

Chlorido{1-[2-(methylsulfonyl)phenyl-diazenyl]naphtholato- κ^3 O,N,S}nickel(II)

Purak Das* and Achintesh Narayan Biswas

Department of Chemistry, University of North Bengal, Siliguri 734 013, India
Correspondence e-mail: purak_nbu@rediffmail.com

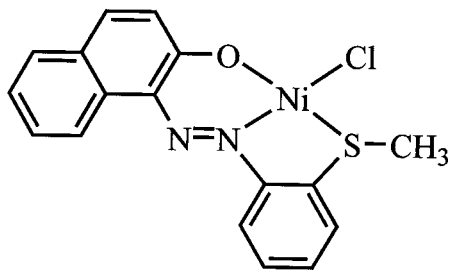
Received 8 October 2007; accepted 10 October 2007

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.045; wR factor = 0.113; data-to-parameter ratio = 13.1.

The Ni atom in the title compound, $[\text{Ni}(\text{C}_{17}\text{H}_{19}\text{N}_2\text{S})\text{Cl}]$, is tetracoordinated by a naphtholate O atom, a diazene N atom, a Cl atom and an S atom in an approximately square-planar geometry. The crystal packing is stabilized by one intermolecular $\text{C}-\text{H}\cdots\text{Cl}$ interaction and two intermolecular $\pi-\pi$ interactions; the centroid-to-centroid distances are 3.745 (3) and 3.744 (3) Å, and the corresponding perpendicular distances are 3.528 and 3.541 Å, respectively.

Related literature

For related literature, see: Ali *et al.* (2002); Bagchi *et al.* (2007); Das *et al.* (2006); Barber *et al.* (1992); Lu *et al.* (1993).



Experimental

Crystal data

$[\text{Ni}(\text{C}_{17}\text{H}_{19}\text{N}_2\text{S})\text{Cl}]$	$V = 1546.2$ (3) Å ³
$M_r = 387.51$	$Z = 4$
Orthorhombic, $Pn2_1a$	Mo $K\alpha$ radiation
$a = 28.717$ (4) Å	$\mu = 1.57$ mm ⁻¹
$b = 11.5393$ (14) Å	$T = 293$ (2) K
$c = 4.6660$ (6) Å	$0.42 \times 0.30 \times 0.19$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	13677 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	2728 independent reflections
$T_{\min} = 0.581$, $T_{\max} = 0.744$	2579 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.050$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$	H-atom parameters constrained
$wR(F^2) = 0.113$	$\Delta\rho_{\text{max}} = 0.64$ e Å ⁻³
$S = 1.19$	$\Delta\rho_{\text{min}} = -0.51$ e Å ⁻³
2728 reflections	Absolute structure: Flack (1983),
209 parameters	with 1292 Freidel pairs
1 restraint	Flack parameter: 0.04 (2)

Table 1

Selected geometric parameters (Å, °).

Ni1—O1	1.836 (4)	Ni1—S1	2.1516 (14)
Ni1—N2	1.860 (4)	Ni1—Cl1	2.2009 (15)
O1—Ni1—N2	94.14 (16)	O1—Ni1—Cl1	89.69 (12)
N2—Ni1—S1	89.52 (12)	S1—Ni1—Cl1	87.04 (6)

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C17}-\text{H17C}\cdots\text{Cl1}^i$	0.96	2.70	3.628 (6)	163

Symmetry code: (i) $x, y, z - 1$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXTL.

Financial support in the form of a fellowship to PD from CSIR (India) is gratefully acknowledged. The authors thank Dr P. Bandyopadhyay, Department of Chemistry, University of North Bengal, for providing laboratory facilities, and Mr Vivek Bagchi, Department of Chemistry, IIT Delhi, for the X-ray crystallographic data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2422).

References

- Ali, M. A., Mirza, A. H., Nazimuddin, M., Dhar, P. K. & Butcher, R. J. (2002). *Transition Met. Chem.* **27**, 27–33.
- Bagchi, V., Das, P. & Bandyopadhyay, D. (2007). *Acta Cryst.* **E63**, m2130.
- Barber, D., Lu, Z., Richardson, T. & Crabtree, R. (1992). *Inorg. Chem.* **31**, 4709–4711.
- Bruker (1997). SHELXTL. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (1998). SMART. Version 5.054. Bruker AXS Inc. Madison, Wisconsin, USA.
- Bruker (2000). SAINT (Version 6.02a). Bruker AXS Inc. Madison, Wisconsin, USA.
- Das, P., Biswas, A. N., Neogi, D. N., Bhawmick, R. & Bandyopadhyay, P. (2006). *Acta Cryst.* **E62**, o5536–o5538.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Lu, Z., White, C., Rheingol, A. & Crabtree, R. (1993). *Angew. Chem. Int. Ed. Engl.* **32**, 92–94.
- Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.

supplementary materials

Acta Cryst. (2007). E63, m2740 [doi:10.1107/S1600536807049719]

Chlorido{1-[2-(methylsulfanyl)phenyldiazenyl]naphtholato- κ^3 O,N,S}nickel(II)

P. Das and A. N. Biswas

Comment

Due to their potential biological activities, square planar Ni(II) complexes of various tridentate ONS ligands have been the subject of recent studies (Ali *et al.* 2002). Some of them have also been found to catalyse important reactions related to CO-dehydrogenase and silane alcoholysis (Lu *et al.*, 1993; Barber *et al.*, 1992). Against this background, we report here the crystal structure of (**I**).

The molecular structure of the title compound, (**I**), is shown in Fig. 1, with the atom numbering scheme. The nickel atom along with donor set of four atoms lie nearly in a plane. Selected bond lengths, bond angles and torsion angles are listed in Table 1. The packing arrangement of (**I**) is shown in Fig. 2. The N=N bond length 1.286 (5) is slightly greater than that in the free azoarenes (Das *et al.*, 2006). Two nearly planar fragment in the molecular structure of (**I**) may be identified: the nickel atom, diazene unit, the chlorine atom and the naphtholato unit (*A*), the sulfur atom and the phenyl moiety (*B*). The dihedral angle between the planes *A/B* is 4.15 (16)°. The crystal packing is stabilized by one intermolecular C—H...Clⁱ [Symmetry code: (i) *x*, *y*, -1 + *z*.] interaction (Fig. 3; Table 2) and two intermolecular π — π interactions (Bagchi *et al.*, 2007); the *Cg3*—*Cg4*ⁱⁱ and *Cg4*—*Cg3*ⁱⁱⁱ [Symmetry codes: (ii) *x*, *y*, 1 + *z*; (iii) *x*, *y*, -1 + *z*. *Cg3* and *Cg4* are the centroids of C1—C10 and C5—C9 rings respectively.] distances are 3.745 (3) and 3.744 (3) Å (Fig. 4); the corresponding perpendicular distances are 3.528 and 3.541 Å respectively. No C—H... π (arene) interaction is present in (**I**).

Experimental

The title compound was synthesized by boiling 1-{2-(methylsulfanyl)phenyldiazenyl}naphthol and NiCl₂·2H₂O in aqueous ethanol on water bath for one hour. The resulting precipitate was recrystallized from dichloromethane–hexane(1:4 v/v) producing crystals suitable for X-ray crystallography. Yield: 65%.

Refinement

H atoms were included at calculated positions as riding atoms with C—H set to 0.93 Å for (aromatic) and 0.96 Å for (CH₃) H atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ (1.5 U_{eq} for methyl group).

Figures

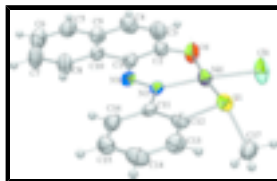


Fig. 1. The asymmetric unit of (**I**), with displacement ellipsoids drawn at the 50% probability level.

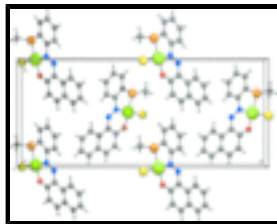


Fig. 2. The molecular arrangement of (I) in the *ab* plane.

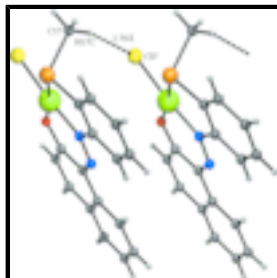


Fig. 3. The intra molecular C—H...Cl interaction in (I) shown by dotted line [Symmetry code: (i) $x, y, -1 + z$].

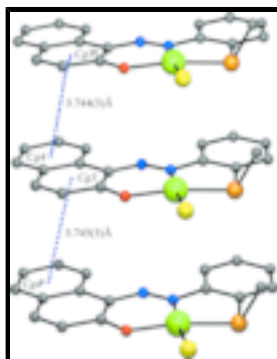


Fig. 4. The inter molecular π — π interaction for (I), indicated by the dotted line. [Symmetry codes: (ii) $x, y, 1 + z$; (iii) $x, y, -1 + z$. *Cg3* & *Cg4* are the centroids of C1—C10 & C5—C9 rings respectively.], H atoms are omitted for clarity.

Chlorido{1-[2-(methylsulfanyl)phenyldiazenyl]naphtholato- $\kappa^3 O, N, S$ }nickel(II)

Crystal data

[Ni(C₁₇H₁₉N₂S)Cl]

$M_r = 387.51$

Orthorhombic, $Pn2_1a$

Hall symbol: P -2ac -2n

$a = 28.717$ (4) Å

$b = 11.5393$ (14) Å

$c = 4.6660$ (6) Å

$V = 1546.2$ (3) Å³

$Z = 4$

$F_{000} = 792$

$D_x = 1.665$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 2728 reflections

$\theta = 1.4$ – 25.0°

$\mu = 1.57$ mm⁻¹

$T = 293$ (2) K

Block, brown

$0.42 \times 0.30 \times 0.19$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

2728 independent reflections

2579 reflections with $I > 2\sigma(I)$

$R_{int} = 0.050$

$T = 293(2)$ K
 $\theta_{\max} = 25.0^\circ$
 φ and ω scans
 $\theta_{\min} = 1.4^\circ$
Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)
 $h = -34 \rightarrow 34$
 $T_{\min} = 0.581$, $T_{\max} = 0.744$
 $k = -13 \rightarrow 13$
13677 measured reflections
 $l = -5 \rightarrow 5$

Refinement

Refinement on F^2
Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full
H-atom parameters constrained
 $R[F^2 > 2\sigma(F^2)] = 0.045$
 $w = 1/[\sigma^2(F_o^2) + (0.0638P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $wR(F^2) = 0.113$
 $(\Delta/\sigma)_{\max} = 0.001$
 $S = 1.19$
 $\Delta\rho_{\max} = 0.64 \text{ e } \text{\AA}^{-3}$
2728 reflections
 $\Delta\rho_{\min} = -0.50 \text{ e } \text{\AA}^{-3}$
209 parameters
Extinction correction: none
1 restraint
Absolute structure: Flack (1983), with 1292 Freidel pairs
Primary atom site location: structure-invariant direct methods
Flack parameter: 0.04 (2)
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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.56150 (2)	0.00129 (5)	0.28733 (11)	0.03227 (19)
S1	0.54404 (5)	0.18260 (11)	0.2816 (3)	0.0355 (3)
O1	0.57767 (14)	-0.1511 (3)	0.3416 (8)	0.0424 (9)
C12	0.58366 (17)	0.2283 (5)	0.0137 (10)	0.0347 (11)
C2	0.61100 (19)	-0.2046 (5)	0.2164 (10)	0.0359 (12)
C1	0.64243 (17)	-0.1529 (4)	0.0188 (11)	0.0328 (11)
C11	0.61433 (15)	0.1454 (4)	-0.0855 (10)	0.0284 (10)
N1	0.64058 (13)	-0.0413 (3)	-0.0621 (8)	0.0315 (9)
C8	0.7118 (2)	-0.1748 (5)	-0.3035 (12)	0.0465 (14)

supplementary materials

H8	0.7099	-0.0971	-0.3552	0.056*
C3	0.6169 (2)	-0.3253 (5)	0.2821 (12)	0.0470 (14)
H3	0.5963	-0.3608	0.4083	0.056*
C16	0.64729 (18)	0.1740 (5)	-0.2918 (11)	0.0390 (12)
H16	0.6678	0.1184	-0.3621	0.047*
C4	0.6514 (2)	-0.3882 (5)	0.1664 (11)	0.0472 (15)
H4	0.6542	-0.4658	0.2174	0.057*
C14	0.6185 (2)	0.3707 (5)	-0.2884 (11)	0.0488 (15)
H14	0.6200	0.4462	-0.3576	0.059*
C10	0.67968 (17)	-0.2211 (5)	-0.1069 (11)	0.0344 (11)
C15	0.64898 (19)	0.2874 (5)	-0.3907 (12)	0.0408 (13)
H15	0.6710	0.3077	-0.5280	0.049*
C9	0.68426 (19)	-0.3401 (5)	-0.0339 (12)	0.0408 (13)
N2	0.60954 (13)	0.0300 (3)	0.0295 (8)	0.0270 (9)
C17	0.4890 (2)	0.2028 (5)	0.1036 (14)	0.0492 (15)
H17A	0.4859	0.2823	0.0462	0.074*
H17B	0.4642	0.1830	0.2322	0.074*
H17C	0.4876	0.1539	-0.0625	0.074*
C5	0.7201 (2)	-0.4051 (6)	-0.1506 (12)	0.0472 (14)
H5	0.7233	-0.4823	-0.0975	0.057*
C13	0.58585 (19)	0.3419 (4)	-0.0849 (11)	0.0391 (12)
H13	0.5655	0.3977	-0.0140	0.047*
C7	0.7461 (2)	-0.2437 (5)	-0.4200 (15)	0.0557 (16)
H7	0.7666	-0.2127	-0.5541	0.067*
C6	0.7505 (2)	-0.3591 (5)	-0.3389 (13)	0.0548 (16)
H6	0.7742	-0.4045	-0.4146	0.066*
Cl1	0.50075 (5)	-0.02334 (13)	0.5684 (4)	0.0566 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0357 (3)	0.0281 (3)	0.0330 (3)	-0.0016 (3)	0.0049 (2)	0.0013 (4)
S1	0.0442 (8)	0.0305 (7)	0.0318 (7)	0.0008 (6)	0.0014 (5)	-0.0027 (6)
O1	0.042 (2)	0.030 (2)	0.054 (2)	0.0021 (17)	0.0135 (19)	0.0033 (17)
C12	0.041 (3)	0.032 (2)	0.031 (3)	-0.004 (2)	-0.004 (2)	0.003 (2)
C2	0.039 (3)	0.034 (3)	0.035 (3)	0.000 (2)	0.001 (2)	0.002 (2)
C1	0.030 (3)	0.030 (3)	0.038 (3)	-0.002 (2)	0.000 (2)	0.002 (2)
C11	0.025 (2)	0.029 (2)	0.031 (3)	-0.002 (2)	-0.009 (2)	0.006 (2)
N1	0.030 (2)	0.030 (2)	0.035 (2)	0.0012 (17)	-0.0033 (18)	0.0008 (17)
C8	0.045 (3)	0.040 (3)	0.055 (4)	0.002 (3)	0.014 (3)	0.002 (3)
C3	0.054 (4)	0.034 (3)	0.053 (3)	0.001 (3)	0.008 (3)	0.012 (3)
C16	0.032 (3)	0.038 (3)	0.047 (3)	-0.002 (2)	0.000 (2)	0.005 (2)
C4	0.066 (4)	0.031 (3)	0.045 (3)	0.006 (3)	0.002 (3)	0.008 (2)
C14	0.069 (4)	0.034 (3)	0.043 (3)	-0.005 (3)	-0.007 (3)	0.010 (3)
C10	0.030 (3)	0.038 (3)	0.035 (3)	0.001 (2)	-0.002 (2)	0.004 (2)
C15	0.039 (3)	0.041 (3)	0.042 (3)	-0.009 (2)	0.001 (2)	0.012 (2)
C9	0.047 (3)	0.033 (3)	0.042 (3)	0.005 (2)	-0.001 (2)	-0.003 (2)
N2	0.023 (2)	0.028 (2)	0.030 (2)	-0.0004 (17)	-0.0031 (16)	0.0012 (16)

C17	0.043 (3)	0.055 (4)	0.050 (3)	0.012 (3)	-0.001 (3)	-0.013 (3)
C5	0.050 (4)	0.036 (3)	0.056 (3)	0.014 (3)	-0.004 (3)	0.002 (3)
C13	0.050 (3)	0.022 (3)	0.045 (3)	0.008 (2)	-0.001 (3)	0.002 (2)
C7	0.046 (3)	0.051 (4)	0.070 (4)	0.002 (3)	0.021 (3)	0.009 (3)
C6	0.049 (4)	0.051 (4)	0.064 (4)	0.009 (3)	0.010 (3)	-0.013 (3)
C11	0.0605 (9)	0.0400 (8)	0.0694 (10)	-0.0014 (6)	0.0323 (7)	0.0028 (7)

Geometric parameters (Å, °)

Ni1—O1	1.836 (4)	C3—H3	0.9300
Ni1—N2	1.860 (4)	C16—C15	1.388 (8)
Ni1—S1	2.1516 (14)	C16—H16	0.9300
Ni1—C11	2.2009 (15)	C4—C9	1.439 (8)
S1—C12	1.771 (5)	C4—H4	0.9300
S1—C17	1.800 (6)	C14—C13	1.374 (8)
O1—C2	1.280 (6)	C14—C15	1.386 (8)
C12—C11	1.380 (7)	C14—H14	0.9300
C12—C13	1.391 (7)	C10—C9	1.421 (7)
C2—C1	1.421 (7)	C15—H15	0.9300
C2—C3	1.437 (8)	C9—C5	1.385 (8)
C1—N1	1.343 (6)	C17—H17A	0.9600
C1—C10	1.452 (7)	C17—H17B	0.9600
C11—C16	1.390 (7)	C17—H17C	0.9600
C11—N2	1.442 (6)	C5—C6	1.346 (8)
N1—N2	1.286 (5)	C5—H5	0.9300
C8—C7	1.379 (8)	C13—H13	0.9300
C8—C10	1.407 (8)	C7—C6	1.390 (8)
C8—H8	0.9300	C7—H7	0.9300
C3—C4	1.341 (8)	C6—H6	0.9300
O1—Ni1—N2	94.14 (16)	C9—C4—H4	118.8
O1—Ni1—S1	172.66 (13)	C13—C14—C15	120.0 (5)
N2—Ni1—S1	89.52 (12)	C13—C14—H14	120.0
O1—Ni1—C11	89.69 (12)	C15—C14—H14	120.0
N2—Ni1—C11	175.02 (12)	C8—C10—C9	117.6 (5)
S1—Ni1—C11	87.04 (6)	C8—C10—C1	122.7 (5)
C12—S1—C17	101.5 (3)	C9—C10—C1	119.7 (5)
C12—S1—Ni1	98.54 (19)	C14—C15—C16	121.2 (5)
C17—S1—Ni1	109.6 (2)	C14—C15—H15	119.4
C2—O1—Ni1	126.0 (3)	C16—C15—H15	119.4
C11—C12—C13	120.9 (5)	C5—C9—C10	119.8 (5)
C11—C12—S1	116.2 (4)	C5—C9—C4	122.3 (5)
C13—C12—S1	122.9 (4)	C10—C9—C4	117.9 (5)
O1—C2—C1	124.7 (5)	N1—N2—C11	113.7 (4)
O1—C2—C3	117.3 (5)	N1—N2—Ni1	127.9 (3)
C1—C2—C3	118.0 (5)	C11—N2—Ni1	118.4 (3)
N1—C1—C2	124.0 (5)	S1—C17—H17A	109.5
N1—C1—C10	115.8 (5)	S1—C17—H17B	109.5
C2—C1—C10	120.2 (5)	H17A—C17—H17B	109.5
C12—C11—C16	120.2 (5)	S1—C17—H17C	109.5

supplementary materials

C12—C11—N2	117.0 (4)	H17A—C17—H17C	109.5
C16—C11—N2	122.8 (4)	H17B—C17—H17C	109.5
N2—N1—C1	123.2 (4)	C6—C5—C9	121.6 (6)
C7—C8—C10	120.4 (6)	C6—C5—H5	119.2
C7—C8—H8	119.8	C9—C5—H5	119.2
C10—C8—H8	119.8	C14—C13—C12	119.2 (5)
C4—C3—C2	121.8 (5)	C14—C13—H13	120.4
C4—C3—H3	119.1	C12—C13—H13	120.4
C2—C3—H3	119.1	C8—C7—C6	120.6 (6)
C15—C16—C11	118.5 (5)	C8—C7—H7	119.7
C15—C16—H16	120.7	C6—C7—H7	119.7
C11—C16—H16	120.7	C5—C6—C7	119.8 (5)
C3—C4—C9	122.5 (5)	C5—C6—H6	120.1
C3—C4—H4	118.8	C7—C6—H6	120.1
N2—Ni1—S1—C12	5.10 (19)	C2—C1—C10—C8	180.0 (5)
C11—Ni1—S1—C12	-171.29 (17)	N1—C1—C10—C9	-179.9 (5)
N2—Ni1—S1—C17	110.7 (3)	C2—C1—C10—C9	0.7 (7)
C11—Ni1—S1—C17	-65.7 (2)	C13—C14—C15—C16	0.2 (9)
N2—Ni1—O1—C2	-2.0 (4)	C11—C16—C15—C14	-0.3 (8)
C11—Ni1—O1—C2	174.8 (4)	C8—C10—C9—C5	1.5 (8)
C17—S1—C12—C11	-117.6 (4)	C1—C10—C9—C5	-179.2 (5)
Ni1—S1—C12—C11	-5.4 (4)	C8—C10—C9—C4	-179.8 (5)
C17—S1—C12—C13	65.3 (5)	C1—C10—C9—C4	-0.4 (8)
Ni1—S1—C12—C13	177.5 (4)	C3—C4—C9—C5	179.3 (6)
Ni1—O1—C2—C1	2.3 (7)	C3—C4—C9—C10	0.6 (9)
Ni1—O1—C2—C3	-177.9 (4)	C1—N1—N2—C11	179.9 (4)
O1—C2—C1—N1	-0.6 (8)	C1—N1—N2—Ni1	0.6 (6)
C3—C2—C1—N1	179.6 (5)	C12—C11—N2—N1	-176.9 (4)
O1—C2—C1—C10	178.8 (5)	C16—C11—N2—N1	4.5 (6)
C3—C2—C1—C10	-1.0 (7)	C12—C11—N2—Ni1	2.5 (5)
C13—C12—C11—C16	-1.6 (8)	C16—C11—N2—Ni1	-176.1 (4)
S1—C12—C11—C16	-178.8 (4)	O1—Ni1—N2—N1	0.7 (4)
C13—C12—C11—N2	179.8 (4)	S1—Ni1—N2—N1	174.3 (4)
S1—C12—C11—N2	2.6 (6)	O1—Ni1—N2—C11	-178.6 (3)
C2—C1—N1—N2	-0.9 (8)	S1—Ni1—N2—C11	-5.0 (3)
C10—C1—N1—N2	179.7 (4)	C10—C9—C5—C6	-1.7 (9)
O1—C2—C3—C4	-178.6 (5)	C4—C9—C5—C6	179.6 (6)
C1—C2—C3—C4	1.2 (8)	C15—C14—C13—C12	-0.7 (8)
C12—C11—C16—C15	1.0 (8)	C11—C12—C13—C14	1.4 (8)
N2—C11—C16—C15	179.6 (4)	S1—C12—C13—C14	178.4 (4)
C2—C3—C4—C9	-1.0 (9)	C10—C8—C7—C6	-1.9 (10)
C7—C8—C10—C9	0.3 (9)	C9—C5—C6—C7	0.1 (10)
C7—C8—C10—C1	-179.0 (5)	C8—C7—C6—C5	1.7 (10)
N1—C1—C10—C8	-0.6 (8)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C17—H17C \cdots C11 ⁱ	0.96	2.70	3.628 (6)	163

Symmetry codes: (i) $x, y, z-1$.

Fig. 1

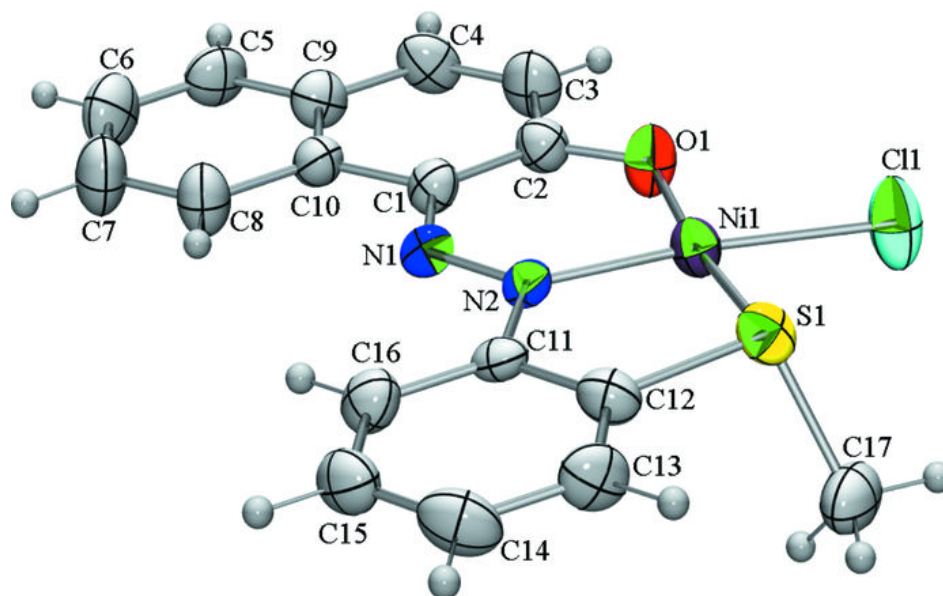


Fig. 2

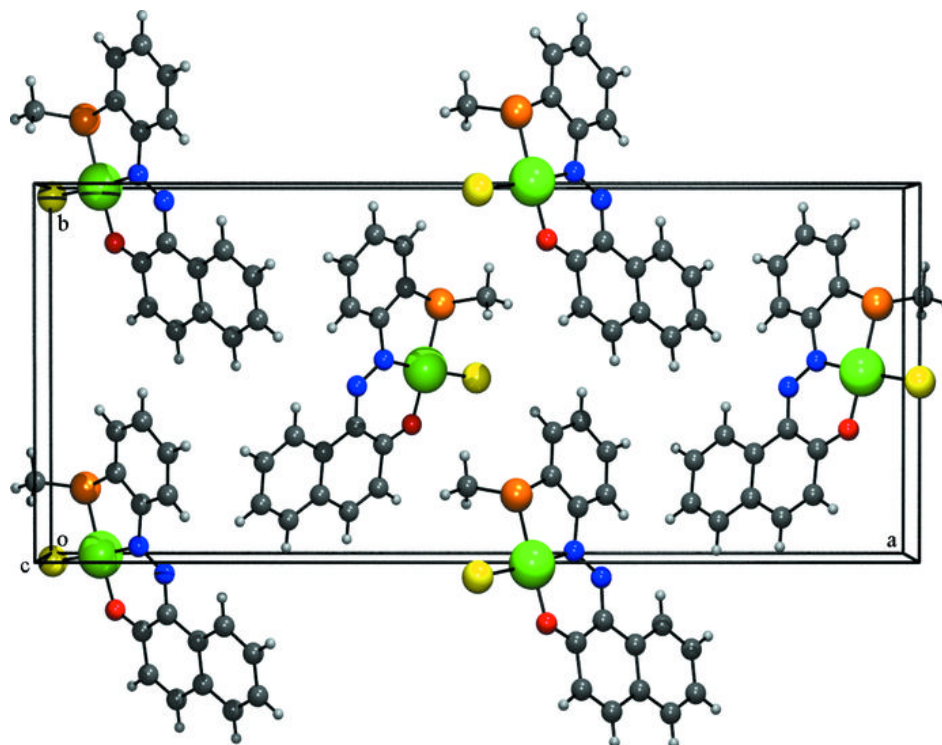


Fig. 3

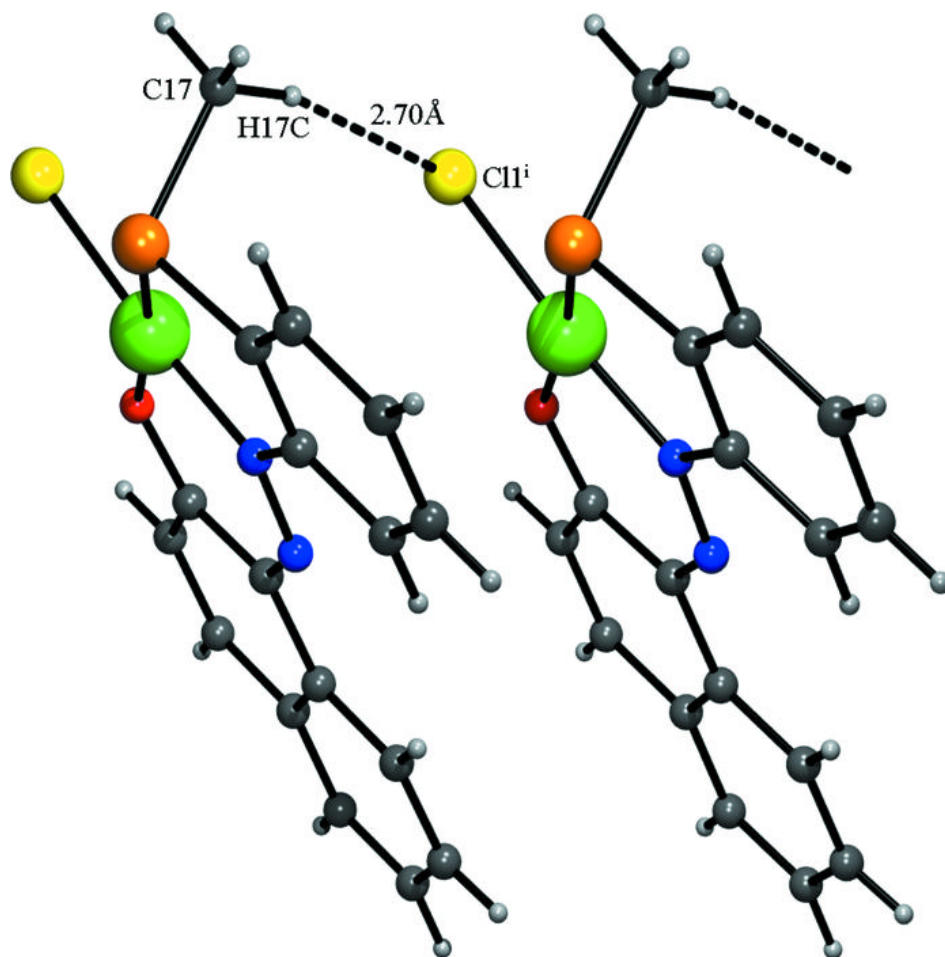


Fig. 4

