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1-(4-Cyanobenzyl)-4-methylpyridinium bis(benzene-1,2-dithiolato)nickelate(III)

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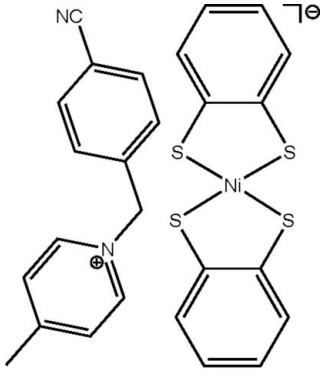
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.010 Å; R factor = 0.060; wR factor = 0.078; data-to-parameter ratio = 14.2.

The asymmetric unit of the title compound, $(C_{14}H_{13}N_2)[Ni(C_6H_4S_2)_2]$, contains two cations, one anion and two half-anions. One of the half-anions has Ni on a twofold rotation axis, while the other has Ni on a centre of symmetry. In the anions, the Ni ions are surrounded by four S atoms in a distorted square-planar geometry. In the crystal structure, the anions exhibit two different packing modes by stacking in face-to-face and side-by-side fashions.

Related literature

For general background, see: de Caro *et al.* (2004); Ray *et al.* (2005); Liu (2007); Liu *et al.* (2005); Wang *et al.* (2006). For related literature, see: Sellmann *et al.* (1991); Xie *et al.* (2002).



Experimental

Crystal data

$(C_{14}H_{13}N_2)[Ni(C_6H_4S_2)_2]$
M_r = 548.40
Monoclinic, $C2/c$
a = 42.344 (3) Å
b = 7.2455 (6) Å
c = 32.768 (2) Å
β = 96.480 (5)°
V = 9988.9 (13) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 1.13 mm^{-1}
T = 294 (2) K
0.20 × 0.12 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.806, T_{max} = 0.896
27982 measured reflections
8530 independent reflections
3392 reflections with $I > 2\sigma(I)$
R_{int} = 0.113

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.078
S = 0.89
8530 reflections
599 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—S6	2.1337 (16)	Ni2—S2	2.1408 (17)
Ni1—S5	2.1477 (14)	Ni2—S1	2.1424 (16)
Ni2—S4	2.1400 (16)	Ni3—S7	2.1424 (15)
Ni2—S3	2.1405 (17)	Ni3—S8	2.1470 (14)
S6—Ni1—S6^{i}	166.03 (9)	S3—Ni2—S2	178.93 (8)
S6—Ni1—S5	91.45 (6)	S4—Ni2—S1	178.82 (6)
S6^{i}—Ni1—S5	89.32 (6)	S3—Ni2—S1	88.26 (6)
S5—Ni1—S5^{i}	173.64 (10)	S2—Ni2—S1	91.66 (6)
S4—Ni2—S3	91.93 (7)	S7—Ni3—S8^{ii}	91.76 (6)
S4—Ni2—S2	88.17 (6)	S7—Ni3—S8	88.25 (6)

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8B···S4^{i}	0.97	2.846	3.721 (3)	150.63

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); 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: HK2244).

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supplementary materials

Acta Cryst. (2007). E**63**, m1707 [**doi:10.1107/S1600536807023847**]

1-(4-Cyanobenzyl)-4-methylpyridinium bis(benzene-1,2-dithiolato)nickelate(III)

G.-X. Liu

Comment

Since their discovery in 1963, square planar bis(benzene-1,2-dithiolato)metal complexes have received considerable attention due to their interesting and often unusual electronic structures. It has been established that the square planar complexes $[M(L)_2]^{2-}$, $[M(L)_2]^{-}$, and $[M(L)_2]^{0}$ (where M = Ni, Pt) form a three membered electron-transfer series, where the neutral species and the dianionic forms are diamagnetic (S = 0), whereas the monoanions are paramagnetic (S = 1/2) (de Caro *et al.*, 2004; Ray *et al.*, 2005). In our previous research using benzylpyridinium derivatives ($[RBzPy]^{+}$) as the counter-cation of $TCNQ^{-}$ (where TCNQ = 7,7,8,8-tetracyanoquinodimethanide), a series of ion-pair compounds with segregated columnar stacks of cations and anions has been prepared (Liu, 2007; Liu *et al.*, 2005; Wang *et al.*, 2006). The quasi one-dimensional magnetic nature of these compounds was attributed to intermolecular-orbital interactions within the anionic columns. As an extension of our work on this series of complexes, we herein report the crystal structure of the title compound, (I).

The asymmetric unit of (I), contains two $(C_{14}H_{13}N_2)^{+}$ cations, one and two halves centrosymmetric $[Ni(C_6H_4S_2)_2]$ anions. In the anions, the Ni ions are surrounded by four S atoms in a distorted square-planar geometry. The dihedral angle between (Ni1/S5/S6/C41/C46) and (Ni1/S5A/S6A/C41A/C46A) planes is 18.98 (2)° [symmetry code (A): −*x*, *y*, 1/2 − *z*]. It is peculiar and interesting. The Ni—S bond lengths and S—Ni—S bond angles (Table 1) are in agreement with the corresponding values in analogous complexes (Sellmann *et al.*, 1991; Xie *et al.*, 2002). The cations have Λ-shaped conformations with the dihedral angles of A/B = 65.03 (3), A/C = 46.37 (4), B/C = 86.96 (4) ° and D/E = 60.62 (3), D/F = 59.72 (3), E/F = 83.56 (4) ° between A (C5/C8/N1), B (C2—C7), C (N1/C9—C13) and D (C19/C22/N2), E (C16—C21), F (N2/C23—C28) planes.

In the crystal structure, the packing of the two anions is different (Fig. 2). The Ni1, Ni3-containing anions stack in a face-to-face fashion with an alternating arrangement of anions and cations, such that the pyridine ring of the cation lies above the benzene ring of the anion. The shortest distance between the adjacent Ni^{III} ions is 7.245 (2) Å. The Ni2-containing anions stack in a side by side fashion with C—H···S interactions (Table 2).

Experimental

Benzene-1,2-dithiol (142 mg, 1.0 mmol) was added to a solution of sodium metal (46 mg, 2.0 mmol) in absolute ethanol (25 ml), under nitrogen atmosphere at room temperature, and then a solution of $NiCl_2{\cdot}6H_2O$ (120 mg, 0.5 mmol) in ethanol (25 ml) was added, resulting in a mixture turning a muddy red–brown color. Following this, $[NCBzPyCH_3]Br$ (289 mg, 1.0 mmol) was added and the mixture allowed to stand with stirring for 1 h, and then stirred for an additional 24 h in air. The color of the mixture gradually turned green, indicating oxidation from a dianionic species to the more stable monoanionic form. The precipitate was washed with absolute ethanol and diethyl ether and then dried. The crude product was recrystallized twice from dichloromethane to give the title compound (yield; 241 mg, 69%, m.p. 483–485 K).

Refinement

H atoms were positioned geometrically, with C—H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xUeq(C), where x = 1.5 for methyl H, and x = 1.2 for all other H atoms.

Figures

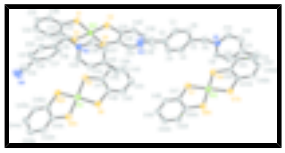

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The symmetry codes A in Ni1 and Ni3 anions are (−x, y, 1/2 − z) and (1/2 − x, 1/2 − y, 1 − z), respectively.

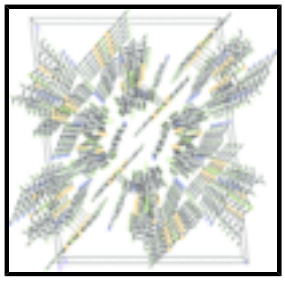

Fig. 2. A packing diagram of (I). The C—H···S interactions are shown as dashed lines.

1-(4-Cyanobenzyl)-4-methylpyridinium bis(benzene-1,2-dithiolato)nickelate(III)

Crystal data

$(C_{14}H_{13}N_2)[Ni(C_6H_4S_2)_2]$	F_{000} = 4528
M_r = 548.40	D_x = 1.459 Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 1320 reflections
a = 42.344 (3) Å	θ = 2.9–16.5º
b = 7.2455 (6) Å	μ = 1.13 mm^{-1}
c = 32.768 (2) Å	T = 294 (2) K
β = 96.480 (5)º	Prism, dark green
V = 9988.9 (13) Å^3	0.20 × 0.12 × 0.10 mm
Z = 16	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	8530 independent reflections
Radiation source: sealed tube	3392 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.113
T = 294(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.5º
Absorption correction: multi-scan	h = −50→47

(SADABS; Bruker, 2000)

T_{min} = 0.806, T_{max} = 0.896

27982 measured reflections

k = −8→7

l = −36→36

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.060

$wR(F^2)$ = 0.078

S = 0.89

8530 reflections

599 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2)]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 0.34 e Å^{-3}

$\Delta\rho_{min}$ = −0.27 e Å^{-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 $F^2 > 2$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	0.0000	0.56508 (13)	0.2500	0.0602 (3)
Ni2	0.125597 (16)	0.62664 (10)	0.12628 (2)	0.0551 (2)
Ni3	0.2500	0.2500	0.5000	0.0615 (3)
S1	0.11139 (3)	0.88755 (19)	0.09943 (4)	0.0620 (4)
S2	0.09055 (4)	0.48396 (19)	0.08584 (5)	0.0667 (5)
S3	0.16124 (4)	0.7690 (2)	0.16585 (5)	0.0700 (5)
S4	0.13900 (3)	0.3664 (2)	0.15386 (4)	0.0641 (4)
S5	0.04314 (4)	0.5815 (2)	0.22143 (4)	0.0647 (5)
S6	0.02601 (4)	0.5293 (2)	0.30913 (4)	0.0737 (5)
S7	0.22258 (4)	0.1943 (2)	0.44230 (4)	0.0718 (5)
S8	0.29206 (4)	0.19526 (19)	0.47107 (5)	0.0646 (5)
N1	0.31857 (14)	0.6691 (6)	0.45220 (15)	0.0574 (13)
N2	0.06481 (13)	1.1024 (6)	0.20015 (15)	0.0563 (13)
N3	0.17638 (18)	0.9953 (13)	0.3108 (2)	0.177 (4)
N4	−0.06790 (18)	0.6563 (12)	0.0635 (2)	0.162 (3)

C1	0.1980 (2)	0.9276 (13)	0.3264 (2)	0.118 (3)
C2	0.2261 (2)	0.8448 (13)	0.3481 (2)	0.082 (2)
C3	0.22698 (19)	0.6628 (13)	0.3573 (2)	0.098 (3)
H3	0.2091	0.5914	0.3494	0.118*
C4	0.2529 (2)	0.5804 (10)	0.3775 (2)	0.087 (2)
H4	0.2526	0.4552	0.3837	0.105*
C5	0.27987 (16)	0.6851 (10)	0.38877 (17)	0.0586 (17)
C6	0.27969 (15)	0.8707 (9)	0.37946 (17)	0.0627 (17)
H6	0.2976	0.9424	0.3871	0.075*
C7	0.25306 (19)	0.9490 (9)	0.35900 (19)	0.072 (2)
H7	0.2531	1.0738	0.3524	0.087*
C8	0.30959 (14)	0.5990 (7)	0.40965 (16)	0.0659 (17)
H8A	0.3066	0.4664	0.4107	0.079*
H8B	0.3269	0.6229	0.3934	0.079*
C9	0.29658 (14)	0.6769 (7)	0.4786 (2)	0.0640 (18)
H9	0.2755	0.6482	0.4698	0.077*
C10	0.30535 (18)	0.7270 (7)	0.5183 (2)	0.071 (2)
H10	0.2899	0.7319	0.5363	0.085*
C11	0.3359 (2)	0.7703 (8)	0.5326 (3)	0.074 (2)
C12	0.35750 (19)	0.7611 (8)	0.5045 (3)	0.084 (2)
H12	0.3787	0.7897	0.5127	0.101*
C13	0.34874 (17)	0.7113 (8)	0.4649 (2)	0.073 (2)
H13	0.3639	0.7065	0.4465	0.088*
C14	0.34560 (16)	0.8237 (8)	0.57622 (19)	0.102 (2)
H14A	0.3680	0.8039	0.5828	0.152*
H14B	0.3342	0.7499	0.5940	0.152*
H14C	0.3408	0.9517	0.5800	0.152*
C15	−0.0476 (2)	0.7422 (13)	0.0787 (3)	0.124 (3)
C16	−0.0223 (2)	0.8514 (12)	0.09821 (19)	0.076 (2)
C17	0.00624 (19)	0.7662 (8)	0.11170 (19)	0.0665 (19)
H17	0.0088	0.6403	0.1077	0.080*
C18	0.03053 (14)	0.8689 (9)	0.13096 (16)	0.0612 (17)
H18	0.0498	0.8122	0.1400	0.073*
C19	0.02699 (17)	1.0549 (9)	0.13723 (16)	0.0556 (17)
C20	−0.0010 (2)	1.1392 (9)	0.1235 (2)	0.081 (2)
H20	−0.0036	1.2654	0.1272	0.097*
C21	−0.02549 (17)	1.0359 (12)	0.1041 (2)	0.088 (2)
H21	−0.0446	1.0933	0.0948	0.106*
C22	0.05457 (14)	1.1652 (8)	0.15794 (17)	0.0750 (19)
H22A	0.0723	1.1558	0.1418	0.090*
H22B	0.0485	1.2941	0.1586	0.090*
C23	0.04440 (14)	1.1099 (7)	0.2284 (2)	0.0643 (17)
H23	0.0237	1.1489	0.2208	0.077*
C24	0.05327 (16)	1.0622 (7)	0.2678 (2)	0.0666 (19)
H24	0.0386	1.0658	0.2869	0.080*
C25	0.08412 (19)	1.0082 (7)	0.2799 (2)	0.0576 (18)
C26	0.09546 (15)	0.9591 (7)	0.32383 (18)	0.092 (2)
H26A	0.1087	0.8512	0.3244	0.137*
H26B	0.0775	0.9347	0.3384	0.137*

H26C	0.1075	1.0600	0.3366	0.137*
C27	0.10478 (18)	0.9985 (7)	0.2500 (3)	0.076 (2)
H27	0.1256	0.9598	0.2568	0.091*
C28	0.09443 (17)	1.0457 (8)	0.2108 (2)	0.0685 (19)
H28	0.1084	1.0383	0.1908	0.082*
C29	0.08084 (13)	0.8376 (9)	0.06148 (16)	0.0535 (15)
C30	0.06495 (15)	0.9756 (8)	0.0381 (2)	0.0685 (19)
H30	0.0707	1.0985	0.0426	0.082*
C31	0.04077 (15)	0.9301 (10)	0.00835 (19)	0.074 (2)
H31	0.0302	1.0234	−0.0072	0.089*
C32	0.03178 (15)	0.7498 (10)	0.0011 (2)	0.082 (2)
H32	0.0154	0.7214	−0.0193	0.099*
C33	0.04738 (15)	0.6106 (9)	0.02449 (19)	0.0724 (18)
H33	0.0415	0.4881	0.0197	0.087*
C34	0.07160 (13)	0.6535 (8)	0.05490 (16)	0.0526 (15)
C35	0.18004 (13)	0.5986 (9)	0.19720 (17)	0.0573 (16)
C36	0.16966 (13)	0.4172 (9)	0.19115 (16)	0.0563 (16)
C37	0.18521 (16)	0.2797 (8)	0.2164 (2)	0.074 (2)
H37	0.1786	0.1577	0.2130	0.089*
C38	0.20967 (17)	0.3218 (10)	0.2457 (2)	0.085 (2)
H38	0.2196	0.2293	0.2621	0.102*
C39	0.21959 (16)	0.5034 (11)	0.2507 (2)	0.086 (2)
H39	0.2363	0.5324	0.2705	0.103*
C40	0.20502 (15)	0.6400 (9)	0.2270 (2)	0.0742 (18)
H40	0.2119	0.7614	0.2307	0.089*
C41	0.07300 (17)	0.5359 (6)	0.2607 (2)	0.0542 (17)
C42	0.1047 (2)	0.5224 (7)	0.2529 (2)	0.070 (2)
H42	0.1099	0.5408	0.2263	0.084*
C43	0.12827 (17)	0.4822 (8)	0.2840 (3)	0.085 (2)
H43	0.1493	0.4726	0.2786	0.102*
C44	0.12051 (17)	0.4560 (7)	0.3236 (2)	0.079 (2)
H44	0.1363	0.4280	0.3448	0.095*
C45	0.0897 (2)	0.4715 (7)	0.3313 (2)	0.073 (2)
H45	0.0847	0.4551	0.3580	0.088*
C46	0.06564 (16)	0.5109 (7)	0.3005 (2)	0.0590 (18)
C47	0.18323 (15)	0.2118 (7)	0.4527 (2)	0.0563 (17)
C48	0.15871 (19)	0.1752 (7)	0.42208 (19)	0.0690 (19)
H48	0.1633	0.1424	0.3959	0.083*
C49	0.12791 (17)	0.1871 (8)	0.4301 (2)	0.0752 (19)
H49	0.1115	0.1633	0.4094	0.090*
C50	0.32329 (17)	0.2401 (6)	0.50796 (18)	0.0539 (18)
C51	0.35497 (18)	0.2307 (7)	0.5006 (2)	0.064 (2)
H51	0.3598	0.2000	0.4745	0.077*
C52	0.37907 (16)	0.2653 (7)	0.5308 (2)	0.078 (2)
H52	0.4001	0.2571	0.5253	0.094*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0747 (9)	0.0539 (7)	0.0541 (7)	0.000	0.0170 (6)	0.000
Ni2	0.0557 (5)	0.0523 (5)	0.0574 (5)	−0.0065 (4)	0.0069 (4)	−0.0029 (4)
Ni3	0.0682 (9)	0.0607 (7)	0.0576 (8)	−0.0042 (6)	0.0156 (6)	0.0002 (5)
S1	0.0613 (11)	0.0554 (10)	0.0674 (11)	−0.0082 (9)	−0.0007 (9)	−0.0025 (8)
S2	0.0686 (13)	0.0552 (10)	0.0733 (12)	−0.0089 (8)	−0.0053 (10)	−0.0027 (8)
S3	0.0744 (13)	0.0597 (11)	0.0725 (12)	−0.0112 (9)	−0.0062 (10)	−0.0029 (9)
S4	0.0635 (12)	0.0553 (10)	0.0717 (11)	−0.0046 (8)	0.0000 (9)	−0.0001 (8)
S5	0.0771 (13)	0.0637 (11)	0.0550 (10)	−0.0004 (9)	0.0154 (9)	0.0043 (8)
S6	0.0834 (14)	0.0861 (13)	0.0541 (11)	0.0030 (9)	0.0185 (10)	0.0024 (8)
S7	0.0742 (13)	0.0874 (13)	0.0560 (11)	−0.0049 (9)	0.0170 (10)	−0.0041 (8)
S8	0.0729 (13)	0.0640 (11)	0.0586 (11)	0.0006 (9)	0.0149 (9)	−0.0025 (8)
N1	0.065 (4)	0.049 (3)	0.062 (4)	0.009 (3)	0.023 (4)	0.008 (2)
N2	0.064 (4)	0.049 (3)	0.056 (4)	−0.007 (3)	0.009 (3)	−0.004 (3)
N3	0.097 (7)	0.267 (10)	0.159 (7)	0.039 (6)	−0.030 (5)	0.070 (6)
N4	0.128 (7)	0.229 (9)	0.125 (6)	−0.074 (6)	−0.003 (5)	−0.019 (6)
C1	0.090 (8)	0.183 (9)	0.079 (6)	0.028 (7)	−0.001 (6)	0.031 (6)
C2	0.072 (7)	0.118 (7)	0.057 (5)	0.003 (6)	0.016 (5)	0.013 (5)
C3	0.082 (7)	0.134 (8)	0.075 (6)	−0.035 (6)	−0.013 (5)	0.002 (5)
C4	0.097 (7)	0.085 (6)	0.080 (6)	−0.027 (6)	0.008 (5)	0.004 (4)
C5	0.061 (5)	0.068 (5)	0.050 (4)	0.006 (4)	0.017 (4)	0.003 (4)
C6	0.067 (5)	0.057 (5)	0.065 (4)	0.004 (4)	0.007 (4)	−0.006 (4)
C7	0.072 (6)	0.080 (5)	0.066 (5)	0.024 (5)	0.012 (4)	0.006 (4)
C8	0.092 (5)	0.061 (4)	0.046 (4)	0.012 (4)	0.013 (4)	−0.003 (3)
C9	0.058 (5)	0.084 (5)	0.052 (5)	0.004 (3)	0.012 (4)	0.010 (4)
C10	0.087 (6)	0.075 (5)	0.053 (5)	0.002 (4)	0.019 (5)	0.008 (4)
C11	0.082 (7)	0.049 (4)	0.087 (7)	0.009 (4)	−0.001 (6)	0.005 (4)
C12	0.075 (7)	0.078 (5)	0.093 (7)	0.002 (4)	−0.011 (6)	−0.012 (4)
C13	0.053 (5)	0.069 (5)	0.100 (7)	0.005 (4)	0.021 (5)	0.003 (4)
C14	0.156 (8)	0.077 (5)	0.065 (5)	−0.002 (5)	−0.016 (5)	−0.011 (4)
C15	0.120 (10)	0.169 (10)	0.082 (7)	−0.052 (7)	0.011 (6)	−0.018 (6)
C16	0.082 (7)	0.100 (7)	0.046 (4)	−0.014 (6)	0.002 (4)	−0.005 (4)
C17	0.078 (6)	0.066 (5)	0.058 (5)	−0.005 (5)	0.018 (4)	0.009 (4)
C18	0.055 (5)	0.071 (5)	0.056 (4)	−0.010 (4)	0.003 (3)	0.009 (4)
C19	0.070 (6)	0.057 (5)	0.039 (4)	−0.007 (4)	0.004 (4)	0.001 (3)
C20	0.089 (6)	0.070 (5)	0.080 (5)	0.025 (5)	−0.004 (5)	−0.006 (4)
C21	0.052 (6)	0.126 (8)	0.083 (6)	0.025 (5)	−0.006 (4)	−0.002 (5)
C22	0.104 (6)	0.072 (5)	0.049 (4)	−0.014 (4)	0.009 (4)	0.008 (3)
C23	0.069 (5)	0.065 (4)	0.060 (5)	0.005 (4)	0.012 (4)	0.001 (4)
C24	0.071 (6)	0.062 (4)	0.068 (5)	0.007 (4)	0.012 (4)	−0.009 (4)
C25	0.081 (6)	0.043 (4)	0.045 (5)	−0.009 (4)	−0.011 (5)	−0.004 (3)
C26	0.127 (7)	0.069 (5)	0.073 (5)	−0.006 (4)	−0.017 (5)	0.011 (4)
C27	0.067 (6)	0.081 (5)	0.076 (6)	−0.005 (4)	−0.005 (5)	0.004 (4)
C28	0.065 (6)	0.067 (5)	0.075 (6)	−0.002 (4)	0.015 (5)	−0.006 (4)
C29	0.042 (4)	0.070 (5)	0.049 (4)	−0.004 (4)	0.005 (3)	0.000 (3)

C30	0.061 (5)	0.076 (5)	0.068 (5)	0.007 (4)	0.007 (4)	0.008 (4)
C31	0.057 (5)	0.098 (6)	0.065 (5)	0.011 (4)	−0.005 (4)	0.003 (4)
C32	0.058 (5)	0.098 (6)	0.088 (6)	−0.006 (5)	−0.004 (4)	−0.020 (5)
C33	0.059 (5)	0.076 (5)	0.081 (5)	−0.002 (4)	0.002 (4)	−0.007 (4)
C34	0.042 (4)	0.064 (4)	0.050 (4)	−0.010 (3)	−0.003 (3)	−0.009 (3)
C35	0.037 (4)	0.075 (5)	0.061 (4)	−0.001 (4)	0.009 (3)	−0.003 (4)
C36	0.049 (4)	0.062 (4)	0.058 (4)	0.003 (4)	0.009 (3)	0.004 (4)
C37	0.074 (6)	0.075 (5)	0.071 (5)	0.012 (4)	0.003 (4)	0.005 (4)
C38	0.074 (6)	0.099 (6)	0.080 (6)	0.014 (5)	−0.005 (4)	0.016 (5)
C39	0.057 (5)	0.117 (7)	0.080 (6)	0.005 (5)	−0.007 (4)	0.004 (5)
C40	0.058 (5)	0.085 (5)	0.077 (5)	−0.004 (4)	−0.005 (4)	−0.009 (4)
C41	0.065 (6)	0.040 (4)	0.058 (5)	0.001 (3)	0.008 (4)	−0.004 (3)
C42	0.085 (7)	0.062 (5)	0.066 (6)	0.008 (4)	0.019 (5)	0.002 (3)
C43	0.084 (7)	0.083 (5)	0.091 (6)	−0.001 (4)	0.021 (6)	−0.005 (4)
C44	0.076 (6)	0.074 (5)	0.085 (6)	0.013 (4)	−0.001 (5)	−0.004 (4)
C45	0.099 (7)	0.059 (4)	0.062 (5)	0.009 (4)	0.011 (5)	0.004 (3)
C46	0.068 (6)	0.049 (4)	0.062 (5)	0.001 (3)	0.014 (4)	−0.001 (3)
C47	0.051 (5)	0.049 (4)	0.068 (5)	−0.004 (3)	0.001 (4)	0.011 (3)
C48	0.083 (6)	0.065 (5)	0.063 (5)	0.000 (4)	0.026 (5)	0.012 (3)
C49	0.081 (6)	0.081 (5)	0.061 (5)	−0.005 (4)	−0.004 (4)	0.010 (4)
C50	0.078 (6)	0.046 (4)	0.039 (5)	0.002 (3)	0.013 (4)	0.006 (3)
C51	0.069 (6)	0.075 (5)	0.054 (5)	0.005 (4)	0.024 (5)	0.003 (3)
C52	0.065 (6)	0.082 (5)	0.086 (6)	−0.010 (4)	0.000 (5)	0.012 (4)

Geometric parameters (Å, °)

Ni1—S6	2.1337 (16)	C19—C20	1.365 (7)
Ni1—S6^{i}	2.1338 (16)	C19—C22	1.511 (7)
Ni1—S5	2.1477 (14)	C20—C21	1.374 (8)
Ni1—S5^{i}	2.1478 (14)	C20—H20	0.9300
Ni2—S4	2.1400 (16)	C21—H21	0.9300
Ni2—S3	2.1405 (17)	C22—H22A	0.9700
Ni2—S2	2.1408 (17)	C22—H22B	0.9700
Ni2—S1	2.1424 (16)	C23—C24	1.348 (7)
Ni3—S7	2.1424 (15)	C23—H23	0.9300
Ni3—S7^{ii}	2.1424 (15)	C24—C25	1.378 (7)
Ni3—S8^{ii}	2.1470 (14)	C24—H24	0.9300
Ni3—S8	2.1470 (14)	C25—C27	1.387 (8)
S1—C29	1.728 (6)	C25—C26	1.508 (7)
S2—C34	1.731 (6)	C26—H26A	0.9600
S3—C35	1.741 (6)	C26—H26B	0.9600
S4—C36	1.719 (6)	C26—H26C	0.9600
S5—C41	1.732 (6)	C27—C28	1.354 (8)
S6—C46	1.738 (6)	C27—H27	0.9300
S7—C47	1.742 (6)	C28—H28	0.9300
S8—C50	1.719 (6)	C29—C30	1.387 (7)
N1—C13	1.333 (6)	C29—C34	1.400 (6)
N1—C9	1.342 (6)	C30—C31	1.371 (7)

N1—C8	1.492 (6)	C30—H30	0.9300
N2—C28	1.328 (6)	C31—C32	1.374 (7)
N2—C23	1.338 (6)	C31—H31	0.9300
N2—C22	1.474 (6)	C32—C33	1.388 (7)
N3—C1	1.109 (8)	C32—H32	0.9300
N4—C15	1.129 (8)	C33—C34	1.383 (7)
C1—C2	1.449 (9)	C33—H33	0.9300
C2—C3	1.352 (9)	C35—C40	1.388 (7)
C2—C7	1.381 (8)	C35—C36	1.393 (7)
C3—C4	1.356 (8)	C36—C37	1.410 (7)
C3—H3	0.9300	C37—C38	1.364 (7)
C4—C5	1.385 (8)	C37—H37	0.9300
C4—H4	0.9300	C38—C39	1.386 (7)
C5—C6	1.379 (7)	C38—H38	0.9300
C5—C8	1.499 (7)	C39—C40	1.363 (7)
C6—C7	1.369 (7)	C39—H39	0.9300
C6—H6	0.9300	C40—H40	0.9300
C7—H7	0.9300	C41—C46	1.386 (7)
C8—H8A	0.9700	C41—C42	1.400 (8)
C8—H8B	0.9700	C42—C43	1.375 (8)
C9—C10	1.361 (7)	C42—H42	0.9300
C9—H9	0.9300	C43—C44	1.387 (7)
C10—C11	1.363 (8)	C43—H43	0.9300
C10—H10	0.9300	C44—C45	1.360 (7)
C11—C12	1.370 (9)	C44—H44	0.9300
C11—C14	1.494 (8)	C45—C46	1.381 (8)
C12—C13	1.357 (8)	C45—H45	0.9300
C12—H12	0.9300	C47—C48	1.385 (7)
C13—H13	0.9300	C47—C50^{ii}	1.394 (7)
C14—H14A	0.9600	C48—C49	1.362 (7)
C14—H14B	0.9600	C48—H48	0.9300
C14—H14C	0.9600	C49—C52^{ii}	1.389 (7)
C15—C16	1.426 (9)	C49—H49	0.9300
C16—C21	1.359 (8)	C50—C51	1.391 (7)
C16—C17	1.384 (8)	C50—C47^{ii}	1.394 (7)
C17—C18	1.365 (7)	C51—C52	1.362 (8)
C17—H17	0.9300	C51—H51	0.9300
C18—C19	1.374 (7)	C52—C49^{ii}	1.389 (7)
C18—H18	0.9300	C52—H52	0.9300
S6—Ni1—S6^{i}	166.03 (9)	N2—C22—H22A	109.0
S6—Ni1—S5	91.45 (6)	C19—C22—H22A	109.0
S6^{i}—Ni1—S5	89.32 (6)	N2—C22—H22B	109.0
S6—Ni1—S5^{i}	89.33 (6)	C19—C22—H22B	109.0
S6^{i}—Ni1—S5^{i}	91.45 (6)	H22A—C22—H22B	107.8
S5—Ni1—S5^{i}	173.64 (10)	N2—C23—C24	121.4 (6)
S4—Ni2—S3	91.93 (7)	N2—C23—H23	119.3
S4—Ni2—S2	88.17 (6)	C24—C23—H23	119.3

S3—Ni2—S2	178.93 (8)	C23—C24—C25	120.0 (6)
S4—Ni2—S1	178.82 (6)	C23—C24—H24	120.0
S3—Ni2—S1	88.26 (6)	C25—C24—H24	120.0
S2—Ni2—S1	91.66 (6)	C24—C25—C27	117.7 (7)
S7—Ni3—S7^{ii}	179.998 (1)	C24—C25—C26	122.0 (7)
S7—Ni3—S8^{ii}	91.76 (6)	C27—C25—C26	120.3 (7)
S7^{ii}—Ni3—S8^{ii}	88.25 (6)	C25—C26—H26A	109.5
S7—Ni3—S8	88.25 (6)	C25—C26—H26B	109.5
S7^{ii}—Ni3—S8	91.75 (6)	H26A—C26—H26B	109.5
S8^{ii}—Ni3—S8	179.998 (1)	C25—C26—H26C	109.5
C29—S1—Ni2	105.3 (2)	H26A—C26—H26C	109.5
C34—S2—Ni2	105.2 (2)	H26B—C26—H26C	109.5
C35—S3—Ni2	105.1 (2)	C28—C27—C25	119.7 (7)
C36—S4—Ni2	104.7 (2)	C28—C27—H27	120.2
C41—S5—Ni1	104.5 (2)	C25—C27—H27	120.2
C46—S6—Ni1	105.7 (3)	N2—C28—C27	121.4 (6)
C47—S7—Ni3	104.4 (3)	N2—C28—H28	119.3
C50—S8—Ni3	105.4 (2)	C27—C28—H28	119.3
C13—N1—C9	120.0 (6)	C30—C29—C34	119.5 (6)
C13—N1—C8	120.2 (5)	C30—C29—S1	121.6 (5)
C9—N1—C8	119.6 (6)	C34—C29—S1	118.9 (5)
C28—N2—C23	119.7 (6)	C31—C30—C29	119.8 (6)
C28—N2—C22	120.7 (6)	C31—C30—H30	120.1
C23—N2—C22	119.5 (6)	C29—C30—H30	120.1
N3—C1—C2	177.6 (12)	C30—C31—C32	121.4 (6)
C3—C2—C7	118.4 (8)	C30—C31—H31	119.3
C3—C2—C1	120.9 (9)	C32—C31—H31	119.3
C7—C2—C1	120.7 (9)	C31—C32—C33	119.4 (7)
C2—C3—C4	122.5 (8)	C31—C32—H32	120.3
C2—C3—H3	118.7	C33—C32—H32	120.3
C4—C3—H3	118.7	C34—C33—C32	120.1 (7)
C3—C4—C5	119.1 (7)	C34—C33—H33	119.9
C3—C4—H4	120.4	C32—C33—H33	119.9
C5—C4—H4	120.4	C33—C34—C29	119.8 (6)
C6—C5—C4	119.4 (6)	C33—C34—S2	121.3 (5)
C6—C5—C8	119.3 (6)	C29—C34—S2	118.9 (5)
C4—C5—C8	121.2 (7)	C40—C35—C36	120.5 (6)
C7—C6—C5	119.8 (6)	C40—C35—S3	121.5 (5)
C7—C6—H6	120.1	C36—C35—S3	118.0 (5)
C5—C6—H6	120.1	C35—C36—C37	117.6 (6)
C6—C7—C2	120.7 (7)	C35—C36—S4	120.3 (5)
C6—C7—H7	119.6	C37—C36—S4	122.1 (5)
C2—C7—H7	119.6	C38—C37—C36	121.5 (6)
N1—C8—C5	113.4 (5)	C38—C37—H37	119.3
N1—C8—H8A	108.9	C36—C37—H37	119.3
C5—C8—H8A	108.9	C37—C38—C39	119.5 (7)
N1—C8—H8B	108.9	C37—C38—H38	120.3
C5—C8—H8B	108.9	C39—C38—H38	120.3

H8A—C8—H8B	107.7	C40—C39—C38	120.6 (7)
N1—C9—C10	119.5 (6)	C40—C39—H39	119.7
N1—C9—H9	120.2	C38—C39—H39	119.7
C10—C9—H9	120.2	C39—C40—C35	120.3 (7)
C9—C10—C11	122.4 (7)	C39—C40—H40	119.8
C9—C10—H10	118.8	C35—C40—H40	119.8
C11—C10—H10	118.8	C46—C41—C42	119.1 (7)
C10—C11—C12	116.0 (8)	C46—C41—S5	120.1 (6)
C10—C11—C14	122.4 (8)	C42—C41—S5	120.8 (6)
C12—C11—C14	121.6 (8)	C43—C42—C41	120.6 (7)
C13—C12—C11	121.6 (8)	C43—C42—H42	119.7
C13—C12—H12	119.2	C41—C42—H42	119.7
C11—C12—H12	119.2	C42—C43—C44	119.7 (7)
N1—C13—C12	120.5 (7)	C42—C43—H43	120.2
N1—C13—H13	119.7	C44—C43—H43	120.2
C12—C13—H13	119.7	C45—C44—C43	119.7 (7)
C11—C14—H14A	109.5	C45—C44—H44	120.2
C11—C14—H14B	109.5	C43—C44—H44	120.2
H14A—C14—H14B	109.5	C44—C45—C46	121.7 (7)
C11—C14—H14C	109.5	C44—C45—H45	119.2
H14A—C14—H14C	109.5	C46—C45—H45	119.2
H14B—C14—H14C	109.5	C45—C46—C41	119.3 (7)
N4—C15—C16	179.3 (11)	C45—C46—S6	122.9 (6)
C21—C16—C17	119.4 (7)	C41—C46—S6	117.8 (6)
C21—C16—C15	121.8 (9)	C48—C47—C50^{ii}	120.4 (6)
C17—C16—C15	118.8 (9)	C48—C47—S7	120.0 (6)
C18—C17—C16	119.3 (7)	C50^{ii}—C47—S7	119.5 (6)
C18—C17—H17	120.3	C49—C48—C47	120.3 (6)
C16—C17—H17	120.3	C49—C48—H48	119.9
C17—C18—C19	121.0 (6)	C47—C48—H48	119.9
C17—C18—H18	119.5	C48—C49—C52^{ii}	120.1 (6)
C19—C18—H18	119.5	C48—C49—H49	119.9
C20—C19—C18	119.7 (6)	C52^{ii}—C49—H49	119.9
C20—C19—C22	120.7 (7)	C51—C50—C47^{ii}	117.9 (6)
C18—C19—C22	119.6 (6)	C51—C50—S8	123.3 (5)
C19—C20—C21	119.4 (7)	C47^{ii}—C50—S8	118.8 (6)
C19—C20—H20	120.3	C52—C51—C50	121.5 (7)
C21—C20—H20	120.3	C52—C51—H51	119.2
C16—C21—C20	121.3 (7)	C50—C51—H51	119.2
C16—C21—H21	119.4	C51—C52—C49^{ii}	119.7 (7)
C20—C21—H21	119.4	C51—C52—H52	120.2
N2—C22—C19	112.9 (5)	C49^{ii}—C52—H52	120.2
S3—Ni2—S1—C29	178.71 (17)	C24—C25—C27—C28	1.5 (8)
S2—Ni2—S1—C29	−0.22 (17)	C26—C25—C27—C28	−179.0 (5)
S4—Ni2—S2—C34	179.64 (18)	C23—N2—C28—C27	−1.4 (8)
S1—Ni2—S2—C34	0.82 (19)	C22—N2—C28—C27	175.8 (5)
S4—Ni2—S3—C35	−0.44 (18)	C25—C27—C28—N2	0.4 (9)

S1—Ni2—S3—C35	178.39 (18)	Ni2—S1—C29—C30	178.1 (4)
S3—Ni2—S4—C36	0.29 (18)	Ni2—S1—C29—C34	−0.6 (4)
S2—Ni2—S4—C36	179.22 (18)	C34—C29—C30—C31	−1.1 (8)
S6—Ni1—S5—C41	5.32 (18)	S1—C29—C30—C31	−179.8 (4)
S6^{i}—Ni1—S5—C41	−160.73 (17)	C29—C30—C31—C32	0.1 (9)
S6^{i}—Ni1—S6—C46	87.36 (18)	C30—C31—C32—C33	0.3 (10)
S5—Ni1—S6—C46	−5.65 (19)	C31—C32—C33—C34	0.4 (9)
S5^{i}—Ni1—S6—C46	−179.34 (19)	C32—C33—C34—C29	−1.4 (8)
S8^{ii}—Ni3—S7—C47	−3.25 (18)	C32—C33—C34—S2	177.6 (4)
S8—Ni3—S7—C47	176.75 (18)	C30—C29—C34—C33	1.8 (8)
S7—Ni3—S8—C50	176.17 (17)	S1—C29—C34—C33	−179.5 (4)
S7^{ii}—Ni3—S8—C50	−3.83 (17)	C30—C29—C34—S2	−177.3 (4)
C7—C2—C3—C4	1.5 (10)	S1—C29—C34—S2	1.4 (6)
C1—C2—C3—C4	179.9 (6)	Ni2—S2—C34—C33	179.5 (4)
C2—C3—C4—C5	−1.0 (11)	Ni2—S2—C34—C29	−1.5 (4)
C3—C4—C5—C6	0.4 (9)	Ni2—S3—C35—C40	179.4 (4)
C3—C4—C5—C8	−177.5 (6)	Ni2—S3—C35—C36	0.6 (4)
C4—C5—C6—C7	−0.4 (8)	C40—C35—C36—C37	0.5 (8)
C8—C5—C6—C7	177.5 (5)	S3—C35—C36—C37	179.4 (4)
C5—C6—C7—C2	1.0 (9)	C40—C35—C36—S4	−179.3 (4)
C3—C2—C7—C6	−1.5 (9)	S3—C35—C36—S4	−0.4 (6)
C1—C2—C7—C6	−179.9 (6)	Ni2—S4—C36—C35	0.0 (4)
C13—N1—C8—C5	−136.2 (6)	Ni2—S4—C36—C37	−179.8 (4)
C9—N1—C8—C5	48.6 (7)	C35—C36—C37—C38	−0.3 (8)
C6—C5—C8—N1	66.0 (6)	S4—C36—C37—C38	179.5 (5)
C4—C5—C8—N1	−116.1 (6)	C36—C37—C38—C39	−0.2 (10)
C13—N1—C9—C10	−0.4 (8)	C37—C38—C39—C40	0.4 (11)
C8—N1—C9—C10	174.9 (5)	C38—C39—C40—C35	−0.2 (10)
N1—C9—C10—C11	0.0 (9)	C36—C35—C40—C39	−0.3 (9)
C9—C10—C11—C12	0.2 (9)	S3—C35—C40—C39	−179.2 (5)
C9—C10—C11—C14	−179.4 (5)	Ni1—S5—C41—C46	−3.9 (4)
C10—C11—C12—C13	−0.2 (9)	Ni1—S5—C41—C42	175.7 (4)
C14—C11—C12—C13	179.5 (6)	C46—C41—C42—C43	1.0 (8)
C9—N1—C13—C12	0.4 (8)	S5—C41—C42—C43	−178.6 (4)
C8—N1—C13—C12	−174.8 (5)	C41—C42—C43—C44	−0.4 (9)
C11—C12—C13—N1	−0.2 (10)	C42—C43—C44—C45	−0.4 (9)
C21—C16—C17—C18	0.6 (9)	C43—C44—C45—C46	0.7 (9)
C15—C16—C17—C18	−179.1 (6)	C44—C45—C46—C41	−0.2 (8)
C16—C17—C18—C19	0.2 (8)	C44—C45—C46—S6	179.3 (4)
C17—C18—C19—C20	−1.0 (8)	C42—C41—C46—C45	−0.7 (8)
C17—C18—C19—C22	−178.8 (5)	S5—C41—C46—C45	178.9 (4)
C18—C19—C20—C21	0.9 (9)	C42—C41—C46—S6	179.8 (4)
C22—C19—C20—C21	178.8 (5)	S5—C41—C46—S6	−0.6 (6)
C17—C16—C21—C20	−0.7 (10)	Ni1—S6—C46—C45	−174.7 (4)
C15—C16—C21—C20	179.1 (6)	Ni1—S6—C46—C41	4.8 (4)
C19—C20—C21—C16	−0.1 (10)	Ni3—S7—C47—C48	−177.0 (4)
C28—N2—C22—C19	121.6 (6)	Ni3—S7—C47—C50^{ii}	1.9 (4)

C23—N2—C22—C19	−61.2 (7)	C50^{ii}—C47—C48—C49	0.5 (8)
C20—C19—C22—N2	120.5 (6)	S7—C47—C48—C49	179.4 (4)
C18—C19—C22—N2	−61.7 (7)	C47—C48—C49—C52^{ii}	−0.5 (9)
C28—N2—C23—C24	0.4 (8)	Ni3—S8—C50—C51	−176.4 (4)
C22—N2—C23—C24	−176.8 (5)	Ni3—S8—C50—C47^{ii}	3.7 (4)
N2—C23—C24—C25	1.5 (9)	C47^{ii}—C50—C51—C52	0.6 (8)
C23—C24—C25—C27	−2.4 (8)	S8—C50—C51—C52	−179.3 (4)
C23—C24—C25—C26	178.1 (5)	C50—C51—C52—C49^{ii}	−0.6 (9)

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

Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8B···S4^{i}	0.97	2.846	3.721 (3)	150.63

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

Fig. 1

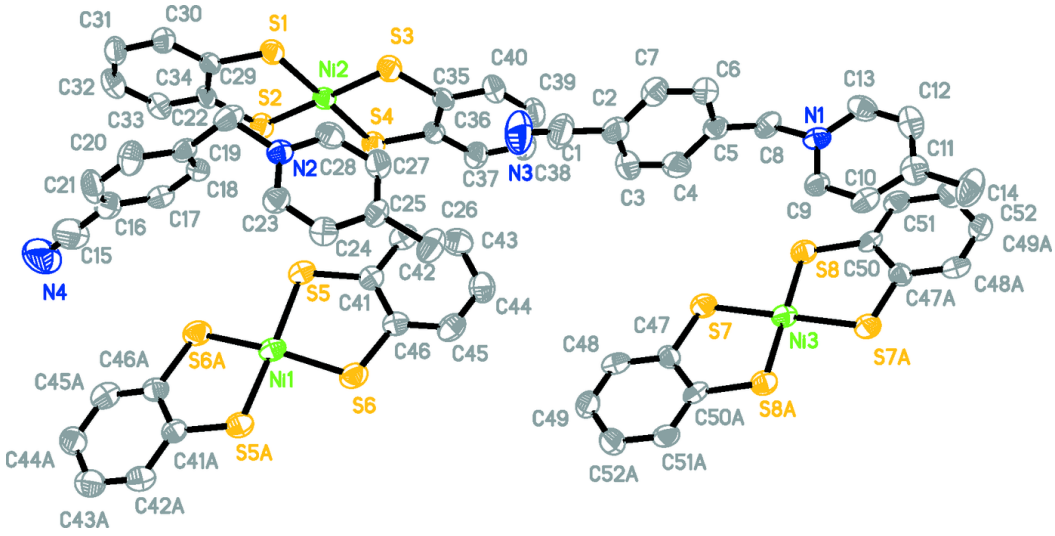
C31
C30
S1
S3
C40
C7
C6
C13
C12
C32
C34
C29
Ni2
C35
C39
C2
N1
S2
S4
C36
C33
C22
C1
C5
C8
C11
C20
C19
N2
C28
C27
C37
N3
C38
C3
C4
C10
C14
C21
C18
C9
C51
C52
C16
C17
C23
C25
C26
C49A
C15
C24
C43
S8
C50
C48A
N4
S5
C42
C41
C44
C47A
C47
S7
Ni3
S7A
C46A
S6A
Ni1
C46
C45
C48
C45A
S6
C50A
S8A
C49
C44A
C41A
S5A
C52A
C51A
C43A
C42A

Fig. 2