
C2	0.7687 (9)	0.4916 (6)	0.5255 (4)	0.0385 (17)
C3	0.8289 (10)	0.5530 (7)	0.5919 (4)	0.051 (2)
H3	0.8572	0.5139	0.6376	0.061*
C4	0.8469 (10)	0.6701 (8)	0.5906 (5)	0.056 (2)
H4	0.8896	0.7100	0.6348	0.067*
C5	0.8020 (10)	0.7266 (7)	0.5245 (4)	0.051 (2)
H5	0.8110	0.8061	0.5242	0.061*
C6	0.7432 (9)	0.6705 (6)	0.4571 (4)	0.0454 (19)
H6	0.7166	0.7117	0.4121	0.055*
C21	0.7525 (9)	0.3699 (6)	0.5302 (4)	0.0416 (18)
H21	0.7820	0.3364	0.5778	0.050*
C22	0.6905 (10)	0.1786 (6)	0.4877 (5)	0.053 (2)
H22A	0.5692	0.1585	0.5041	0.064*
H22B	0.7903	0.1556	0.5268	0.064*
C23	0.7149 (10)	0.1201 (6)	0.4129 (4)	0.048 (2)
H23A	0.8472	0.1201	0.4042	0.058*
H23B	0.6708	0.0415	0.4133	0.058*
C24	0.6345 (10)	0.1642 (6)	0.2747 (4)	0.0479 (19)
H24A	0.5831	0.0902	0.2580	0.058*
H24B	0.7693	0.1647	0.2704	0.058*
C25	0.5361 (10)	0.2590 (5)	0.2279 (4)	0.0427 (19)
H25A	0.5694	0.2569	0.1763	0.051*
H25B	0.3997	0.2515	0.2261	0.051*
Cl1	0.2875 (3)	0.52634 (16)	0.14998 (11)	0.0494 (5)
N1	0.7000 (7)	0.3025 (5)	0.4737 (3)	0.0395 (14)
N2	0.5992 (8)	0.1873 (5)	0.3525 (3)	0.0426 (15)
H2A	0.488 (5)	0.167 (6)	0.364 (4)	0.051*
N3	0.6022 (8)	0.3689 (4)	0.2664 (3)	0.0357 (14)
H3A	0.507 (4)	0.405 (5)	0.247 (3)	0.043*

supplementary materials

H3B	0.711 (4)	0.384 (5)	0.253 (3)	0.043*
O1	0.6663 (6)	0.5003 (4)	0.3910 (2)	0.0374 (11)
O2	0.4176 (8)	0.6467 (4)	0.3029 (3)	0.0581 (14)
H2B	0.386 (12)	0.617 (6)	0.261 (2)	0.087*
H2C	0.484 (11)	0.599 (5)	0.327 (3)	0.087*
O3	0.5374 (8)	0.8703 (5)	0.2971 (4)	0.0741 (18)
H3C	0.508 (12)	0.803 (2)	0.300 (6)	0.111*
H3D	0.446 (8)	0.906 (6)	0.308 (6)	0.111*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0315 (5)	0.0318 (5)	0.0368 (5)	0.0024 (4)	0.0045 (4)	0.0000 (4)
C1	0.028 (4)	0.046 (5)	0.033 (4)	-0.002 (3)	0.003 (3)	-0.005 (4)
C2	0.029 (4)	0.053 (5)	0.034 (4)	0.005 (3)	0.004 (3)	-0.002 (4)
C3	0.036 (4)	0.076 (6)	0.038 (5)	0.010 (4)	-0.002 (4)	0.002 (4)
C4	0.048 (5)	0.071 (7)	0.047 (5)	-0.008 (4)	-0.002 (4)	-0.014 (5)
C5	0.046 (5)	0.055 (5)	0.051 (6)	0.001 (4)	0.010 (4)	-0.020 (4)
C6	0.036 (4)	0.049 (5)	0.051 (5)	-0.004 (4)	0.004 (3)	-0.013 (4)
C21	0.037 (4)	0.054 (5)	0.034 (4)	0.015 (4)	0.005 (3)	0.014 (4)
C22	0.037 (4)	0.045 (5)	0.076 (6)	-0.005 (4)	0.003 (4)	0.007 (4)
C23	0.040 (4)	0.027 (4)	0.078 (6)	0.009 (3)	0.006 (4)	0.004 (4)
C24	0.045 (4)	0.043 (4)	0.057 (5)	-0.005 (4)	0.012 (4)	-0.015 (4)
C25	0.047 (5)	0.043 (5)	0.038 (4)	-0.009 (4)	0.003 (4)	-0.011 (3)
Cl1	0.0508 (12)	0.0435 (11)	0.0529 (12)	0.0020 (9)	0.0017 (10)	0.0043 (9)
N1	0.032 (3)	0.038 (3)	0.049 (4)	0.008 (3)	0.005 (3)	0.004 (3)
N2	0.041 (4)	0.042 (4)	0.045 (4)	-0.010 (3)	0.007 (3)	0.012 (3)
N3	0.030 (3)	0.032 (4)	0.044 (4)	0.001 (3)	0.003 (3)	-0.007 (3)
O1	0.042 (3)	0.035 (3)	0.033 (3)	0.003 (2)	-0.003 (2)	0.000 (2)
O2	0.071 (4)	0.046 (3)	0.056 (3)	0.009 (3)	-0.001 (3)	-0.002 (3)
O3	0.066 (4)	0.042 (3)	0.118 (5)	0.003 (3)	0.027 (4)	-0.004 (4)

Geometric parameters (\AA , $^\circ$)

Ni1—N1	1.825 (6)	C22—H22A	0.9700
Ni1—O1	1.842 (4)	C22—H22B	0.9700
Ni1—N2	1.894 (6)	C23—N2	1.492 (9)
Ni1—N3	1.920 (6)	C23—H23A	0.9700
C1—O1	1.329 (7)	C23—H23B	0.9700
C1—C2	1.392 (9)	C24—N2	1.452 (9)
C1—C6	1.410 (9)	C24—C25	1.504 (9)
C2—C3	1.398 (10)	C24—H24A	0.9700
C2—C21	1.429 (9)	C24—H24B	0.9700
C3—C4	1.373 (10)	C25—N3	1.501 (8)
C3—H3	0.9300	C25—H25A	0.9700
C4—C5	1.346 (10)	C25—H25B	0.9700
C4—H4	0.9300	N2—H2A	0.87 (2)
C5—C6	1.381 (9)	N3—H3A	0.84 (4)
C5—H5	0.9300	N3—H3B	0.854 (19)

C6—H6	0.9300	O2—H2B	0.83 (2)
C21—N1	1.292 (8)	O2—H2C	0.82 (6)
C21—H21	0.9300	O3—H3C	0.82 (2)
C22—N1	1.469 (8)	O3—H3D	0.81 (7)
C22—C23	1.515 (10)		
N1—Ni1—O1	96.1 (2)	C22—C23—H23A	110.5
N1—Ni1—N2	86.9 (3)	N2—C23—H23B	110.5
O1—Ni1—N2	176.9 (2)	C22—C23—H23B	110.5
N1—Ni1—N3	169.4 (2)	H23A—C23—H23B	108.7
O1—Ni1—N3	90.7 (2)	N2—C24—C25	105.3 (6)
N2—Ni1—N3	86.4 (2)	N2—C24—H24A	110.7
O1—C1—C2	124.4 (6)	C25—C24—H24A	110.7
O1—C1—C6	117.1 (6)	N2—C24—H24B	110.7
C2—C1—C6	118.5 (6)	C25—C24—H24B	110.7
C1—C2—C3	119.5 (7)	H24A—C24—H24B	108.8
C1—C2—C21	121.8 (6)	N3—C25—C24	106.1 (5)
C3—C2—C21	118.6 (7)	N3—C25—H25A	110.5
C4—C3—C2	121.0 (7)	C24—C25—H25A	110.5
C4—C3—H3	119.5	N3—C25—H25B	110.5
C2—C3—H3	119.5	C24—C25—H25B	110.5
C5—C4—C3	119.2 (7)	H25A—C25—H25B	108.7
C5—C4—H4	120.4	C21—N1—C22	118.9 (6)
C3—C4—H4	120.4	C21—N1—Ni1	126.3 (5)
C4—C5—C6	122.3 (8)	C22—N1—Ni1	114.7 (5)
C4—C5—H5	118.9	C24—N2—C23	116.0 (6)
C6—C5—H5	118.9	C24—N2—Ni1	109.9 (4)
C5—C6—C1	119.3 (7)	C23—N2—Ni1	108.2 (4)
C5—C6—H6	120.3	C24—N2—H2A	116 (5)
C1—C6—H6	120.3	C23—N2—H2A	97 (5)
N1—C21—C2	125.4 (6)	Ni1—N2—H2A	109 (5)
N1—C21—H21	117.3	C25—N3—Ni1	109.0 (4)
C2—C21—H21	117.3	C25—N3—H3A	93 (4)
N1—C22—C23	106.5 (6)	Ni1—N3—H3A	119 (4)
N1—C22—H22A	110.4	C25—N3—H3B	107 (4)
C23—C22—H22A	110.4	Ni1—N3—H3B	107 (4)
N1—C22—H22B	110.4	H3A—N3—H3B	120 (4)
C23—C22—H22B	110.4	C1—O1—Ni1	126.0 (4)
H22A—C22—H22B	108.6	H2B—O2—H2C	104 (3)
N2—C23—C22	106.1 (5)	H3C—O3—H3D	105 (8)
N2—C23—H23A	110.5		
O1—C1—C2—C3	179.6 (6)	N3—Ni1—N1—C21	128.3 (13)
C6—C1—C2—C3	1.0 (9)	O1—Ni1—N1—C22	178.7 (4)
O1—C1—C2—C21	-1.4 (10)	N2—Ni1—N1—C22	-0.8 (5)
C6—C1—C2—C21	179.9 (6)	N3—Ni1—N1—C22	-51.1 (15)
C1—C2—C3—C4	-1.0 (10)	C25—C24—N2—C23	-167.6 (5)
C21—C2—C3—C4	-180.0 (6)	C25—C24—N2—Ni1	-44.5 (6)
C2—C3—C4—C5	1.4 (11)	C22—C23—N2—C24	166.1 (6)
C3—C4—C5—C6	-1.8 (11)	C22—C23—N2—Ni1	42.1 (6)

supplementary materials

C4—C5—C6—C1	1.9 (11)	N1—Ni1—N2—C24	-151.6 (5)
O1—C1—C6—C5	179.9 (6)	N3—Ni1—N2—C24	20.3 (5)
C2—C1—C6—C5	-1.4 (10)	N1—Ni1—N2—C23	-24.0 (4)
C1—C2—C21—N1	1.5 (11)	N3—Ni1—N2—C23	147.9 (5)
C3—C2—C21—N1	-179.5 (6)	C24—C25—N3—Ni1	-35.4 (6)
N1—C22—C23—N2	-42.0 (7)	N1—Ni1—N3—C25	59.6 (15)
N2—C24—C25—N3	51.1 (7)	O1—Ni1—N3—C25	-169.8 (4)
C2—C21—N1—C22	179.9 (6)	N2—Ni1—N3—C25	9.2 (4)
C2—C21—N1—Ni1	0.6 (10)	C2—C1—O1—Ni1	-0.6 (9)
C23—C22—N1—C21	-154.8 (6)	C6—C1—O1—Ni1	178.0 (4)
C23—C22—N1—Ni1	24.7 (7)	N1—Ni1—O1—C1	2.0 (5)
O1—Ni1—N1—C21	-1.9 (6)	N3—Ni1—O1—C1	-170.0 (5)
N2—Ni1—N1—C21	178.6 (6)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N2—H2A \cdots C11 ⁱ	0.87 (2)	2.55 (4)	3.325 (6)	149 (6)
N3—H3A \cdots C11	0.84 (4)	2.60 (3)	3.397 (6)	160 (5)
N3—H3B \cdots O3 ⁱⁱ	0.85 (2)	2.09 (3)	2.914 (8)	162 (6)
O2—H2B \cdots C11	0.83 (2)	2.27 (5)	3.091 (5)	176 (9)
O2—H2C \cdots O1	0.82 (6)	1.99 (6)	2.797 (6)	172 (8)
O3—H3C \cdots O2	0.82 (2)	1.93 (2)	2.750 (8)	175 (9)
O3—H3D \cdots C11 ⁱⁱⁱ	0.81 (7)	2.36 (7)	3.166 (6)	172 (9)
C25—H25B \cdots O2 ⁱ	0.97	2.56	3.464 (9)	154

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

Fig. 1

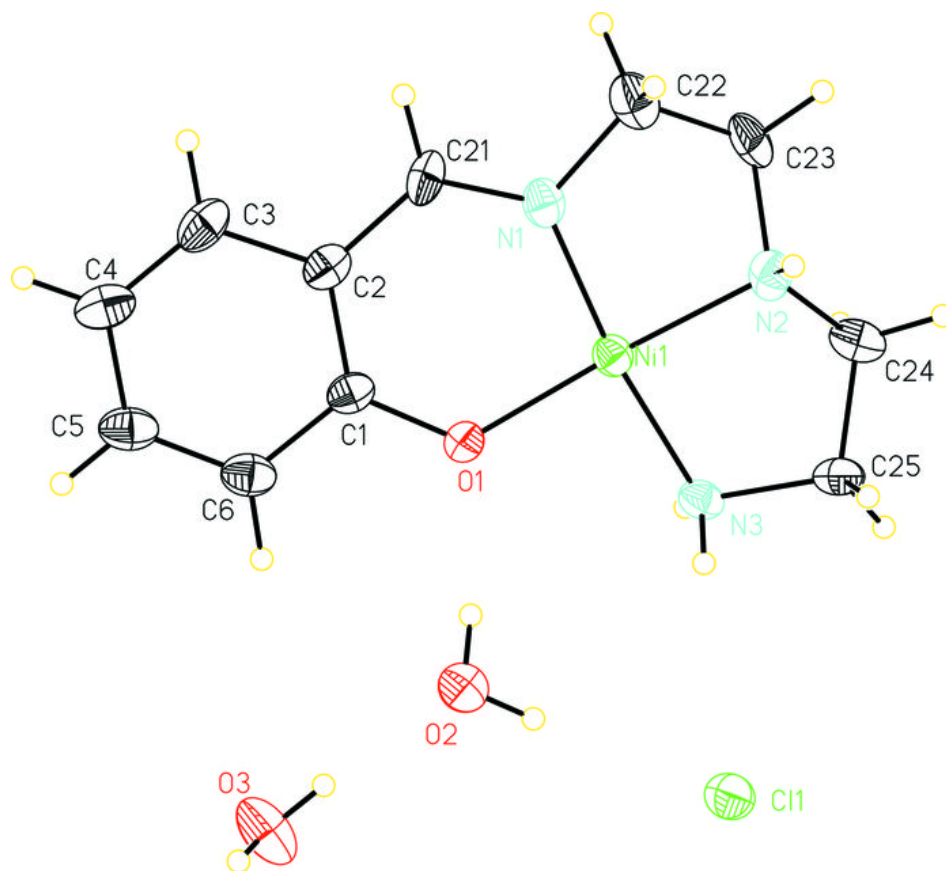


Fig. 2

