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Aqua(2,2′-bipyridine)(2-formyl-4,6-dinitrophenolato)nickel(II) perchlorate

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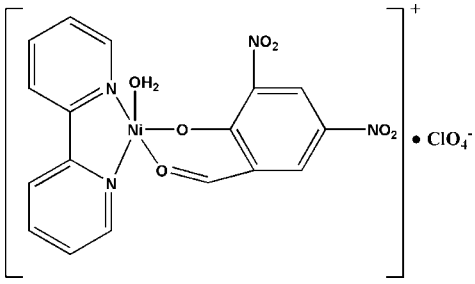
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.052; wR factor = 0.161; data-to-parameter ratio = 12.6.

In the title complex, $[Ni(C_7H_3N_2O_6)(C_{10}H_8N_2)(H_2O)]ClO_4$, the Ni^{II} ion adopts a distorted square-pyramidal coordination geometry, with the coordinated water molecule occupying the apical position. The Ni^{II} complex cation is linked to the ClO_4^- anion by O—H···O hydrogen bonding.

Related literature

For general background, see Huang & Gladysz (1988); Li & Chen (2006); Wang *et al.* (2001); Wu & Lu (2003). For a related structure, see Das *et al.* (1997).



Experimental

Crystal data

$[Ni(C_7H_3N_2O_6)(C_{10}H_8N_2)(H_2O)]ClO_4$
M_r = 543.47
Monoclinic, $P2_1/c$
a = 7.4481 (3) Å
b = 24.1832 (9) Å
c = 11.6691 (4) Å
β = 98.021 (2)°
V = 2081.26 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.13 mm^{-1}
T = 293 (2) K
0.28 × 0.22 × 0.16 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.742, T_{max} = 0.840
11140 measured reflections
3862 independent reflections
2976 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.161
S = 1.05
3862 reflections
307 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···O6^{i}	0.84	2.39	3.149 (8)	151
O1W—H1W···O8^{i}	0.84	2.42	3.159 (9)	148
O1W—H2W···O9	0.89	2.02	2.906 (8)	175

Symmetry code: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2289).

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supplementary materials

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Aqua(2,2'-bipyridine)(2-formyl-4,6-dinitrophenolato)nickel(II) perchlorate

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Comment

Synthesis of transition metal complexes with aldehyde groups has been a subject of considerable importance (Huang & Gladysz, 1998). A series complexes of this type has been report (Li & Chen, 2006; Das *et al.*, 1997; Wang *et al.*, 2001). Recent years, research effort has been devoted to the study of substituted bis(salicylaldehydato)nickel(II) complexes because of their catalytic activity in the dimerization of propylene and in olefin oligomerization when used together with an aluminium co-catalyst and/or phosphine ligand (Wu & Lu, 2003). In order to study the structure of bis(salicylaldehydato)nickel(II) complexes, We reported here the synthesis and crystal structure of a new nickle(II) complex.

As shown in Fig. 1, the title compound contains one Ni(II) ion, one 2-formyl-4,6-dinitrophenolate (*L*) ligand, one 2,2'-bipyridine, one coordinated water molecules and one ClO_4^- anion. This compound exhibits a mononuclear structure. The Ni atom is five coordinated by two O atoms from the *L* ligand, two N atoms from the bidentate ligand (bipy) and one O atom from the coordinated water molecule, forming a slightly distorted square pyramidal geometry, with N1, N2, O10, O1 in the basal plane and O1W in the axial position. The bond lengths of Ni—O or Ni—N are similar to those reported for other Ni complexes (Das *et al.*, 1997). The $[Ni(2,2'\text{-bipy})(L)(H_2O)]^+$ cations and the ClO_4^- anions are interlinked into a supramolecular structure by the O···O hydrogen bond which exists between the oxygen atoms of the water molecule and the oxygen atoms of the perchlorate (Fig. 2).

Experimental

An aqueous solution (10 ml) nickel perchloride (0.46 g, 1 mmol) was added dropwise inyo an ethanol-water solution of 2-hydroxy-3,5-dinitrobenzaldehyde (0.21 g, 1 mmol). Then an ethanol solution (3 ml) of 2,2'-bipy (0.16 g, 1 mmol) was mixed with the above solution. The mixture was stirred for 1 h at room temperature. The green crystal was separated by slow evaporation of the solvent at room temperature over a period of about two weeks.

Refinement

Water H atoms ere located in a difference Fourier map and refined as riding in their as-found relative positions with $U_{iso}(H) = 1.5U_{eq}(O)$. Aromatic H atoms were generated geometrically with C—H = 0.93 Å and refined in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

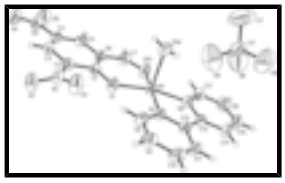

Fig. 1. The molecular structure of the title compound with 30% probability displacement ellipsoids.

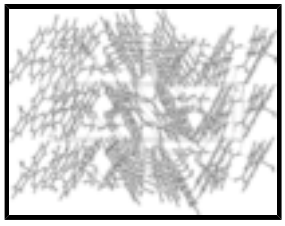

Fig. 2. Projection of the title compound viewed down the *c* axis.

Aqua(2,2'-bipyridine)(2-formyl-4,6-dinitrophenolato)nickel(II) perchlorate

Crystal data

$[Ni(C_7H_3N_2O_6)(C_{10}H_8N_2)(H_2O)]ClO_4$	F_{000} = 1104
M_r = 543.47	D_x = 1.734 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3862 reflections
a = 7.4481 (3) Å	θ = 2.0–25.5º
b = 24.1832 (9) Å	μ = 1.13 mm^{-1}
c = 11.6691 (4) Å	T = 293 (2) K
β = 98.021 (2)º	Block, green
V = 2081.26 (13) Å^3	0.28 × 0.22 × 0.16 mm
Z = 4	

Data collection

Bruker APEX area-detector diffractometer	3862 independent reflections
Radiation source: fine-focus sealed tube	2976 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.036
T = 293(2) K	θ_{max} = 25.5º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 2002)	h = −8→9
T_{min} = 0.742, T_{max} = 0.840	k = −25→29
11140 measured reflections	l = −13→14

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.052$	H-atom parameters constrained
$wR(F^2) = 0.161$	$w = 1/[\sigma^2(F_o^2) + (0.0899P)^2 + 1.1617P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.002$
3862 reflections	$\Delta\rho_{max} = 0.53$ e Å^{-3}
307 parameters	$\Delta\rho_{min} = -0.42$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
Ni1	0.38844 (6)	0.12807 (2)	0.36590 (4)	0.0515 (2)
Cl1	0.72075 (18)	0.29702 (6)	0.25988 (10)	0.0786 (4)
N1	0.5932 (4)	0.10590 (14)	0.2851 (3)	0.0552 (8)
N2	0.3009 (5)	0.16174 (13)	0.2129 (3)	0.0602 (8)
N3	0.6769 (5)	0.02080 (16)	0.6778 (3)	0.0671 (9)
N4	0.2015 (7)	0.05604 (18)	0.9129 (4)	0.0847 (12)
O1	0.4707 (4)	0.08100 (12)	0.4955 (2)	0.0634 (7)
O2	0.7174 (5)	−0.02028 (15)	0.7391 (3)	0.0905 (10)
O3	0.7727 (5)	0.03745 (18)	0.6097 (3)	0.1009 (13)
O4	0.2983 (7)	0.03533 (18)	0.9933 (3)	0.1120 (14)
O5	0.0433 (7)	0.0705 (2)	0.9158 (4)	0.1288 (17)
O6	0.8095 (11)	0.3113 (3)	0.1710 (6)	0.206 (3)
O7	0.7424 (13)	0.3400 (3)	0.3349 (6)	0.223 (4)
O8	0.5391 (9)	0.2903 (3)	0.2204 (7)	0.212 (4)
O9	0.7850 (8)	0.2486 (3)	0.3140 (7)	0.181 (3)
O10	0.1627 (4)	0.14491 (14)	0.4282 (3)	0.0718 (8)
O1W	0.5206 (5)	0.20274 (14)	0.4487 (3)	0.0907 (11)
H1W	0.5704	0.2073	0.5167	0.136*
H2W	0.5965	0.2181	0.4059	0.136*
C1	0.4103 (5)	0.07758 (15)	0.5925 (3)	0.0510 (8)
C2	0.5053 (5)	0.04762 (16)	0.6876 (3)	0.0548 (9)
C3	0.4404 (6)	0.04219 (16)	0.7917 (3)	0.0601 (10)

H3	0.5072	0.0230	0.8524	0.072*
C4	0.2758 (6)	0.06537 (16)	0.8056 (3)	0.0603 (10)
C5	0.1757 (6)	0.09459 (16)	0.7184 (4)	0.0611 (10)
H5	0.0649	0.1099	0.7297	0.073*
C6	0.2406 (5)	0.10143 (16)	0.6121 (3)	0.0541 (9)
C7	0.1301 (6)	0.13249 (18)	0.5261 (4)	0.0667 (11)
H7	0.0203	0.1450	0.5457	0.080*
C8	0.7379 (6)	0.07741 (19)	0.3332 (4)	0.0669 (11)
H8	0.7462	0.0670	0.4105	0.080*
C9	0.8763 (6)	0.0629 (2)	0.2709 (5)	0.0772 (13)
H9	0.9765	0.0432	0.3055	0.093*
C10	0.8616 (7)	0.0785 (2)	0.1571 (5)	0.0804 (14)
H10	0.9532	0.0693	0.1138	0.096*
C11	0.7148 (7)	0.1070 (2)	0.1069 (4)	0.0756 (13)
H11	0.7039	0.1167	0.0291	0.091*
C12	0.5786 (6)	0.12171 (16)	0.1738 (4)	0.0616 (11)
C13	0.4126 (6)	0.15312 (17)	0.1330 (3)	0.0618 (10)
C14	0.3683 (8)	0.1739 (2)	0.0216 (4)	0.0780 (13)
H14	0.4454	0.1680	−0.0335	0.094*
C15	0.2122 (10)	0.2028 (2)	−0.0067 (4)	0.0951 (18)
H15	0.1825	0.2171	−0.0810	0.114*
C16	0.0993 (8)	0.2109 (2)	0.0742 (5)	0.0856 (15)
H16	−0.0089	0.2302	0.0556	0.103*
C17	0.1483 (6)	0.18994 (18)	0.1844 (4)	0.0693 (11)
H17	0.0722	0.1957	0.2401	0.083*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0540 (3)	0.0636 (3)	0.0395 (3)	0.0065 (2)	0.0162 (2)	0.0060 (2)
Cl1	0.0865 (8)	0.0984 (9)	0.0533 (6)	−0.0131 (7)	0.0182 (5)	−0.0012 (6)
N1	0.061 (2)	0.0607 (17)	0.0473 (18)	−0.0045 (16)	0.0191 (15)	−0.0026 (14)
N2	0.074 (2)	0.0582 (19)	0.0496 (18)	−0.0063 (17)	0.0124 (16)	0.0028 (15)
N3	0.060 (2)	0.082 (2)	0.060 (2)	0.0082 (18)	0.0111 (17)	0.0163 (18)
N4	0.115 (4)	0.085 (3)	0.059 (2)	0.011 (3)	0.031 (2)	0.002 (2)
O1	0.0602 (16)	0.0836 (19)	0.0509 (15)	0.0152 (14)	0.0231 (13)	0.0131 (14)
O2	0.084 (2)	0.099 (2)	0.091 (2)	0.0278 (19)	0.0200 (18)	0.034 (2)
O3	0.068 (2)	0.143 (3)	0.099 (3)	0.027 (2)	0.036 (2)	0.050 (2)
O4	0.164 (4)	0.118 (3)	0.059 (2)	0.019 (3)	0.032 (2)	0.018 (2)
O5	0.138 (4)	0.169 (4)	0.095 (3)	0.036 (3)	0.073 (3)	0.026 (3)
O6	0.253 (8)	0.236 (7)	0.159 (5)	−0.084 (6)	0.134 (6)	−0.007 (5)
O7	0.321 (10)	0.208 (7)	0.140 (5)	0.025 (7)	0.034 (6)	−0.081 (5)
O8	0.131 (5)	0.253 (8)	0.234 (8)	−0.073 (5)	−0.039 (5)	0.082 (7)
O9	0.146 (5)	0.164 (5)	0.243 (7)	0.041 (4)	0.070 (5)	0.066 (5)
O10	0.0678 (19)	0.096 (2)	0.0543 (17)	0.0221 (16)	0.0180 (14)	0.0176 (15)
O1W	0.129 (3)	0.085 (2)	0.0584 (19)	−0.018 (2)	0.0141 (19)	−0.0086 (16)
C1	0.057 (2)	0.054 (2)	0.045 (2)	−0.0015 (16)	0.0182 (16)	0.0034 (16)
C2	0.053 (2)	0.059 (2)	0.054 (2)	0.0031 (17)	0.0145 (17)	0.0046 (17)

C3	0.074 (3)	0.061 (2)	0.046 (2)	0.001 (2)	0.0104 (18)	0.0061 (17)
C4	0.081 (3)	0.059 (2)	0.045 (2)	0.000 (2)	0.025 (2)	−0.0009 (17)
C5	0.066 (3)	0.063 (2)	0.060 (2)	0.0050 (19)	0.027 (2)	−0.0043 (19)
C6	0.057 (2)	0.063 (2)	0.045 (2)	0.0048 (18)	0.0161 (16)	0.0024 (16)
C7	0.062 (3)	0.083 (3)	0.060 (3)	0.016 (2)	0.025 (2)	0.005 (2)
C8	0.065 (3)	0.080 (3)	0.059 (2)	0.001 (2)	0.021 (2)	−0.002 (2)
C9	0.064 (3)	0.086 (3)	0.088 (3)	0.002 (2)	0.035 (2)	−0.011 (3)
C10	0.076 (3)	0.088 (3)	0.087 (3)	−0.009 (3)	0.048 (3)	−0.019 (3)
C11	0.093 (4)	0.084 (3)	0.058 (3)	−0.018 (3)	0.040 (3)	−0.011 (2)
C12	0.077 (3)	0.060 (2)	0.051 (2)	−0.017 (2)	0.023 (2)	−0.0082 (18)
C13	0.083 (3)	0.055 (2)	0.050 (2)	−0.018 (2)	0.018 (2)	−0.0012 (18)
C14	0.113 (4)	0.076 (3)	0.048 (2)	−0.012 (3)	0.021 (2)	0.009 (2)
C15	0.140 (5)	0.090 (4)	0.052 (3)	−0.014 (4)	0.002 (3)	0.019 (3)
C16	0.096 (4)	0.077 (3)	0.080 (3)	0.003 (3)	−0.006 (3)	0.022 (3)
C17	0.078 (3)	0.069 (3)	0.060 (3)	0.004 (2)	0.006 (2)	0.007 (2)

Geometric parameters (Å, °)

Ni1—O1	1.924 (3)	C2—C3	1.375 (5)
Ni1—O10	1.965 (3)	C3—C4	1.378 (6)
Ni1—N1	1.975 (3)	C3—H3	0.9300
Ni1—N2	1.988 (3)	C4—C5	1.371 (6)
Ni1—O1W	2.213 (3)	C5—C6	1.402 (5)
Cl1—O6	1.351 (5)	C5—H5	0.9300
Cl1—O7	1.355 (6)	C6—C7	1.421 (6)
Cl1—O9	1.384 (6)	C7—H7	0.9300
Cl1—O8	1.377 (6)	C8—C9	1.386 (6)
N1—C8	1.335 (5)	C8—H8	0.9300
N1—C12	1.344 (5)	C9—C10	1.370 (7)
N2—C17	1.328 (5)	C9—H9	0.9300
N2—C13	1.349 (5)	C10—C11	1.355 (8)
N3—O3	1.209 (5)	C10—H10	0.9300
N3—O2	1.237 (5)	C11—C12	1.410 (6)
N3—C2	1.452 (5)	C11—H11	0.9300
N4—O4	1.209 (6)	C12—C13	1.472 (7)
N4—O5	1.235 (6)	C13—C14	1.390 (6)
N4—C4	1.455 (5)	C14—C15	1.358 (8)
O1—C1	1.278 (4)	C14—H14	0.9300
O10—C7	1.238 (5)	C15—C16	1.364 (8)
O1W—H1W	0.8354	C15—H15	0.9300
O1W—H2W	0.8863	C16—C17	1.383 (7)
C1—C2	1.427 (5)	C16—H16	0.9300
C1—C6	1.437 (5)	C17—H17	0.9300
O1—Ni1—O10	91.56 (11)	C5—C4—C3	121.5 (4)
O1—Ni1—N1	91.83 (12)	C5—C4—N4	119.1 (4)
O10—Ni1—N1	171.87 (14)	C3—C4—N4	119.3 (4)
O1—Ni1—N2	167.74 (13)	C4—C5—C6	119.9 (4)
O10—Ni1—N2	93.27 (13)	C4—C5—H5	120.0
N1—Ni1—N2	82.00 (14)	C6—C5—H5	120.0

O1—Ni1—O1W	93.80 (13)	C5—C6—C7	116.8 (4)
O10—Ni1—O1W	91.19 (14)	C5—C6—C1	120.9 (4)
N1—Ni1—O1W	95.96 (14)	C7—C6—C1	122.4 (3)
N2—Ni1—O1W	97.36 (13)	O10—C7—C6	127.7 (4)
O6—Cl1—O7	105.8 (5)	O10—C7—H7	116.1
O6—Cl1—O9	113.1 (5)	C6—C7—H7	116.1
O7—Cl1—O9	110.6 (5)	N1—C8—C9	121.7 (4)
O6—Cl1—O8	109.7 (5)	N1—C8—H8	119.1
O7—Cl1—O8	109.3 (6)	C9—C8—H8	119.1
O9—Cl1—O8	108.3 (4)	C10—C9—C8	118.3 (5)
C8—N1—C12	120.3 (4)	C10—C9—H9	120.8
C8—N1—Ni1	124.9 (3)	C8—C9—H9	120.8
C12—N1—Ni1	114.8 (3)	C11—C10—C9	120.6 (4)
C17—N2—C13	119.7 (4)	C11—C10—H10	119.7
C17—N2—Ni1	126.7 (3)	C9—C10—H10	119.7
C13—N2—Ni1	113.6 (3)	C10—C11—C12	119.3 (4)
O3—N3—O2	122.0 (4)	C10—C11—H11	120.4
O3—N3—C2	120.6 (4)	C12—C11—H11	120.4
O2—N3—C2	117.4 (3)	N1—C12—C11	119.7 (4)
O4—N4—O5	124.4 (5)	N1—C12—C13	114.2 (4)
O4—N4—C4	118.3 (5)	C11—C12—C13	126.0 (4)
O5—N4—C4	117.3 (5)	N2—C13—C14	120.1 (4)
C1—O1—Ni1	128.5 (2)	N2—C13—C12	115.3 (4)
C7—O10—Ni1	125.4 (3)	C14—C13—C12	124.6 (4)
Ni1—O1W—H1W	129.3	C15—C14—C13	119.8 (5)
Ni1—O1W—H2W	112.1	C15—C14—H14	120.1
H1W—O1W—H2W	104.2	C13—C14—H14	120.1
O1—C1—C2	121.6 (3)	C16—C15—C14	119.7 (5)
O1—C1—C6	122.8 (3)	C16—C15—H15	120.1
C2—C1—C6	115.6 (3)	C14—C15—H15	120.1
C3—C2—C1	122.6 (4)	C15—C16—C17	118.9 (5)
C3—C2—N3	116.6 (4)	C15—C16—H16	120.6
C1—C2—N3	120.8 (3)	C17—C16—H16	120.6
C2—C3—C4	119.5 (4)	N2—C17—C16	121.8 (5)
C2—C3—H3	120.2	N2—C17—H17	119.1
C4—C3—H3	120.2	C16—C17—H17	119.1

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W···O6^{i}	0.84	2.39	3.149 (8)	151
O1W—H1W···O8^{i}	0.84	2.42	3.159 (9)	148
O1W—H2W···O9	0.89	2.02	2.906 (8)	175

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

Fig. 1

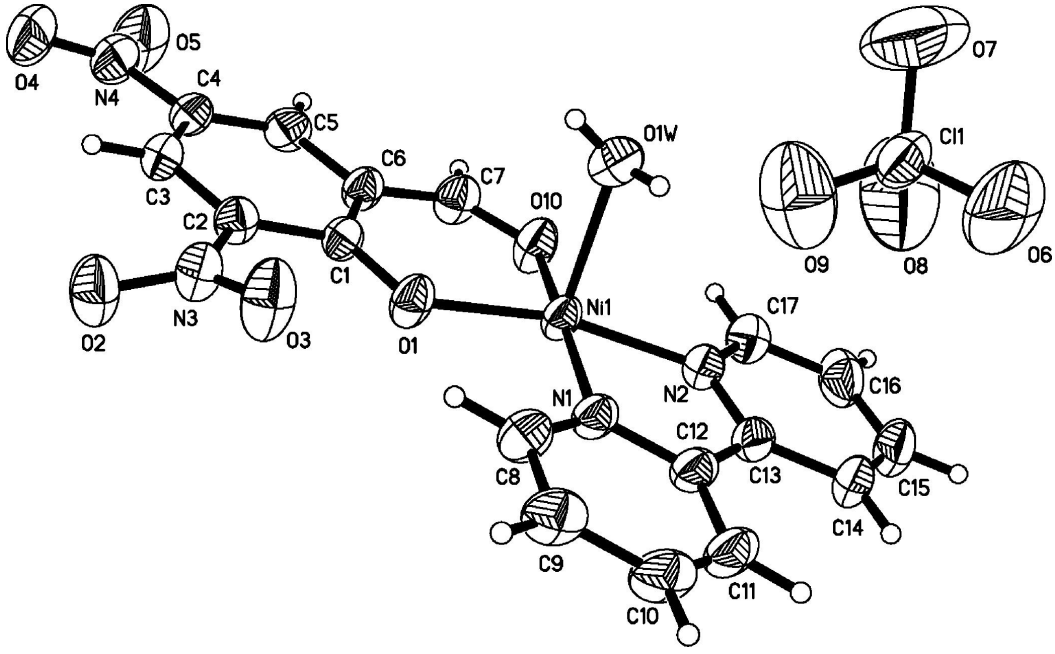
O5
O4
N4
C4
C5
C6
C7
O10
O1W
C3
C2
C1
Ni1
C17
O7
Cl1
O9
O8
O6
N3
O2
O3
O1
N1
N2
C16
C12
C8
C13
C15
C14
C9
C11
C10

Fig. 2