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Bis[1,2-bis(3,5-dimethylphenyl)ethylene-1,2-dithiolato(1—)]nickel(II)

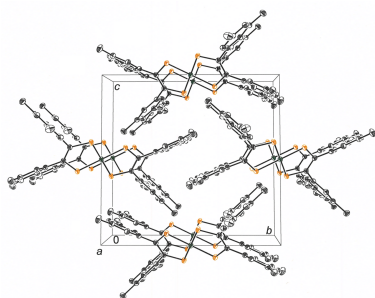
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The title compound, $[\text{Ni}(\text{C}_{18}\text{H}_{18}\text{S}_2)_2]$, **1**, crystallizes upon an inversion center in monoclinic $P2_1/c$ with intraligand C—S and C—C_{chelate} bond lengths that are indicative of the radical monoanionic redox level for the dithiolene ligand. The arene rings are canted at angles of 43.54 (4) and 71.36 (3)° with respect to the NiS₄ plane. Molecules of **1** form columnar stacks along the *a* axis of the cell with a $\sim 59^\circ$ angle between the molecular plane and the stacking axis. Adjacent stacks alternate in the directionality of their cant relative to the stacking axis such that a 37.2° angle is defined by the core NiS₄ planes of molecules from adjoining columns. Intermolecular interactions are governed by methyl C—H→ π_{arene} hydrogen bonds, with each molecule enjoying four such interactions as acceptor and providing four such interactions as donor.

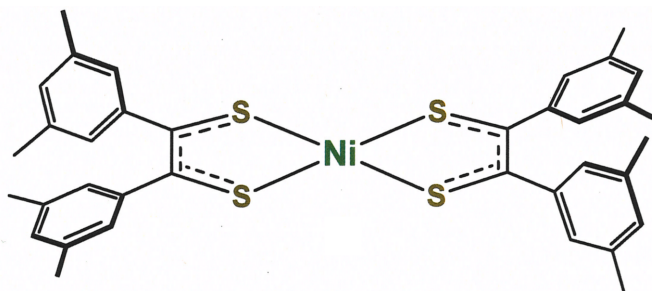
1. Chemical context

First synthesized in the middle 1960s, transition-metal dithiolene complexes elicited interest initially because their electronic structures did not conform to classical descriptive formalisms and led to the recognition that complexes with redox-active ligands define a category of coordination compounds that distinctively differ from those with metal-based frontier MOs (Eisenberg & Gray, 2011). For dithiolene complexes of the Group 10 metals particularly, their potential as novel, engineered materials for a broad range of applications has motivated steady effort aimed at the development of new synthetic methods and at characterization of their optical, electronic, and magnetic properties. Examples of the important behavior manifested by this compound class include the reversible bleaching of nickel dithiolene dyes under intense radiation (Mueller-Westerhoff *et al.*, 1991), superconductivity in molecular Group 10 bis(dithiolene) complexes (Kato, 2004), sensing of organophosphate toxins by platinum dithiolene 1,2-bis(diphenylphosphino)ethane complexes (Van Houten *et al.*, 1998), ferromagnetism (Robertson & Cronin, 2002; Faulmann & Cassoux, 2004), and catalytic H₂-evolution by nickel bis(dithiolene) complexes under photolysis (Zarkadoulas *et al.*, 2016). Because the redox, electronic, and optical properties that support many of these applications are directly and rationally influenced by the chemical nature of the dithiolene substituents, the development and characterization of new ligand derivatives and their complexes with Group 10 metals is of continuing interest. In this report, we detail the synthesis and crystal structure of nickel bis(3,5-dimethylphenyl)dithiolene, a coordination compound and a dithiolene ligand variant that have not previously been reported.



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2. Structural commentary

Bis[1,2-bis(3,5-dimethylphenyl)ethylene-1,2-dithiolato(1-)]nickel(II), **1**, is prepared in 38% yield using the phosphorus sulfide-benzil/benzoin protocol first disclosed by Schrauzer (Schrauzer & Mayweg, 1965). The separation of **1** from the solution as a microcrystalline precipitate is enabled by its hydrocarbon-rich periphery, its centrosymmetry and the polar, mixed aqueous-organic medium in which it forms. Its purity at this point is sufficient for most further purposes, but it is readily tractable to preparative-scale recrystallization by vapor diffusion methods.

The NiS₄ interior of **1** is rigorously planar, a feature necessitated by the occurrence of the molecule upon a crystallographic inversion center (Fig. 1). The placement of the Ni²⁺ ion upon an inversion center has the additional consequence that only half of the coordination complex is unique. The angles at which the arene substituents join the C₂S₂Ni chelate ring are 43.54 (4) and 71.36 (3)°. The 1.7063 (8) Å S—C_{ave} and 1.393 (2) C—C_{chelate} bond lengths in **1** are similar to the 1.714 (1) and 1.365 (9) Å observed for the corresponding bonds in Me₂C₂S₂²⁻ in [Ni(S₂C₂Me₂)₂] (Fig. 2; Lim *et al.*, 2001). This fact, in conjunction with the observation that these interatomic distances lie between those for the C—S and C—C_{chelate} bonds in [Ni(S₂C₂Me₂)₂]²⁻ (Lim *et al.*, 2001) and [Ni((S=C)₂(NMeCH₂)₂)₂]²⁺ (Bigoli, *et al.*, 2001), in which the

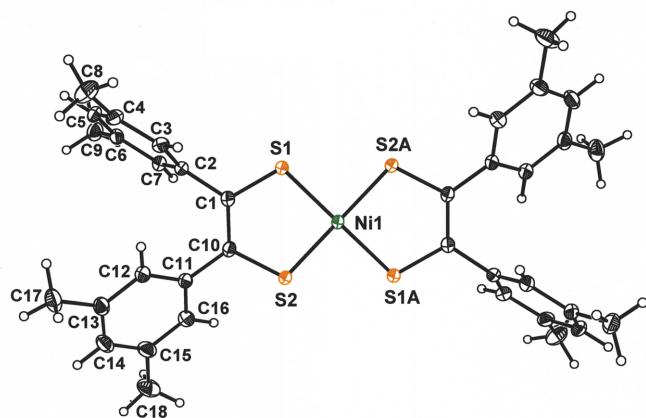


Figure 1

Displacement ellipsoid plot of **1** at the 50% probability level with atom labeling. Symmetry-related atoms other than S1A and S2A are not labeled. Symmetry code: (A) $-x, 2 - y, 1 - z$.

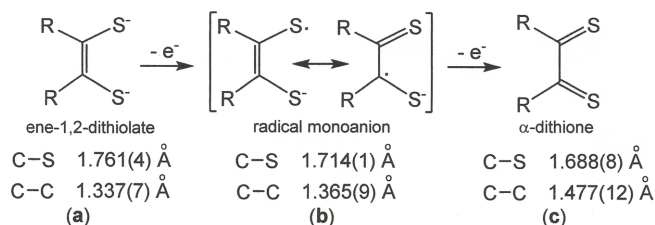


Figure 2

Redox levels of the dithiolene ligand shown with the S—C and C—C intra-ligand bond lengths that are typical for each redox state. The S—C and C—C bond lengths decrease and increase, respectively, as the redox series is traversed from ene-1,2-dithiolate(2-) (a) to α -dithione (c).

ligand redox levels are fully reduced ene-1,2-dithiolate and fully oxidized α -dithione, respectively, affirms a radical monoanionic description of the ligands in **1** (*cf.* Fig. 2).

3. Supramolecular features

The packing arrangement places molecules of **1** into columnar stacks along the *a*-axis direction of the cell with aryl rings of neighboring molecules forming both parallel planar and near orthogonal interactions (Fig. 3). When adjacent columns of molecules are viewed from the perspective of the edge of the NiS₄ plane (Fig. 4), an alternation is evident in the disposition angle of the molecular plane with respect to the stacking axis. The centermost stack in Fig. 4 reveals molecules whose planar core is rotated clockwise approximately 31° from orthogonality to the stacking axis, while the adjoining columns of **1** have the molecular plane inclined in the opposite direction by an equal magnitude. Regardless of the directionality of the tilt, the molecular planes form an angle of about 59° with the *a* axis. From the vantage point presented in Fig. 4, molecules from neighboring stacks are canted at a 37.2° angle relative to

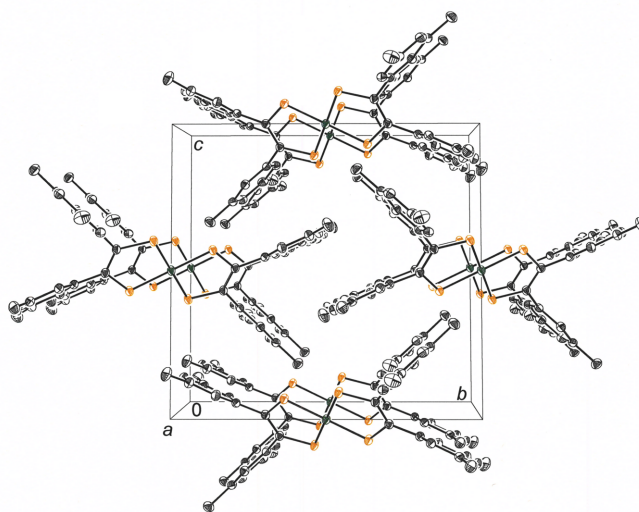


Figure 3

View along the *a* axis of the unit cell, revealing columnar stacks of **1**. Displacement ellipsoids are shown at the 50% level, and all H atoms are omitted for clarity.

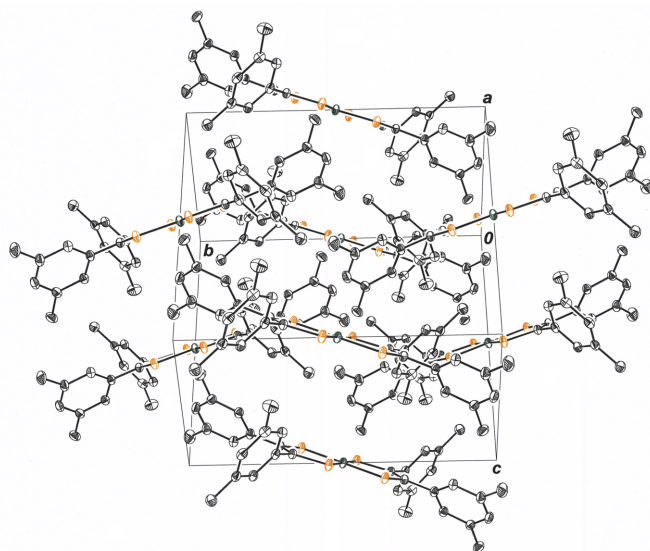


Figure 4

A 'side-on' perspective of the columnar stacks of **1** illustrating the alternating orientation of the molecular plane relative to the stacking axis. The view is approximately along the direction of the *ac* face diagonal of the cell. Displacement ellipsoids are drawn at the 50% level, and all H atoms are omitted for clarity.

one another such that a herringbone-like motif to the packing arrangement is created. A perspective view down the *c* axis of the cell again shows a zigzag pattern formed as rows of **1** that are canted in the other direction as they are also replicated by translation along *b* (Fig. 5).

Intermolecular interactions between stacks are governed by methyl C—H→ π_{arene} non-classical hydrogen bonds rather than by aliphatic dispersion forces. The distance between the C2—C7 ring centroid and H17C of an adjoining molecule is 2.97 Å, while H18B from a different neighboring molecule is positioned 2.87 Å from the C11—C16 ring centroid. This pattern is replicated on the molecule's other side such that each molecule functions as an acceptor of four such

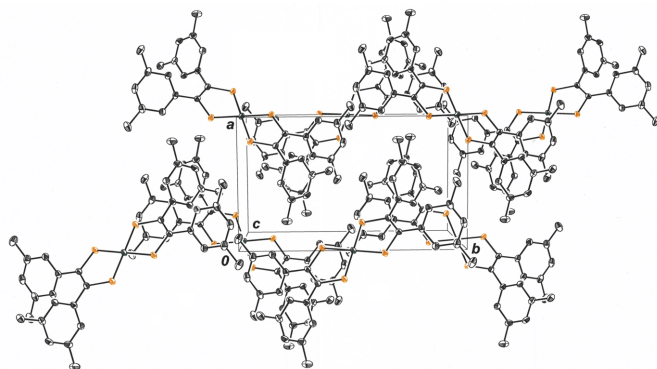


Figure 5

View of the molecular packing for **1** along the *c* axis of the unit cell. A sawtoothed appearance to the packing motif is again evident but with more acute angle in the pattern. Displacement ellipsoids are drawn at the 50% level, and all H atoms are omitted for clarity.

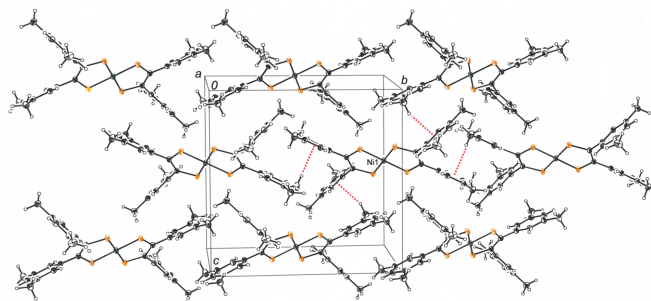


Figure 6

Packing arrangement of **1** in rows along the *b* axis (left-to-right) as viewed down the *a* axis of the cell. The four C—H→ π_{arene} interactions in which the molecule with the Ni1 label serves as acceptor are illustrated with heavy dashed red lines. Displacement ellipsoids are presented at the 50% level.

C—H→ π_{arene} hydrogen bonds, one with each 3,5-dimethylphenyl ring (Fig. 6). The heavy red dashed lines that depict these interactions evoke a windmill-like symmetry in Fig. 6. Additionally, both H17C and H18B from each end of **1** serve as donors of C—H→ π_{arene} hydrogen bonds to adjacent molecules, providing each molecule of **1** with an additional four C—H→ π_{arene} hydrogen bonds as C—H donor. While such interactions are individually weak with an interaction strength in the range of 1.5–2.5 kcal mol^{−1} (Nishio, 2012), their collective effect appears to be decisive in guiding the interleaved arrangement of 3,5-dimethylphenyl rings.

4. Database survey

The bis(3,5-dimethylphenyl)dithiolene ligand does not appear in any structurally characterized coordination compound of the transition metals or any other element (CSD, Version 2024.3; Groom *et al.*, 2016), nor does any report of its use occur in other information databases. The set of structurally characterized homoleptic nickel bis(dithiolene) complexes with aryl-type substituents, [Ni(S₂C₂Ar₂)₂], to which **1** is now joined includes those where Ar = Ph (Megnamisi-Belombe & Nuber, 1989; Kuramoto & Asao, 1990; Miao *et al.*, 2011), Me-4-C₆H₄ (Miao *et al.*, 2011), ^tBu-4-C₆H₄ (Das Gupta *et al.*, 2023), Cl-4-C₆H₄ (Koehne *et al.*, 2022), MeO-4-C₆H₄ (Arumugam *et al.*, 2007), and 3,5-(MeO)₂-4-ⁿBuO-C₆H₂ (Nakazumi *et al.*, 1992). Among these complexes, the largest twist angle between an aryl ring substituent and the NiS₄C₄ plane is 65.77° in the monoclinic polymorph of [Ni(S₂C₂Ph₂)₂] (Miao *et al.*, 2011), a value that is appreciably less than the 71.36 (3)° twist angle in **1**. While C—H→ π_{arene} hydrogen-bond interactions are very apparent in this *P*₂/*1*/*n* form of [Ni(S₂C₂Ph₂)₂], close approach of H atoms to the ring centroids of neighboring molecules easily occurs with lessened rotation of the aryl substituent from the planar core.

5. Synthesis and crystallization

Phosphorus sulfide (P₄S₁₀, 0.379 g, 0.853 mmol) and 1,2-bis-(3,5-dimethylphenyl)ethane-1,2-dione (0.353 g, 1.32 mmol)

Table 1

Experimental details.

Crystal data	
Chemical formula	[Ni(C ₁₈ H ₁₈ S ₂) ₂]
<i>M_r</i>	655.60
Crystal system, space group	Monoclinic, <i>P</i> ₂ ₁ / <i>c</i>
Temperature (K)	150
<i>a</i> , <i>b</i> , <i>c</i> (Å)	8.4446 (2), 14.0911 (2), 13.5880 (2)
β (°)	96.133 (1)
<i>V</i> (Å ³)	1607.63 (5)
<i>Z</i>	2
Radiation type	Cu <i>K</i> α
μ (mm ^{−1})	3.47
Crystal size (mm)	0.14 × 0.14 × 0.04
Data collection	
Diffractometer	Bruker D8 QUEST PHOTON 3 diffractometer
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T</i> _{min} , <i>T</i> _{max}	0.77, 0.88
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	33748, 3139, 2827
<i>R</i> _{int}	0.077
(sin θ /λ) _{max} (Å ^{−1})	0.618
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.024, 0.066, 1.08
No. of reflections	3139
No. of parameters	191
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ^{−3})	0.29, −0.30

Computer programs: *APEX4* and *SAINT* (Bruker, 2021), *SHELXT* (Sheldrick, 2015a), *SHELXL2018/1* (Sheldrick, 2015b) and *SHELXTL* (Sheldrick, 2008).

were dissolved in 1,4-dioxane (50 ml) and refluxed under a N₂ atmosphere for 3.5 h. The resulting mixture was cooled to ambient temperature, filtered to remove unreacted solids, transferred to a solution of [Ni(OH₂)₆]Cl₂ (0.129 g, 0.541 mmol) in deionized H₂O (5 ml) and brought to reflux again for 3 h under N₂. Upon cooling, the reaction mixture deposited crude **1** as a dark microcrystalline solid, which was collected by vacuum filtration, washed in succession with portions of deionized H₂O, EtOH, and Et₂O and then dried overnight under vacuum. Yield: 0.135 g, 0.206 mmol, 38%. Diffraction quality, prism-shaped black crystals were grown by the diffusion of MeOH vapor into a benzene solution. ¹H NMR (δ, p.p.m. in CDCl₃): 7.00 (s, 3 H, *ortho* and *para* aromatic C—H), 2.25 (s, 24 H, —CH₃). ¹³C NMR (δ, p.p.m. in CDCl₃): 181.9, 141.3, 137.8, 130.6, 126.9, 21.3. UV-vis [CH₂Cl₂, λ_{max}, nm (ε_M, M^{−1}·cm^{−1}): 270 (11800), 320 (15000), 605 (670), 875 (10200). Cyclic voltammetry (CH₂Cl₂, [Bu₄N][PF₆] supporting electrolyte, Cp₂Fe⁺/Cp₂Fe as reference): **1** − e[−] → [**1**]⁺, +0.611 V; **1** + e[−] → [**1**][−], −0.509 V; [**1**][−] − e[−] → [**1**]^{2−}, −1.323 V. Analysis calculated for C₃₆H₃₆S₄Ni: C, 65.95; H, 5.53; S, 19.56. Found: C, 65.86; H, 5.49; S, 19.49.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. Hydrogen atoms were added in

calculated positions and refined with isotropic displacement parameters that were approximately 1.2 times (for aromatic C—H) or 1.5 times (for —CH₃) those of the carbon atoms to which they were attached. The C—H distances assumed were 0.95 and 0.98 Å for the aromatic C—H and —CH₃ types of hydrogen atoms, respectively. Rotation around the CH₃—C_{aromatic} bonds was used to identify the positional variant that best modeled the experimental electron-density map.

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Computing details

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Crystal data

[Ni(C₁₈H₁₈S₂)₂]
 $M_r = 655.60$
 Monoclinic, $P2_1/c$
 $a = 8.4446$ (2) Å
 $b = 14.0911$ (2) Å
 $c = 13.5880$ (2) Å
 $\beta = 96.133$ (1)°
 $V = 1607.63$ (5) Å³
 $Z = 2$

$F(000) = 688$
 $D_x = 1.354$ Mg m^{−3}
 Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
 Cell parameters from 9778 reflections
 $\theta = 6.3$ – 72.3 °
 $\mu = 3.47$ mm^{−1}
 $T = 150$ K
 Prism, black
 $0.14 \times 0.14 \times 0.04$ mm

Data collection

Bruker D8 QUEST PHOTON 3
 diffractometer
 Radiation source: INCOATEC I μ S micro—
 focus source
 Mirror monochromator
 Detector resolution: 7.3910 pixels mm^{−1}
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.77$, $T_{\max} = 0.88$
 33748 measured reflections
 3139 independent reflections
 2827 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.077$
 $\theta_{\max} = 72.4$ °, $\theta_{\min} = 5.3$ °
 $h = -10 \rightarrow 9$
 $k = -17 \rightarrow 17$
 $l = -16 \rightarrow 16$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.024$
 $wR(F^2) = 0.066$
 $S = 1.08$
 3139 reflections
 191 parameters
 0 restraints
 Primary atom site location: dual

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0406P)^2 + 0.231P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.29$ e Å^{−3}
 $\Delta\rho_{\min} = -0.30$ e Å^{−3}

Special details

Experimental. The diffraction data were obtained from 18 sets of frames, each of width 0.50° in ω or φ , collected with scan parameters determined by the "strategy" routine in *APEX4*. The scan time was 1.00 to 2.00 sec/frame.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.000000	1.000000	0.500000	0.01729 (9)
S1	0.19671 (3)	0.95781 (2)	0.60078 (2)	0.02015 (9)
S2	−0.00937 (3)	0.86456 (2)	0.43113 (2)	0.01909 (9)
C1	0.23361 (13)	0.84300 (9)	0.57198 (9)	0.0178 (2)
C2	0.36518 (14)	0.79450 (8)	0.63520 (8)	0.0185 (2)
C3	0.52354 (14)	0.81955 (9)	0.62757 (9)	0.0204 (2)
H3	0.547341	0.869239	0.584243	0.025*
C4	0.64722 (14)	0.77144 (10)	0.68374 (9)	0.0227 (2)
C5	0.60798 (14)	0.70147 (9)	0.74937 (9)	0.0220 (2)
H5	0.691341	0.669344	0.788443	0.026*
C6	0.45082 (14)	0.67694 (9)	0.75972 (9)	0.0205 (2)
C7	0.32915 (14)	0.72416 (9)	0.70087 (9)	0.0198 (2)
H7	0.221118	0.707946	0.705910	0.024*
C8	0.81906 (16)	0.79350 (13)	0.67185 (11)	0.0347 (3)
H8A	0.884086	0.784314	0.735298	0.052*
H8B	0.828065	0.859488	0.650366	0.052*
H8C	0.856592	0.751012	0.622164	0.052*
C9	0.41374 (16)	0.60121 (10)	0.83200 (10)	0.0267 (3)
H9A	0.299904	0.602821	0.840280	0.040*
H9B	0.475912	0.612633	0.896001	0.040*
H9C	0.441270	0.538868	0.806746	0.040*
C10	0.14043 (13)	0.79976 (8)	0.49382 (8)	0.0175 (2)
C11	0.16772 (14)	0.70341 (9)	0.45561 (9)	0.0194 (2)
C12	0.32241 (15)	0.67305 (9)	0.44488 (9)	0.0209 (2)
H12	0.409948	0.712794	0.466938	0.025*
C13	0.35040 (16)	0.58592 (9)	0.40260 (9)	0.0235 (2)
C14	0.22139 (17)	0.52790 (9)	0.37169 (9)	0.0274 (3)
H14	0.239969	0.467764	0.343480	0.033*
C15	0.06530 (17)	0.55596 (10)	0.38116 (10)	0.0265 (3)
C16	0.03943 (15)	0.64417 (9)	0.42290 (9)	0.0230 (2)
H16	−0.066303	0.664398	0.429274	0.028*
C17	0.51798 (17)	0.55730 (11)	0.38711 (11)	0.0317 (3)
H17A	0.524013	0.488055	0.381859	0.048*

H17B	0.591452	0.578953	0.443336	0.048*
H17C	0.547411	0.586274	0.326076	0.048*
C18	−0.0720 (2)	0.49193 (11)	0.34582 (13)	0.0379 (3)
H18A	−0.157674	0.529667	0.310700	0.057*
H18B	−0.111446	0.460583	0.402777	0.057*
H18C	−0.036098	0.443897	0.300991	0.057*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.01736 (15)	0.01340 (15)	0.01985 (15)	0.00354 (9)	−0.00388 (11)	−0.00123 (10)
S1	0.02112 (15)	0.01491 (15)	0.02242 (15)	0.00378 (9)	−0.00688 (11)	−0.00326 (10)
S2	0.01952 (15)	0.01512 (14)	0.02085 (14)	0.00370 (9)	−0.00609 (10)	−0.00226 (10)
C1	0.0185 (5)	0.0148 (5)	0.0197 (5)	0.0022 (4)	0.0003 (4)	0.0000 (4)
C2	0.0192 (5)	0.0171 (5)	0.0180 (5)	0.0042 (4)	−0.0035 (4)	−0.0030 (4)
C3	0.0218 (6)	0.0206 (6)	0.0180 (5)	0.0002 (4)	−0.0020 (4)	−0.0008 (4)
C4	0.0188 (5)	0.0277 (6)	0.0207 (5)	0.0023 (5)	−0.0025 (4)	−0.0037 (5)
C5	0.0198 (6)	0.0252 (6)	0.0198 (5)	0.0083 (4)	−0.0039 (4)	−0.0017 (5)
C6	0.0246 (6)	0.0188 (6)	0.0175 (5)	0.0063 (4)	−0.0001 (4)	−0.0011 (4)
C7	0.0184 (5)	0.0184 (5)	0.0218 (5)	0.0027 (4)	−0.0015 (4)	−0.0013 (4)
C8	0.0205 (6)	0.0495 (9)	0.0334 (7)	−0.0008 (6)	−0.0012 (5)	0.0055 (7)
C9	0.0289 (6)	0.0257 (6)	0.0251 (6)	0.0056 (5)	0.0009 (5)	0.0052 (5)
C10	0.0167 (5)	0.0158 (5)	0.0194 (5)	0.0027 (4)	−0.0008 (4)	0.0013 (4)
C11	0.0248 (6)	0.0155 (6)	0.0168 (5)	0.0036 (4)	−0.0019 (4)	0.0006 (4)
C12	0.0245 (6)	0.0184 (6)	0.0191 (5)	0.0036 (4)	−0.0008 (4)	0.0011 (4)
C13	0.0326 (6)	0.0203 (6)	0.0178 (5)	0.0074 (5)	0.0036 (5)	0.0027 (4)
C14	0.0437 (8)	0.0167 (6)	0.0218 (6)	0.0046 (5)	0.0030 (5)	−0.0028 (5)
C15	0.0358 (7)	0.0192 (6)	0.0237 (6)	−0.0023 (5)	−0.0006 (5)	−0.0029 (5)
C16	0.0252 (6)	0.0188 (6)	0.0243 (6)	0.0006 (4)	−0.0008 (5)	−0.0014 (5)
C17	0.0381 (7)	0.0276 (7)	0.0311 (7)	0.0123 (6)	0.0114 (6)	0.0006 (5)
C18	0.0447 (8)	0.0272 (7)	0.0411 (8)	−0.0108 (6)	0.0004 (7)	−0.0107 (6)

Geometric parameters (Å, °)

Ni1—S1 ⁱ	2.1218 (3)	C9—H9A	0.9800
Ni1—S1	2.1218 (3)	C9—H9B	0.9800
Ni1—S2 ⁱ	2.1233 (3)	C9—H9C	0.9800
Ni1—S2	2.1233 (3)	C10—C11	1.4804 (16)
S1—C1	1.7010 (12)	C11—C12	1.3969 (17)
S2—C10	1.7115 (11)	C11—C16	1.4018 (18)
C1—C10	1.3927 (16)	C12—C13	1.3865 (18)
C1—C2	1.4952 (15)	C12—H12	0.9500
C2—C7	1.3889 (17)	C13—C14	1.391 (2)
C2—C3	1.3976 (17)	C13—C17	1.5077 (18)
C3—C4	1.4009 (17)	C14—C15	1.395 (2)
C3—H3	0.9500	C14—H14	0.9500
C4—C5	1.3929 (19)	C15—C16	1.3932 (18)
C4—C8	1.5095 (18)	C15—C18	1.5064 (19)

C5—C6	1.3931 (18)	C16—H16	0.9500
C5—H5	0.9500	C17—H17A	0.9800
C6—C7	1.4009 (17)	C17—H17B	0.9800
C6—C9	1.5057 (17)	C17—H17C	0.9800
C7—H7	0.9500	C18—H18A	0.9800
C8—H8A	0.9800	C18—H18B	0.9800
C8—H8B	0.9800	C18—H18C	0.9800
C8—H8C	0.9800		
S1 ⁱ —Ni1—S1	180.0	H9A—C9—H9B	109.5
S1 ⁱ —Ni1—S2 ⁱ	91.279 (10)	C6—C9—H9C	109.5
S1—Ni1—S2 ⁱ	88.723 (10)	H9A—C9—H9C	109.5
S1 ⁱ —Ni1—S2	88.721 (10)	H9B—C9—H9C	109.5
S1—Ni1—S2	91.278 (10)	C1—C10—C11	124.90 (10)
S2 ⁱ —Ni1—S2	180.0	C1—C10—S2	118.26 (9)
C1—S1—Ni1	105.55 (4)	C11—C10—S2	116.69 (8)
C10—S2—Ni1	105.63 (4)	C12—C11—C16	118.96 (11)
C10—C1—C2	124.25 (11)	C12—C11—C10	119.99 (11)
C10—C1—S1	119.28 (9)	C16—C11—C10	120.89 (11)
C2—C1—S1	116.46 (9)	C13—C12—C11	121.14 (12)
C7—C2—C3	120.32 (10)	C13—C12—H12	119.4
C7—C2—C1	119.67 (11)	C11—C12—H12	119.4
C3—C2—C1	120.01 (11)	C12—C13—C14	118.88 (12)
C2—C3—C4	120.06 (12)	C12—C13—C17	119.92 (13)
C2—C3—H3	120.0	C14—C13—C17	121.15 (12)
C4—C3—H3	120.0	C13—C14—C15	121.53 (12)
C5—C4—C3	118.48 (11)	C13—C14—H14	119.2
C5—C4—C8	120.76 (11)	C15—C14—H14	119.2
C3—C4—C8	120.75 (12)	C16—C15—C14	118.76 (12)
C4—C5—C6	122.32 (11)	C16—C15—C18	121.02 (13)
C4—C5—H5	118.8	C14—C15—C18	120.22 (13)
C6—C5—H5	118.8	C15—C16—C11	120.72 (12)
C5—C6—C7	118.23 (12)	C15—C16—H16	119.6
C5—C6—C9	120.56 (11)	C11—C16—H16	119.6
C7—C6—C9	121.20 (11)	C13—C17—H17A	109.5
C2—C7—C6	120.53 (11)	C13—C17—H17B	109.5
C2—C7—H7	119.7	H17A—C17—H17B	109.5
C6—C7—H7	119.7	C13—C17—H17C	109.5
C4—C8—H8A	109.5	H17A—C17—H17C	109.5
C4—C8—H8B	109.5	H17B—C17—H17C	109.5
H8A—C8—H8B	109.5	C15—C18—H18A	109.5
C4—C8—H8C	109.5	C15—C18—H18B	109.5
H8A—C8—H8C	109.5	H18A—C18—H18B	109.5
H8B—C8—H8C	109.5	C15—C18—H18C	109.5
C6—C9—H9A	109.5	H18A—C18—H18C	109.5
C6—C9—H9B	109.5	H18B—C18—H18C	109.5
Ni1—S1—C1—C10	1.02 (11)	C2—C1—C10—S2	178.12 (9)

Ni1—S1—C1—C2	−177.97 (8)	S1—C1—C10—S2	−0.78 (14)
C10—C1—C2—C7	−70.01 (16)	Ni1—S2—C10—C1	0.13 (11)
S1—C1—C2—C7	108.92 (11)	Ni1—S2—C10—C11	−175.73 (8)
C10—C1—C2—C3	109.54 (14)	C1—C10—C11—C12	−41.64 (18)
S1—C1—C2—C3	−71.52 (13)	S2—C10—C11—C12	133.91 (10)
C7—C2—C3—C4	2.22 (18)	C1—C10—C11—C16	143.13 (12)
C1—C2—C3—C4	−177.33 (11)	S2—C10—C11—C16	−41.32 (15)
C2—C3—C4—C5	−2.46 (18)	C16—C11—C12—C13	0.06 (18)
C2—C3—C4—C8	176.27 (12)	C10—C11—C12—C13	−175.26 (11)
C3—C4—C5—C6	1.02 (19)	C11—C12—C13—C14	−0.76 (18)
C8—C4—C5—C6	−177.71 (13)	C11—C12—C13—C17	176.79 (11)
C4—C5—C6—C7	0.68 (19)	C12—C13—C14—C15	0.83 (19)
C4—C5—C6—C9	−179.67 (12)	C17—C13—C14—C15	−176.69 (13)
C3—C2—C7—C6	−0.47 (18)	C13—C14—C15—C16	−0.2 (2)
C1—C2—C7—C6	179.08 (11)	C13—C14—C15—C18	179.27 (13)
C5—C6—C7—C2	−0.96 (18)	C14—C15—C16—C11	−0.5 (2)
C9—C6—C7—C2	179.39 (11)	C18—C15—C16—C11	−179.98 (13)
C2—C1—C10—C11	−6.39 (19)	C12—C11—C16—C15	0.60 (18)
S1—C1—C10—C11	174.70 (9)	C10—C11—C16—C15	175.88 (12)

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