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catena-Poly[[diaquabis[(4-chlorophenylsulfinyl)acetato-κO]nickel(II)]-μ-4,4′-bipyridine-$\kappa^2 N:N'$]

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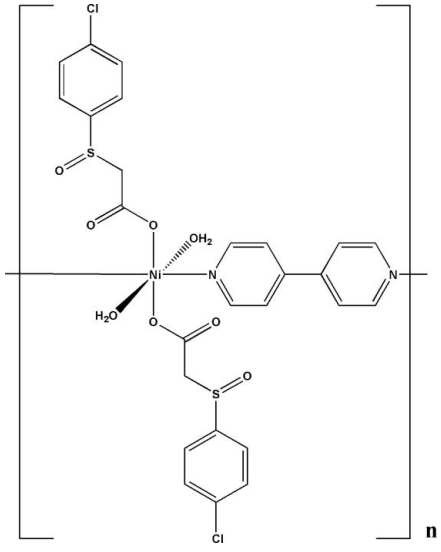
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.031; wR factor = 0.071; data-to-parameter ratio = 16.7.

In the title coordination polymer, $[Ni(C_8H_6ClO_3S)_2(C_{10}H_8N_2)(H_2O)_2]_n$, the Ni^{II} ion exists in an octahedral coordination environment formed by two carboxylate O atoms from two 4-chlorophenylsulfinylacetate ligands, two N atoms from two bipyridine ligands and two water molecules. The Ni^{II} ion lies on a twofold rotation axis. Bridging by the bipyridine ligand leads to a linear chain structure; intermolecular O—H···O hydrogen bonds link the chains into a three-dimensional network.

Related literature

For isostructural compounds, see: Hou, Yu *et al.* (2007*a*,*b*); Hou, Li *et al.* (2007). For related literature, see: Nobles & Thompson (1965).



Experimental

Crystal data

$[Ni(C_8H_6ClO_3S)_2(C_{10}H_8N_2)(H_2O)_2]$
M_r = 686.20
Orthorhombic, *Fdd*2
a = 20.269 (4) Å
b = 25.503 (6) Å
c = 11.345 (11) Å
V = 5865 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.04 mm^{-1}
T = 293 (2) K
0.36 × 0.34 × 0.06 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.699, T_{max} = 0.896
13880 measured reflections
3148 independent reflections
2922 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.071
S = 1.05
3148 reflections
188 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Absolute structure: Flack (1983), 1382 Friedel pairs
Flack parameter: 0.009 (12)

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H11···S1^{i}	0.85	2.98	3.822 (2)	173
O4—H11···O1^{i}	0.85	1.89	2.709 (3)	160
O4—H12···O2^{ii}	0.85	1.85	2.643 (3)	154

Symmetry codes: (i) $x+\frac{1}{4}, -y+\frac{1}{4}, z+\frac{1}{4}$; (ii) $-x, -y, z$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); 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: LH2434).

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supplementary materials

Acta Cryst. (2007). E**63**, m1970 [**doi:10.1107/S1600536807029832**]

catena-Poly[[diaquabis[(4-chlorophenylsulfinyl)acetato-*κO*]nickel(II)]-*μ*-4,4'-bipyridine-κ^2N:*N*']

Y. Su, Y.-J. Hou, Z.-Z. Sun, B.-Y. Li and G.-F. Hou

Comment

Recently, we reported the crystal structures of diaquabis[(4-nitrophenylsulfinylacetato)(4,4'-bipyridine)zinc (Hou *et al.* 2007*a*), diaquabis[(4-chlorophenylsulfinylacetato)(4,4'-bipyridine)cobalt (Hou *et al.* 2007*b*) and diaquabis[(4-chlorophenylsulfinylacetato)(4,4'-bipyridine)zinc (Hou *et al.* 2007*c*); this paper reports the isostructural nickel compound.

In the title compound the nickel bis(4-chlorophenylsulfinylacetate) moiety is bridged by 4,4'-bipyridine into a linear chain (Fig. 1). The Ni^{II} atom shows an all *trans* octahedral coordination. The chains are connected into a three dimensional network *via* intermolecular O—H···O hydrogen bonds (Fig. 2).

Experimental

(4-Chlorophenylsulfanyl)acetic acid was prepared by the nucleophilic reaction of chloroacetic acid and 4-chlorothiophenol under basic conditions. It was then oxidized using 30% aqueous hydrogen peroxide in acetic anhydride solution to produce 4-chlorophenylsulfinyl acetic acid (Nobles & Thompson, 1965). Nickel nitrate hexahydrate (0.592 g, 2 mmol), 4,4'-bipyridine (0.312 g, 2 mmol) and 4-chlorophenylsulfinyl acetic acid (0.437 g, 2 mmol) were dissolved in water and the pH was adjusted to 6 with 0.01 *M* sodium hydroxide; green crystals separated from the filtered solution after several days.

Refinement

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic C) or C—H = 0.97 Å (methylene C), and with U_{iso}(H) = 1.2Ueq(C). Water H atoms were initially located in a difference Fourier map but they were treated as riding on their parent atoms with O—H = 0.85 Å and with U_{iso}(H) = 1.5U_{eq}(O).

The Flack parameter was refined from 1382 Friedel pairs.

Figures

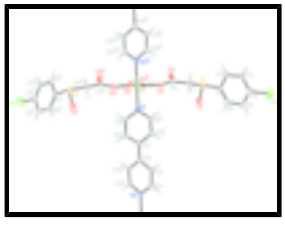

Fig. 1. Part of the polymeric structure of the title complex, with the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as spheres of arbitrary radii. [Symmetry codes: (I) −*x*, −*y* + 2, *z*; (II) *x*, *y*,*z* − 1; (III) −*x*, −*y* + 2, *z* − 1, (IV) *x*, *y*, *z* + 1].

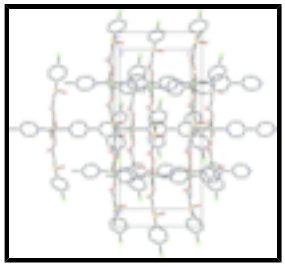

Fig. 2. A partial packing plot of (I). Dashed lines indicate the hydrogen-bonding interactions. H atoms not involved in hydrogen bonds have been omitted.

catena-Poly[[diaquabis[(4-chlorophenylsulfinyl)acetato- κ*O*]nickel(II)]-μ-4,4'-bipyridine-κ^2*N*:*N*']

Crystal data

$[Ni(C_8H_6ClO_3S)_2(C_{10}H_8N_2)(H_2O)_2]$	F_{000} = 2816
M_r = 686.20	D_x = 1.554 Mg m^{-3}
Orthorhombic, *Fdd*2	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: F 2 -2d	Cell parameters from 13082 reflections
a = 20.269 (4) Å	θ = 6.3–54.9º
b = 25.503 (6) Å	μ = 1.04 mm^{-1}
c = 11.345 (11) Å	*T* = 293 (2) K
V = 5865 (6) Å^3	Block, green
Z = 8	0.36 × 0.34 × 0.06 mm

Data collection

Rigaku R-AXIS RAPID diffractometer	3148 independent reflections
Radiation source: fine-focus sealed tube	2922 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.046
T = 293(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 3.2º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	*h* = −25→26
T_{min} = 0.699, T_{max} = 0.896	*k* = −33→32
13880 measured reflections	*l* = −12→14

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.031	$w = 1/[\sigma^2(F_o^2) + (0.0337P)^2 + 3.8506P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.071	$(\Delta/\sigma)_{max}$ = 0.002
S = 1.05	$\Delta\rho_{max}$ = 0.41 e Å^{-3}
3148 reflections	$\Delta\rho_{min}$ = −0.22 e Å^{-3}

188 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 1382 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.009 (12)
Secondary atom site location: difference Fourier map	

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}
C1	0.02738 (12)	0.27432 (10)	1.0801 (2)	0.0288 (5)
C2	0.06467 (13)	0.29286 (11)	1.1730 (3)	0.0384 (6)
H1	0.0610	0.2776	1.2471	0.046*
C3	0.10721 (14)	0.33408 (11)	1.1552 (3)	0.0442 (7)
H2	0.1336	0.3463	1.2163	0.053*
C4	0.11011 (14)	0.35688 (12)	1.0454 (3)	0.0467 (7)
C5	0.07312 (17)	0.33870 (14)	0.9523 (3)	0.0515 (8)
H3	0.0761	0.3544	0.8785	0.062*
C6	0.03164 (16)	0.29673 (13)	0.9708 (3)	0.0461 (7)
H4	0.0065	0.2836	0.9089	0.055*
C7	0.02904 (12)	0.17011 (9)	1.1228 (3)	0.0347 (5)
H5	0.0568	0.1682	1.0532	0.042*
H6	0.0570	0.1775	1.1901	0.042*
C8	−0.00613 (12)	0.11761 (10)	1.1409 (2)	0.0310 (6)
C9	0.02268 (14)	−0.04086 (11)	0.8755 (3)	0.0384 (6)
H7	0.0395	−0.0694	0.9168	0.046*
C10	0.02241 (16)	−0.04277 (12)	0.7538 (3)	0.0423 (7)
H8	0.0372	−0.0726	0.7148	0.051*
C11	0.0000	0.0000	0.6903 (3)	0.0301 (9)
C12	0.0000	0.0000	0.5593 (4)	0.0353 (10)
C13	0.03408 (15)	0.03756 (12)	0.4951 (2)	0.0391 (7)
H9	0.0571	0.0639	0.5339	0.047*
C14	0.03372 (13)	0.03575 (11)	0.3736 (3)	0.0369 (6)
H10	0.0582	0.0607	0.3328	0.044*
Cl1	0.16225 (6)	0.41043 (5)	1.02446 (13)	0.0889 (4)
N1	0.0000	0.0000	0.9364 (2)	0.0260 (7)
N2	0.0000	0.0000	0.3110 (3)	0.0307 (8)
Ni1	0.0000	0.0000	1.12362 (3)	0.02230 (10)

O1	−0.06260 (11)	0.21128 (8)	0.9883 (2)	0.0528 (6)
O2	−0.06426 (9)	0.11872 (8)	1.1772 (2)	0.0493 (5)
O3	0.02798 (8)	0.07784 (6)	1.11784 (15)	0.0296 (4)
O4	0.09886 (8)	−0.02184 (7)	1.12220 (16)	0.0332 (4)
H12	0.1000	−0.0534	1.1464	0.050*
H11	0.1248	−0.0079	1.1720	0.050*
S1	−0.03045 (3)	0.22185 (2)	1.10534 (6)	0.03402 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0316 (12)	0.0244 (12)	0.0304 (15)	0.0017 (9)	−0.0044 (10)	0.0017 (10)
C2	0.0474 (15)	0.0344 (15)	0.0333 (14)	−0.0034 (12)	−0.0117 (12)	0.0059 (12)
C3	0.0444 (15)	0.0378 (16)	0.0503 (18)	−0.0059 (12)	−0.0150 (13)	−0.0006 (13)
C4	0.0391 (14)	0.0369 (16)	0.064 (2)	−0.0068 (12)	0.0044 (13)	0.0072 (14)
C5	0.063 (2)	0.055 (2)	0.0371 (17)	−0.0043 (16)	0.0001 (14)	0.0189 (15)
C6	0.0570 (17)	0.0492 (18)	0.0322 (16)	−0.0065 (14)	−0.0107 (13)	0.0028 (13)
C7	0.0342 (11)	0.0251 (12)	0.0447 (16)	0.0017 (9)	−0.0025 (12)	−0.0017 (11)
C8	0.0391 (13)	0.0285 (12)	0.0256 (17)	−0.0012 (10)	−0.0007 (11)	−0.0022 (10)
C9	0.0581 (16)	0.0359 (14)	0.0213 (14)	0.0107 (12)	0.0051 (12)	0.0039 (11)
C10	0.0677 (18)	0.0350 (16)	0.0242 (16)	0.0131 (14)	0.0077 (13)	−0.0003 (11)
C11	0.037 (2)	0.040 (3)	0.013 (2)	−0.0003 (15)	0.000	0.000
C12	0.046 (2)	0.037 (3)	0.022 (2)	0.0065 (17)	0.000	0.000
C13	0.0530 (16)	0.0443 (18)	0.0200 (14)	−0.0092 (13)	−0.0037 (12)	−0.0026 (12)
C14	0.0452 (14)	0.0401 (16)	0.0255 (15)	−0.0097 (11)	0.0001 (12)	0.0037 (12)
Cl1	0.0792 (6)	0.0642 (7)	0.1232 (11)	−0.0367 (5)	0.0061 (7)	0.0231 (7)
N1	0.0327 (17)	0.0333 (18)	0.0121 (16)	−0.0014 (12)	0.000	0.000
N2	0.0354 (18)	0.0289 (19)	0.028 (2)	0.0015 (12)	0.000	0.000
Ni1	0.03055 (18)	0.02204 (19)	0.01430 (17)	−0.00089 (18)	0.000	0.000
O1	0.0502 (11)	0.0421 (12)	0.0660 (15)	−0.0015 (9)	−0.0291 (11)	−0.0030 (11)
O2	0.0486 (11)	0.0303 (10)	0.0691 (15)	−0.0039 (9)	0.0222 (10)	−0.0093 (10)
O3	0.0389 (8)	0.0236 (8)	0.0265 (9)	−0.0012 (6)	0.0005 (7)	−0.0003 (7)
O4	0.0350 (8)	0.0331 (9)	0.0314 (9)	−0.0026 (7)	−0.0037 (8)	0.0024 (9)
S1	0.0320 (3)	0.0254 (3)	0.0446 (4)	0.0018 (2)	−0.0021 (3)	−0.0017 (3)

Geometric parameters (Å, °)

C1—C6	1.369 (4)	C10—H8	0.9300
C1—C2	1.380 (4)	C11—C10^{i}	1.384 (4)
C1—S1	1.802 (3)	C11—C12	1.486 (4)
C2—C3	1.375 (4)	C12—C13^{i}	1.388 (4)
C2—H1	0.9300	C12—C13	1.388 (4)
C3—C4	1.375 (5)	C13—C14	1.378 (4)
C3—H2	0.9300	C13—H9	0.9300
C4—C5	1.376 (5)	C14—N2	1.343 (3)
C4—Cl1	1.743 (3)	C14—H10	0.9300
C5—C6	1.377 (4)	N1—C9^{i}	1.332 (3)
C5—H3	0.9300	N1—Ni1	2.124 (3)

C6—H4	0.9300	N2—C14^{i}	1.343 (3)
C7—C8	1.531 (3)	N2—Ni1^{ii}	2.125 (4)
C7—S1	1.799 (2)	Ni1—O3^{i}	2.0657 (16)
C7—H5	0.9700	Ni1—O3	2.0657 (17)
C7—H6	0.9700	Ni1—O4	2.0799 (16)
C8—O2	1.249 (3)	Ni1—O4^{i}	2.0799 (16)
C8—O3	1.255 (3)	Ni1—N2^{iii}	2.125 (4)
C9—N1	1.332 (3)	O1—S1	1.503 (2)
C9—C10	1.381 (5)	O4—H12	0.8501
C9—H7	0.9300	O4—H11	0.8500
C10—C11	1.384 (4)		
C6—C1—C2	120.9 (3)	C13^{i}—C12—C11	121.7 (2)
C6—C1—S1	119.7 (2)	C13—C12—C11	121.7 (2)
C2—C1—S1	119.3 (2)	C14—C13—C12	119.9 (3)
C3—C2—C1	119.6 (3)	C14—C13—H9	120.0
C3—C2—H1	120.2	C12—C13—H9	120.0
C1—C2—H1	120.2	N2—C14—C13	123.7 (3)
C2—C3—C4	118.9 (3)	N2—C14—H10	118.2
C2—C3—H2	120.6	C13—C14—H10	118.2
C4—C3—H2	120.6	C9—N1—C9^{i}	117.5 (3)
C3—C4—C5	122.0 (3)	C9—N1—Ni1	121.27 (17)
C3—C4—Cl1	118.7 (3)	C9^{i}—N1—Ni1	121.27 (17)
C5—C4—Cl1	119.3 (3)	C14—N2—C14^{i}	116.1 (4)
C4—C5—C6	118.5 (3)	C14—N2—Ni1^{ii}	121.96 (18)
C4—C5—H3	120.7	C14^{i}—N2—Ni1^{ii}	121.96 (18)
C6—C5—H3	120.7	O3^{i}—Ni1—O3	176.36 (10)
C1—C6—C5	120.1 (3)	O3^{i}—Ni1—O4	90.39 (7)
C1—C6—H4	120.0	O3—Ni1—O4	89.58 (7)
C5—C6—H4	120.0	O3^{i}—Ni1—O4^{i}	89.58 (7)
C8—C7—S1	110.14 (17)	O3—Ni1—O4^{i}	90.39 (7)
C8—C7—H5	109.6	O4—Ni1—O4^{i}	179.11 (10)
S1—C7—H5	109.6	O3^{i}—Ni1—N1	88.18 (5)
C8—C7—H6	109.6	O3—Ni1—N1	88.18 (5)
S1—C7—H6	109.6	O4—Ni1—N1	89.56 (5)
H5—C7—H6	108.1	O4^{i}—Ni1—N1	89.56 (5)
O2—C8—O3	127.4 (2)	O3^{i}—Ni1—N2^{iii}	91.82 (5)
O2—C8—C7	117.6 (2)	O3—Ni1—N2^{iii}	91.82 (5)
O3—C8—C7	115.0 (2)	O4—Ni1—N2^{iii}	90.44 (5)
N1—C9—C10	123.0 (3)	O4^{i}—Ni1—N2^{iii}	90.44 (5)
N1—C9—H7	118.5	N1—Ni1—N2^{iii}	180.000 (1)
C10—C9—H7	118.5	C8—O3—Ni1	128.23 (15)
C9—C10—C11	119.6 (3)	Ni1—O4—H12	106.1
C9—C10—H8	120.2	Ni1—O4—H11	118.7
C11—C10—H8	120.2	H12—O4—H11	99.4

C10—C11—C10^{i}	117.3 (4)	O1—S1—C7	104.83 (13)
C10—C11—C12	121.4 (2)	O1—S1—C1	105.96 (13)
C10^{i}—C11—C12	121.4 (2)	C7—S1—C1	97.25 (11)
C13^{i}—C12—C13	116.6 (4)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H11···S1^{iv}	0.85	2.98	3.822 (2)	173
O4—H11···O1^{iv}	0.85	1.89	2.709 (3)	160
O4—H12···O2^{i}	0.85	1.85	2.643 (3)	154

Symmetry codes: (iv) *x*+1/4, −*y*+1/4, *z*+1/4; (i) −*x*, −*y*, *z*.

Fig. 1

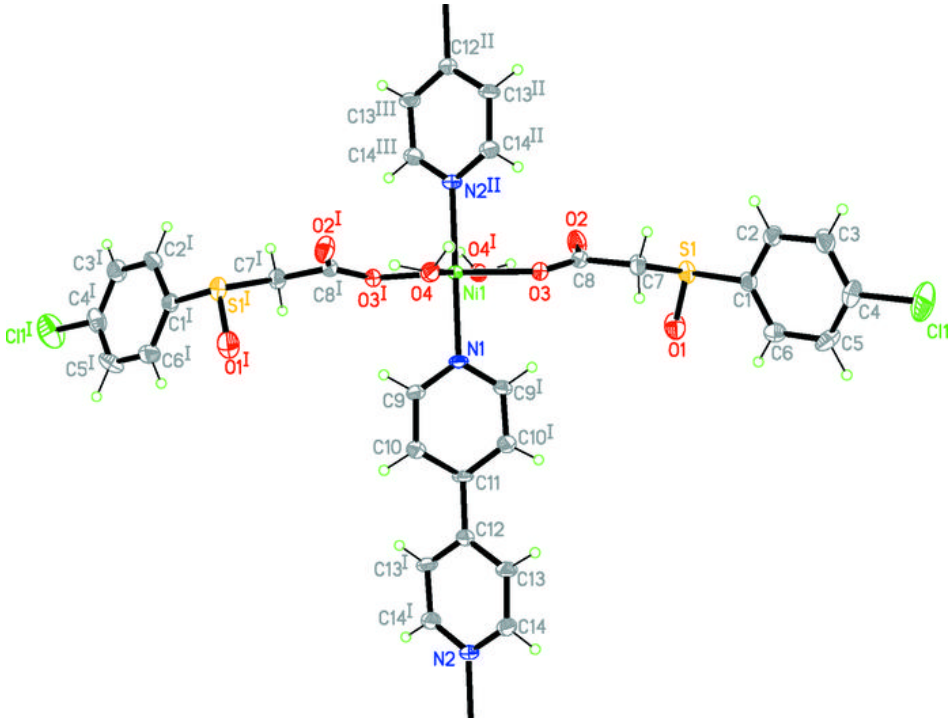
C12II
C13III
C13II
C14III
C14II
N2II
O2I
O4I
O2
S1
C2
C3
C3I
C2I
C7I
C8I
O3I
O4
Ni1
O3
C8
C7
C1
C4
C4I
S1I
C1I
Cl1I
O1I
O1
Cl1
C5I
C6I
C6
C5
N1
C9
C9I
C10
C10I
C11
C12
C13I
C13
C14I
C14
N2

Fig. 2