

Bis(2-dimethylamino-1,10-phenanthroline- κ^2N,N')bis(thiocyanato- κN)nickel(II) methanol disolvate

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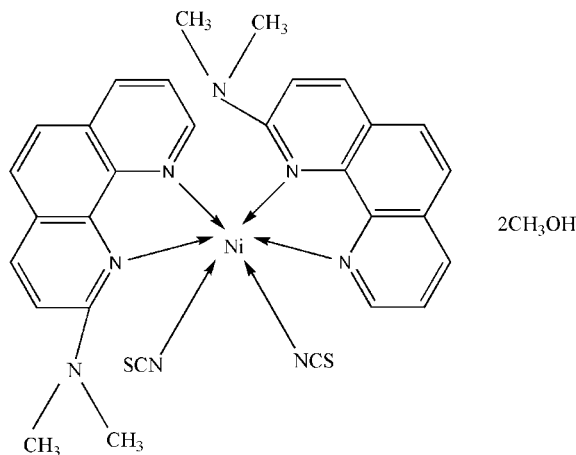
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.041; wR factor = 0.100; data-to-parameter ratio = 14.6.

In the title complex, $[\text{Ni}(\text{NCS})_2(\text{C}_{14}\text{H}_{13}\text{N}_3)_2] \cdot 2\text{CH}_3\text{OH}$, the Ni^{II} atom lies on a crystallographic twofold rotation axis and is in a slightly distorted octahedral NiN_6 coordination environment. The crystal structure is stabilized by a combination of weak π - π stacking interactions between symmetry-related 1,10-phenanthroline ligands [centroid-centroid distance between benzene rings = $3.5936(18)$ Å] and weak $\text{O}-\text{H} \cdots \text{S}$, $\text{C}-\text{H} \cdots \text{O}$ and $\text{C}-\text{H} \cdots \text{S}$ hydrogen bonds between methanol and complex molecules.

Related literature

 For related literature, see: Zhang *et al.* (2006); Liu *et al.* (2008).


Experimental

Crystal data

 $[\text{Ni}(\text{NCS})_2(\text{C}_{14}\text{H}_{13}\text{N}_3)_2] \cdot 2\text{CH}_3\text{OH}$
 $M_r = 685.50$

 Monoclinic, $C2/c$
 $a = 19.573(3)$ Å

 $b = 11.452(3)$ Å
 $c = 16.338(3)$ Å
 $\beta = 117.693(4)^\circ$
 $V = 3242.6(10)$ Å³
 $Z = 4$

 Mo $K\alpha$ radiation
 $\mu = 0.77$ mm⁻¹
 $T = 298(2)$ K
 $0.31 \times 0.24 \times 0.21$ mm

Data collection

 Bruker SMART APEX CCD diffractometer
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\text{min}} = 0.796$, $T_{\text{max}} = 0.855$

 8459 measured reflections
 3064 independent reflections
 2668 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.100$
 $S = 1.05$
 3064 reflections

 210 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.52$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.27$ e Å⁻³
Table 1

Selected geometric parameters (Å, °).

N1—Ni1	2.0569 (19)	N3—Ni1	2.047 (2)
N2—Ni1	2.2556 (18)		
N3 ⁱ —Ni1—N3	90.27 (11)	N1—Ni1—N2	77.31 (7)
N3—Ni1—N1 ⁱ	93.08 (7)	N3—Ni1—N2 ⁱ	167.90 (7)
N3—Ni1—N1	88.63 (7)	N1—Ni1—N2 ⁱ	100.76 (7)
N1 ⁱ —Ni1—N1	177.57 (10)	N2—Ni1—N2 ⁱ	78.13 (9)
N3—Ni1—N2	96.75 (7)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
C14—H14C ⁱⁱ ···S1 ⁱⁱⁱ	0.96	2.86	3.784 (3)	163
O1—H4 ⁱⁱⁱ ···S1 ⁱⁱⁱ	0.82	2.65	3.331 (2)	142
C15—H15B ^{iv} ···O1 ^{iv}	0.96	2.51	3.427 (4)	161

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: LH2613).

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supplementary materials

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S. G. Zhang, T. Q. Hu and H. Li

Comment

The derivatives of 1,10-phenanthroline play a pivotal role in the area of modern coordination chemistry (Zhang *et al.* 2006) and a number of complexes have been reported with derivatives as ligands (Liu *et al.* 2008). Here we report the crystal structure of the title complex, (I), formed using 2-(dimethyl)amine-1,10-phenanthroline as a ligand.

The molecular structure of (I) is shown in Fig. 1. In the mononuclear complex, atom Ni1 is in a slightly distorted octahedral geometry (Table 1). There is a single π - π stacking interaction involving symmetry related 1,10-phenanthroline ligands, with the the relevant distances being $Cg1 \cdots Cg1^i = 3.5936$ (18) Å and $Cg1 \cdots Cg1_{\text{perp}}^i = 3.449$ Å; $\alpha = 0.00^\circ$ [symmetry code: (i) 1-*x*, -*y*, -*z*; Cg1 is the centroid of the C4—C9 ring; $Cg1 \cdots Cg1_{\text{perp}}$ is the perpendicular distance from ring Cg1 to ring $Cg1^i$; α is the dihedral between the two ring planes]. In addition, the crystal structure contains weak O—H \cdots S, C—H \cdots O and C—H \cdots S hydrogen bonds between methanol molecules and complex molecules [Fig. 2 and Table 2]. In addition to the π - π stacking interactions and the hydrogen bonds there is relatively close contact between the H atom of the hydroxyl and symmetry-related pyridine ring [$H \cdots Cg2 = 2.82$, where Cg2 is the centroid of N1/C1—C5 ring]. The combination of the above interactions help stabilize the crystal structure.

Experimental

15 ml methanol solution of $Ni(ClO_4) \cdot 6H_2O$ (0.2503 g, 0.684 mmol) was added into a 10 ml methanol solution containing 2-(dimethyl)amine-1,10-phenanthroline (0.1531 g, 0.686 mmol), and the mixed solution was stirred for a few minutes. Then 10 ml methanol solution of NaSCN (0.1112 g, 1.37 mmol) was added into the mixed solution above. The green single crystals were obtained after the solution had been allowed to stand at room temperature for two weeks.

Refinement

H atom of hydroxyl was located in a difference Fourier map and refined as riding in its as found position with $U_{\text{iso}}(H) = 1.5 U_{\text{eq}}(O)$. Other H atoms were placed in calculated positions (C—H = 0.96 Å for methyl group and C—H = 0.93 Å for other H atoms) and refined as riding with $U_{\text{iso}} = 1.5 U_{\text{eq}}(C)$ for methyl H and $U_{\text{iso}} = 1.2 U_{\text{eq}}(C)$ for other H atoms.

Figures

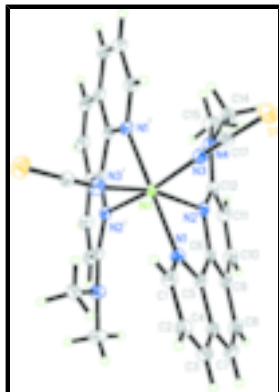


Fig. 1. View of the molecular structure of complex (I), showing the the atom numbering scheme with thermal ellipsoids drawn at the 30% probability level (methanol molecules are not shown). Primed atoms are related by the symmetry operator $(-x+1, y, -z+1/2)$.

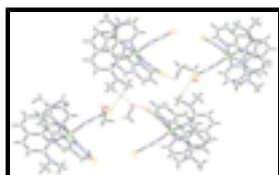


Fig. 2. Part of the crystal structure showing hydrogen bonds between methanol molecules and complex molecules (dashed lines).

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Crystal data

$[\text{Ni}(\text{NCS})_2(\text{C}_{14}\text{H}_{13}\text{N}_3)_2] \cdot 2\text{CH}_4\text{O}$

$M_r = 685.50$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 19.573\ (3)\ \text{\AA}$

$b = 11.452\ (3)\ \text{\AA}$

$c = 16.338\ (3)\ \text{\AA}$

$\beta = 117.693\ (4)^\circ$

$V = 3242.6\ (10)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 1432$

$D_x = 1.404\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3100 reflections

$\theta = 2.4\text{--}27.8^\circ$

$\mu = 0.77\ \text{mm}^{-1}$

$T = 298\ (2)\ \text{K}$

Block, green

$0.31 \times 0.24 \times 0.21\ \text{mm}$

Data collection

Bruker SMART APEX CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298\ (2)\ \text{K}$

ϕ and ω scans

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

$T_{\min} = 0.796$, $T_{\max} = 0.855$

8459 measured reflections

3064 independent reflections

2668 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.030$

$\theta_{\text{max}} = 25.7^\circ$

$\theta_{\text{min}} = 2.1^\circ$

$h = -18 \rightarrow 23$

$k = -12 \rightarrow 13$

$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H-atom parameters constrained
$wR(F^2) = 0.100$	$w = 1/[\sigma^2(F_o^2) + (0.0522P)^2 + 2.7575P]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
3064 reflections	$(\Delta/\sigma)_{\max} < 0.001$
210 parameters	$\Delta\rho_{\max} = 0.52 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.27 \text{ e } \text{\AA}^{-3}$
	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 $F^2 > \sigma(F^2)$ 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	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.38579 (14)	-0.2002 (2)	0.05726 (16)	0.0324 (6)
H1	0.3846	-0.2706	0.0850	0.039*
C2	0.33596 (15)	-0.1849 (2)	-0.03666 (17)	0.0385 (6)
H2	0.3033	-0.2451	-0.0711	0.046*
C3	0.33558 (15)	-0.0809 (3)	-0.07755 (17)	0.0371 (6)
H3	0.3013	-0.0688	-0.1396	0.045*
C4	0.38688 (14)	0.0075 (2)	-0.02593 (16)	0.0310 (5)
C5	0.43824 (13)	-0.01749 (19)	0.06749 (15)	0.0248 (5)
C6	0.49639 (13)	0.06546 (19)	0.12309 (15)	0.0234 (5)
C7	0.38961 (16)	0.1199 (2)	-0.06162 (17)	0.0358 (6)
H7	0.3562	0.1372	-0.1231	0.043*
C8	0.43990 (15)	0.2013 (2)	-0.00747 (17)	0.0359 (6)
H8	0.4391	0.2752	-0.0314	0.043*
C9	0.49437 (14)	0.1764 (2)	0.08600 (16)	0.0296 (5)
C10	0.54844 (15)	0.2582 (2)	0.14486 (18)	0.0351 (6)
H10	0.5475	0.3344	0.1248	0.042*
C11	0.60188 (15)	0.2262 (2)	0.23065 (17)	0.0336 (6)
H11	0.6366	0.2811	0.2701	0.040*

supplementary materials

C12	0.60511 (14)	0.10882 (19)	0.26076 (16)	0.0269 (5)
C14	0.69963 (14)	-0.0403 (2)	0.34968 (18)	0.0340 (6)
H14A	0.6624	-0.0934	0.3064	0.051*
H14B	0.7179	-0.0700	0.4113	0.051*
H14C	0.7422	-0.0324	0.3362	0.051*
C15	0.71573 (17)	0.1587 (2)	0.40742 (18)	0.0445 (7)
H15A	0.7498	0.1885	0.3851	0.067*
H15B	0.7455	0.1225	0.4666	0.067*
H15C	0.6860	0.2216	0.4135	0.067*
C16	0.5917 (2)	0.4773 (3)	0.3971 (3)	0.0682 (10)
H6	0.5532	0.5318	0.3577	0.096 (14)*
H9	0.5911	0.4728	0.4554	0.14 (2)*
H5	0.5809	0.4016	0.3685	0.129 (19)*
C17	0.59639 (13)	-0.3261 (2)	0.21965 (15)	0.0258 (5)
N1	0.43477 (11)	-0.11804 (16)	0.10854 (12)	0.0257 (4)
N2	0.55031 (11)	0.03107 (15)	0.20930 (12)	0.0231 (4)
N3	0.56731 (12)	-0.24797 (17)	0.23466 (13)	0.0290 (4)
N4	0.66394 (12)	0.07266 (17)	0.34233 (13)	0.0305 (5)
Ni1	0.5000	-0.12186 (3)	0.2500	0.02153 (14)
O1	0.66464 (13)	0.5147 (2)	0.41138 (16)	0.0681 (7)
H4	0.6688	0.4940	0.3658	0.102*
S1	0.63832 (4)	-0.43760 (6)	0.19758 (5)	0.0419 (2)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0360 (14)	0.0320 (13)	0.0322 (12)	-0.0045 (11)	0.0184 (11)	-0.0052 (10)
C2	0.0362 (15)	0.0467 (15)	0.0341 (13)	-0.0091 (12)	0.0177 (12)	-0.0138 (12)
C3	0.0300 (14)	0.0549 (16)	0.0236 (12)	0.0040 (12)	0.0102 (11)	-0.0049 (11)
C4	0.0321 (14)	0.0406 (14)	0.0246 (12)	0.0092 (11)	0.0167 (11)	0.0005 (10)
C5	0.0283 (12)	0.0275 (12)	0.0239 (11)	0.0060 (10)	0.0166 (10)	0.0002 (9)
C6	0.0283 (12)	0.0245 (11)	0.0247 (11)	0.0056 (9)	0.0186 (10)	0.0020 (9)
C7	0.0413 (15)	0.0440 (15)	0.0242 (12)	0.0139 (12)	0.0170 (11)	0.0085 (11)
C8	0.0494 (17)	0.0318 (13)	0.0339 (13)	0.0151 (12)	0.0256 (13)	0.0133 (11)
C9	0.0392 (14)	0.0246 (12)	0.0341 (12)	0.0067 (10)	0.0247 (12)	0.0048 (10)
C10	0.0466 (16)	0.0217 (12)	0.0459 (15)	0.0021 (11)	0.0291 (13)	0.0050 (11)
C11	0.0412 (15)	0.0265 (13)	0.0379 (14)	-0.0066 (11)	0.0225 (12)	-0.0033 (10)
C12	0.0316 (13)	0.0272 (12)	0.0286 (12)	-0.0013 (10)	0.0195 (10)	-0.0027 (9)
C14	0.0272 (13)	0.0349 (13)	0.0392 (14)	0.0001 (10)	0.0148 (11)	0.0060 (11)
C15	0.0419 (16)	0.0427 (16)	0.0365 (14)	-0.0094 (13)	0.0078 (13)	-0.0080 (12)
C16	0.060 (2)	0.059 (2)	0.093 (3)	-0.0081 (18)	0.041 (2)	0.012 (2)
C17	0.0264 (12)	0.0272 (12)	0.0234 (11)	0.0000 (10)	0.0112 (10)	0.0046 (9)
N1	0.0286 (11)	0.0259 (10)	0.0239 (9)	0.0002 (8)	0.0134 (8)	-0.0030 (8)
N2	0.0269 (10)	0.0217 (9)	0.0255 (9)	0.0008 (8)	0.0162 (8)	-0.0003 (7)
N3	0.0375 (12)	0.0237 (10)	0.0282 (10)	0.0038 (9)	0.0174 (9)	0.0018 (8)
N4	0.0307 (11)	0.0285 (10)	0.0285 (10)	-0.0030 (9)	0.0105 (9)	-0.0001 (8)
Ni1	0.0277 (2)	0.0178 (2)	0.0207 (2)	0.000	0.01265 (18)	0.000
O1	0.0449 (13)	0.0956 (18)	0.0573 (14)	0.0003 (12)	0.0182 (11)	0.0297 (13)

S1 0.0482 (4) 0.0367 (4) 0.0449 (4) 0.0161 (3) 0.0250 (3) 0.0006 (3)

Geometric parameters (Å, °)

C1—N1	1.326 (3)	C12—N4	1.359 (3)
C1—C2	1.395 (3)	C14—N4	1.449 (3)
C1—H1	0.9300	C14—H14A	0.9600
C2—C3	1.364 (4)	C14—H14B	0.9600
C2—H2	0.9300	C14—H14C	0.9600
C3—C4	1.399 (4)	C15—N4	1.458 (3)
C3—H3	0.9300	C15—H15A	0.9600
C4—C5	1.413 (3)	C15—H15B	0.9600
C4—C7	1.424 (4)	C15—H15C	0.9600
C5—N1	1.350 (3)	C16—O1	1.402 (4)
C5—C6	1.436 (3)	C16—H6	0.9600
C6—N2	1.368 (3)	C16—H9	0.9600
C6—C9	1.400 (3)	C16—H5	0.9600
C7—C8	1.346 (4)	C17—N3	1.146 (3)
C7—H7	0.9300	C17—S1	1.646 (2)
C8—C9	1.427 (3)	N1—Ni1	2.0569 (19)
C8—H8	0.9300	N2—Ni1	2.2556 (18)
C9—C10	1.406 (3)	N3—Ni1	2.047 (2)
C10—C11	1.353 (4)	Ni1—N3 ⁱ	2.047 (2)
C10—H10	0.9300	Ni1—N1 ⁱ	2.0569 (19)
C11—C12	1.422 (3)	Ni1—N2 ⁱ	2.2556 (18)
C11—H11	0.9300	O1—H4	0.8217
C12—N2	1.346 (3)		
N1—C1—C2	122.5 (2)	H14B—C14—H14C	109.5
N1—C1—H1	118.8	N4—C15—H15A	109.5
C2—C1—H1	118.8	N4—C15—H15B	109.5
C3—C2—C1	119.3 (2)	H15A—C15—H15B	109.5
C3—C2—H2	120.3	N4—C15—H15C	109.5
C1—C2—H2	120.3	H15A—C15—H15C	109.5
C2—C3—C4	119.9 (2)	H15B—C15—H15C	109.5
C2—C3—H3	120.1	O1—C16—H6	109.5
C4—C3—H3	120.1	O1—C16—H9	109.5
C3—C4—C5	117.1 (2)	H6—C16—H9	109.5
C3—C4—C7	124.1 (2)	O1—C16—H5	109.5
C5—C4—C7	118.8 (2)	H6—C16—H5	109.5
N1—C5—C4	122.3 (2)	H9—C16—H5	109.5
N1—C5—C6	117.26 (19)	N3—C17—S1	179.6 (2)
C4—C5—C6	120.4 (2)	C1—N1—C5	118.7 (2)
N2—C6—C9	124.0 (2)	C1—N1—Ni1	125.71 (16)
N2—C6—C5	117.80 (19)	C5—N1—Ni1	115.34 (14)
C9—C6—C5	118.2 (2)	C12—N2—C6	117.53 (19)
C8—C7—C4	120.8 (2)	C12—N2—Ni1	131.28 (15)
C8—C7—H7	119.6	C6—N2—Ni1	107.06 (14)
C4—C7—H7	119.6	C17—N3—Ni1	171.3 (2)

supplementary materials

C7—C8—C9	121.3 (2)	C12—N4—C14	120.6 (2)
C7—C8—H8	119.4	C12—N4—C15	119.6 (2)
C9—C8—H8	119.4	C14—N4—C15	113.4 (2)
C6—C9—C10	116.6 (2)	N3 ⁱ —Ni1—N3	90.27 (11)
C6—C9—C8	120.1 (2)	N3 ⁱ —Ni1—N1 ⁱ	88.63 (7)
C10—C9—C8	123.3 (2)	N3—Ni1—N1 ⁱ	93.08 (7)
C11—C10—C9	120.1 (2)	N3 ⁱ —Ni1—N1	93.08 (7)
C11—C10—H10	119.9	N3—Ni1—N1	88.63 (7)
C9—C10—H10	119.9	N1 ⁱ —Ni1—N1	177.57 (10)
C10—C11—C12	120.2 (2)	N3 ⁱ —Ni1—N2	167.90 (7)
C10—C11—H11	119.9	N3—Ni1—N2	96.75 (7)
C12—C11—H11	119.9	N1 ⁱ —Ni1—N2	100.76 (7)
N2—C12—N4	118.5 (2)	N1—Ni1—N2	77.31 (7)
N2—C12—C11	121.0 (2)	N3 ⁱ —Ni1—N2 ⁱ	96.75 (7)
N4—C12—C11	120.5 (2)	N3—Ni1—N2 ⁱ	167.90 (7)
N4—C14—H14A	109.5	N1 ⁱ —Ni1—N2 ⁱ	77.31 (7)
N4—C14—H14B	109.5	N1—Ni1—N2 ⁱ	100.76 (7)
H14A—C14—H14B	109.5	N2—Ni1—N2 ⁱ	78.13 (9)
N4—C14—H14C	109.5	C16—O1—H4	106.5
H14A—C14—H14C	109.5		
N1—C1—C2—C3	-1.8 (4)	C6—C5—N1—Ni1	11.1 (2)
C1—C2—C3—C4	2.3 (4)	N4—C12—N2—C6	-173.0 (2)
C2—C3—C4—C5	1.1 (4)	C11—C12—N2—C6	6.8 (3)
C2—C3—C4—C7	-178.3 (2)	N4—C12—N2—Ni1	33.1 (3)
C3—C4—C5—N1	-5.3 (3)	C11—C12—N2—Ni1	-147.06 (18)
C7—C4—C5—N1	174.2 (2)	C9—C6—N2—C12	-0.8 (3)
C3—C4—C5—C6	175.4 (2)	C5—C6—N2—C12	179.39 (19)
C7—C4—C5—C6	-5.2 (3)	C9—C6—N2—Ni1	158.98 (18)
N1—C5—C6—N2	8.4 (3)	C5—C6—N2—Ni1	-20.8 (2)
C4—C5—C6—N2	-172.2 (2)	N2—C12—N4—C14	41.2 (3)
N1—C5—C6—C9	-171.4 (2)	C11—C12—N4—C14	-138.6 (2)
C4—C5—C6—C9	8.0 (3)	N2—C12—N4—C15	-168.5 (2)
C3—C4—C7—C8	179.1 (2)	C11—C12—N4—C15	11.7 (3)
C5—C4—C7—C8	-0.3 (4)	C1—N1—Ni1—N3 ⁱ	-17.9 (2)
C4—C7—C8—C9	2.8 (4)	C5—N1—Ni1—N3 ⁱ	155.82 (16)
N2—C6—C9—C10	-4.6 (3)	C1—N1—Ni1—N3	72.3 (2)
C5—C6—C9—C10	175.2 (2)	C5—N1—Ni1—N3	-113.98 (16)
N2—C6—C9—C8	174.7 (2)	C1—N1—Ni1—N2	169.6 (2)
C5—C6—C9—C8	-5.5 (3)	C5—N1—Ni1—N2	-16.74 (15)
C7—C8—C9—C6	0.1 (4)	C1—N1—Ni1—N2 ⁱ	-115.3 (2)
C7—C8—C9—C10	179.4 (2)	C5—N1—Ni1—N2 ⁱ	58.34 (17)
C6—C9—C10—C11	3.9 (4)	C12—N2—Ni1—N3 ⁱ	137.6 (3)
C8—C9—C10—C11	-175.4 (2)	C6—N2—Ni1—N3 ⁱ	-18.3 (4)
C9—C10—C11—C12	1.8 (4)	C12—N2—Ni1—N3	-97.3 (2)
C10—C11—C12—N2	-7.5 (4)	C6—N2—Ni1—N3	106.84 (14)

C10—C11—C12—N4	172.3 (2)	C12—N2—Ni1—N1 ⁱ	-2.8 (2)
C2—C1—N1—C5	-2.3 (4)	C6—N2—Ni1—N1 ⁱ	-158.71 (14)
C2—C1—N1—Ni1	171.22 (18)	C12—N2—Ni1—N1	175.7 (2)
C4—C5—N1—C1	5.9 (3)	C6—N2—Ni1—N1	19.77 (14)
C6—C5—N1—C1	-174.8 (2)	C12—N2—Ni1—N2 ⁱ	71.63 (19)
C4—C5—N1—Ni1	-168.28 (17)	C6—N2—Ni1—N2 ⁱ	-84.28 (14)

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

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

<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>
C14—H14C \cdots S1 ⁱⁱ	0.96	2.86	3.784 (3)	163
O1—H4 \cdots S1 ⁱⁱⁱ	0.82	2.65	3.331 (2)	142
C15—H15B \cdots O1 ^{iv}	0.96	2.51	3.427 (4)	161

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

Fig. 1

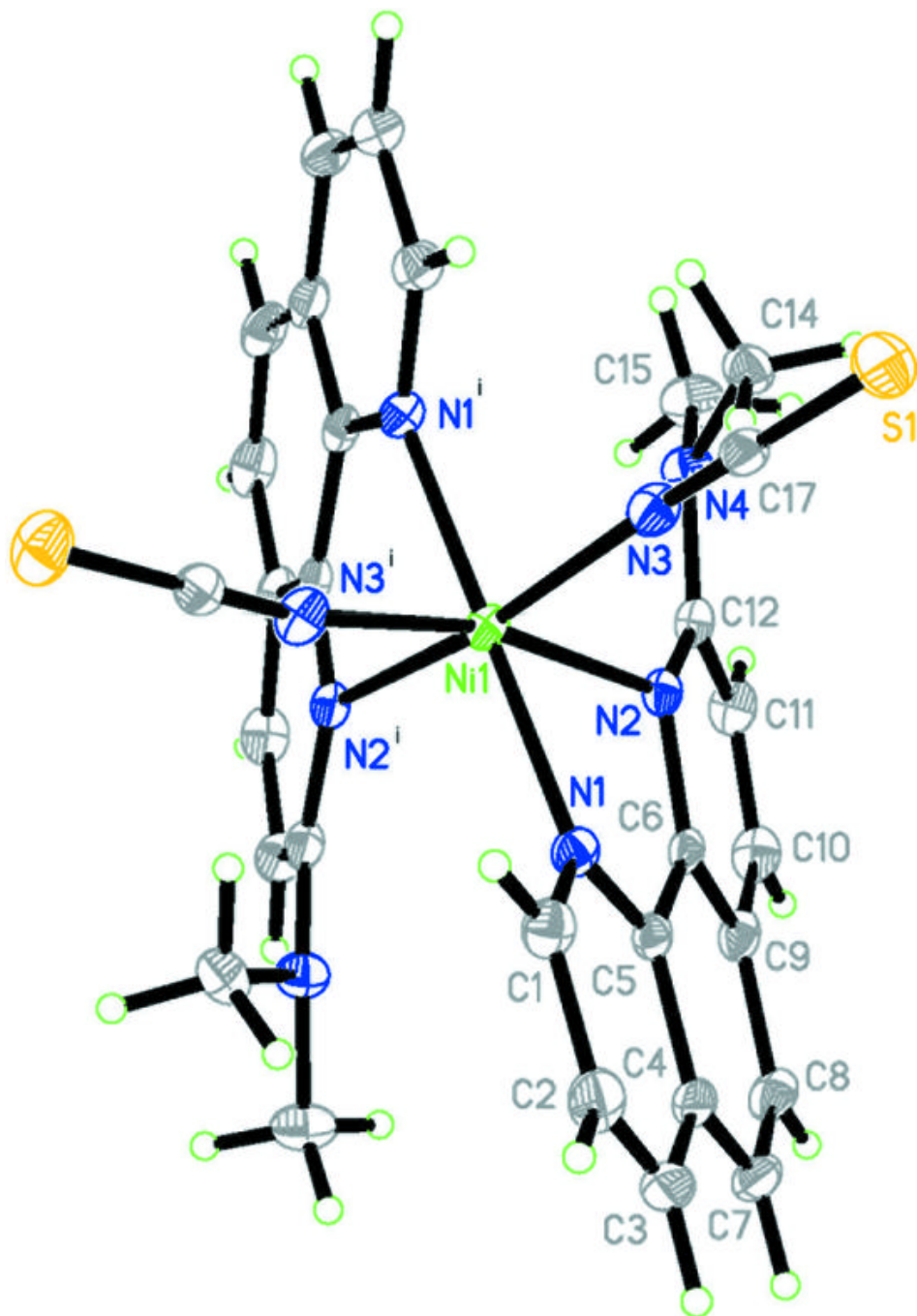


Fig. 2

