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Bis[*S*-octyl 3-(4-methoxybenzylidene)dithiocarbazato-κ^2N^3,S]nickel(II)

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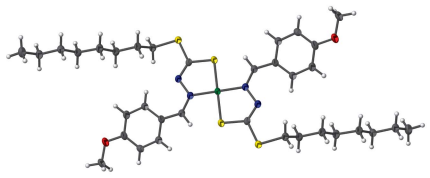
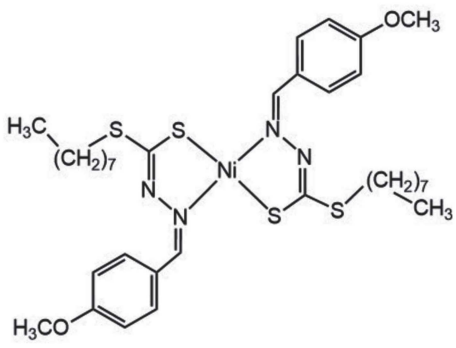
Structural data: full structural data are available from iucrdata.iucr.org

The nickel(II) cation of the title complex, $[Ni(C_{17}H_{25}N_2OS_2)_2]$, is located on a crystallographic inversion centre. It has a square-planar coordination geometry, with a *trans* configuration of the *N*,*S*-chelating ligands, as imposed by the crystal symmetry.

3D view



Chemical scheme



Structure description

Bidentate Schiff bases of *S*-methyl or *S*-benzyl dithiocarbazates and their metal complexes have received considerable attention for their possible bioactivities. As part of our ongoing structural studies of S-containing Schiff bases (Howlader *et al.*, 2015; Islam *et al.*, 2011, 2014), we now report on the structure of the title complex in which the ligand has a long alkyl chain.

The molecular structure of the title complex is illustrated in Fig. 1. The complex has the nickel(II) cation located on a crystallographic inversion centre with the two Schiff bases, in their deprotonated imino thiolate form, chelating through the azomethine nitrogen atom N1 and the thiolate sulfur atom S1 in a *trans*-planar configuration, as imposed by the crystal symmetry. The complex has a coplanar geometry with the exception of the octyl chains that extend above and below the coordination plane (Fig. 1). The Ni—S and Ni—N bond lengths are 2.1796 (6) and 1.9310 (19) Å, respectively, and the S1—Ni1—N1 chelating angle is 85.67 (5)°. These geometrical parameters are comparable to those found in the related bis-chelated nickel(II) complex with the *S*-hexyl 3-(4-methylbenzylidene)dithiocarbazate ligand (Howlader *et al.*, 2015). There the corresponding

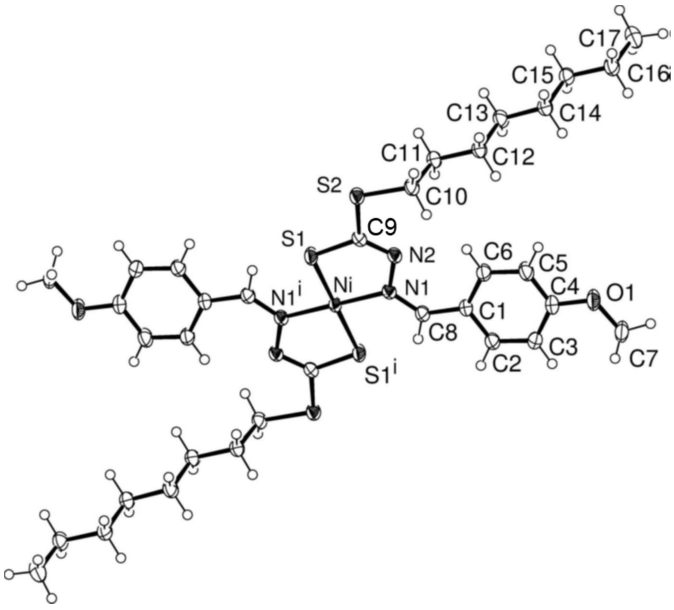


Figure 1
A view of the molecular structure of the title complex, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level. Symmetry code (i) $-x+1, -y+1, -z+1$.

bond lengths and angles are 2.1775 (10) and 1.933 (3) Å, and 86.04 (9)°, respectively, indicating that neither the longer alkyl group nor the different Schiff base affects the coordination bond lengths.

The structure of the title ligand (H*L*), reported by Begum *et al.* (2015), shows that on coordination, a 180° rotation occurs about the C9—N2 bond in order to allow *N*,*S* chelation to the metal atom. Upon coordination, some salient features are also observed with respect to the free ligand. The most significant is an elongation of the C9—S1 bond length from 1.6734 (15) Å in the ligand to 1.7514 (19) Å in the title complex, thus validating the coordination with the deprotonated thiolate sulfur atom. Correspondingly, the N2—C9 bond length of 1.3343 (16) Å in H*L* is shortened to 1.285 (3) Å in the title complex, while the N1—N2 bond length of 1.3829 (17) Å in H*L* is slightly elongated to 1.413 (3) Å in the complex. These geometrical parameters agree with those reported for similar nickel complexes when the ligands assume either a *trans* (Islam *et al.*, 2011, 2014; Zhang *et al.*, 2004) or a *cis* configuration (Chan *et al.*, 2008; Li *et al.*, 2006).

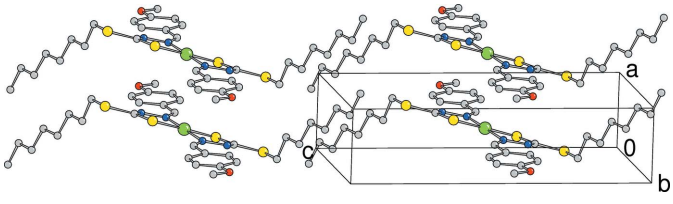


Figure 2
A view approximately along the *b* axis of the crystal packing of the title complex.

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Ni(C_{17}H_{25}N_2OS_2)_2]$
M_r	733.73
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	173
a, b, c (Å)	4.55302 (14), 11.5641 (3), 17.5075 (5)
α, β, γ (°)	84.1436 (7), 85.6165 (10), 76.4084 (10)
V (Å^3)	890.00 (5)
Z	1
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.82
Crystal size (mm)	0.27 × 0.12 × 0.07
Data collection	
Diffractometer	Rigaku R-AXIS RAPID
Absorption correction	Multi-scan (*ABSCOR*; Higashi, 1995)
T_{min}, T_{max}	0.866, 0.944
No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections	8899, 4041, 3705
R_{int}	0.025
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.112, 1.15
No. of reflections	4041
No. of parameters	207
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.17, −0.37

Computer programs: *RAPID-AUTO* (Rigaku, 1999), *SIR92* (Altomare *et al.*, 1994), *SHELXL97* (Sheldrick, 2008) and *CrystalStructure* (Rigaku, 2010).

In the crystal, complex molecules stack up the *a* axis at a distance of 4.55302 (14) Å, thus excluding any significant interactions between the aromatic rings (see Fig. 2).

Synthesis and crystallization

A solution of $Ni(CH_3COO)_2{\cdot}4H_2O$ (0.06 g, 0.25 mmol) in methanol (7 ml) was added to a methanol solution (10 ml) of the *S*-octyl (*E*)-3-(4-methoxybenzylidene)dithiocarbazate ligand (0.17 g, 0.5 mmol). The resulting mixture was stirred at room temperature for 5 h. The dark orange precipitate that formed was filtered off, washed with methanol and dried *in vacuo* over anhydrous $CaCl_2$. Dark orange single crystals of the title complex (m.p. 371 K), suitable for X-ray diffraction analysis, were obtained by slow evaporation from a mixture of chloroform/toluene (6:1 *v*:*v*).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Acknowledgements

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Funding information

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full crystallographic data

IUCrData (2018). **3**, x181684 [https://doi.org/10.1107/S241431461801684X]

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Crystal data

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Triclinic, $P\overline{1}$
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a = 4.55302 (14) Å
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c = 17.5075 (5) Å
α = 84.1436 (7)°
β = 85.6165 (10)°
γ = 76.4084 (10)°
V = 890.00 (5) Å^3
Z = 1
$F(000)$ = 390.00
D_x = 1.369 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 8264 reflections
θ = 3.1–27.5°
μ = 0.82 mm^{-1}
T = 173 K
Platelet, orange
0.27 × 0.12 × 0.07 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
T_{min} = 0.866, T_{max} = 0.944
8899 measured reflections
4041 independent reflections
3705 reflections with $F^2 > 2.0\sigma(F^2)$
R_{int} = 0.025
θ_{max} = 27.5°
h = −5→5
k = −14→14
l = −22→21

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.112
S = 1.15
4041 reflections
207 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0566P)^2 + 0.5813P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY

Refinement. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).

The H atoms were located geometrically and treated as riding atoms: C—H = 0.95–0.99 Å with U_{iso}(H) = 1.5U_{eq}(*C*-methyl) and 1.2U_{eq}(C) for other H atoms.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni	0.5000	0.5000	0.5000	0.02291 (12)
S1	0.53959 (14)	0.35043 (5)	0.58802 (3)	0.03236 (15)
S2	0.72806 (13)	0.33241 (4)	0.74527 (3)	0.02987 (14)
O1	1.3002 (4)	0.96865 (14)	0.71096 (9)	0.0387 (4)
N1	0.6922 (4)	0.57294 (15)	0.57058 (9)	0.0247 (4)
N2	0.7284 (4)	0.52311 (15)	0.64734 (9)	0.0256 (4)
C1	0.9372 (5)	0.73725 (17)	0.59923 (11)	0.0249 (4)
C2	1.0441 (5)	0.82953 (18)	0.55700 (12)	0.0292 (5)
C3	1.1693 (5)	0.90850 (18)	0.59111 (12)	0.0302 (5)
C4	1.1880 (5)	0.89570 (18)	0.67074 (12)	0.0283 (4)
C5	1.0869 (6)	0.8034 (2)	0.71388 (13)	0.0353 (5)
C6	0.9640 (6)	0.72470 (19)	0.67942 (12)	0.0314 (5)
C7	1.3781 (6)	1.0717 (2)	0.66998 (15)	0.0397 (6)
C8	0.8008 (5)	0.66685 (18)	0.55359 (11)	0.0264 (4)
C9	0.6696 (5)	0.41906 (17)	0.65734 (11)	0.0243 (4)
C10	0.8698 (5)	0.42720 (18)	0.80277 (11)	0.0282 (4)
C11	0.6211 (5)	0.51742 (19)	0.84182 (12)	0.0291 (4)
C12	0.7464 (5)	0.58919 (19)	0.89491 (12)	0.0293 (5)
C13	0.5011 (5)	0.6716 (2)	0.94072 (12)	0.0314 (5)
C14	0.6261 (5)	0.73863 (19)	0.99649 (12)	0.0306 (5)
C15	0.3830 (5)	0.82086 (19)	1.04283 (12)	0.0305 (5)
C16	0.5078 (6)	0.8927 (2)	1.09547 (13)	0.0335 (5)
C17	0.2620 (6)	0.9785 (2)	1.13894 (14)	0.0418 (6)
H1	1.0306	0.8386	0.5028	0.0351*
H2	1.2411	0.9701	0.5608	0.0362*
H3	1.1027	0.7943	0.7681	0.0423*
H4	0.8974	0.6620	0.7099	0.0377*
H5	1.5416	1.0465	0.6312	0.0476*
H6	1.4452	1.1184	0.7060	0.0476*
H7	1.2007	1.1208	0.6446	0.0476*
H8	0.7894	0.6958	0.5009	0.0316*
H9	0.9957	0.3763	0.8426	0.0338*
H10	1.0013	0.4706	0.7693	0.0338*
H11	0.4799	0.4749	0.8721	0.0349*
H12	0.5055	0.5730	0.8021	0.0349*
H13	0.8793	0.5331	0.9312	0.0352*
H14	0.8718	0.6376	0.8636	0.0352*

H15	0.3694	0.6238	0.9700	0.0377*
H16	0.3744	0.7304	0.9045	0.0377*
H17	0.7537	0.6798	1.0325	0.0367*
H18	0.7571	0.7866	0.9671	0.0367*
H19	0.2587	0.7722	1.0744	0.0366*
H20	0.2485	0.8769	1.0069	0.0366*
H21	0.6347	0.8368	1.1330	0.0402*
H22	0.6391	0.9388	1.0643	0.0402*
H23	0.1296	1.0319	1.1022	0.0501*
H24	0.3557	1.0259	1.1689	0.0501*
H25	0.1426	0.9331	1.1737	0.0501*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni	0.0282 (2)	0.02338 (19)	0.02004 (18)	−0.01005 (13)	−0.00419 (13)	−0.00357 (13)
S1	0.0511 (4)	0.0275 (3)	0.0245 (3)	−0.0186 (3)	−0.0109 (2)	−0.00139 (19)
S2	0.0432 (3)	0.0257 (3)	0.0235 (3)	−0.0124 (2)	−0.0073 (2)	−0.00067 (18)
O1	0.0545 (11)	0.0323 (8)	0.0371 (9)	−0.0207 (7)	−0.0132 (8)	−0.0064 (7)
N1	0.0302 (9)	0.0249 (8)	0.0207 (8)	−0.0086 (7)	−0.0036 (7)	−0.0027 (6)
N2	0.0322 (9)	0.0259 (8)	0.0206 (8)	−0.0089 (7)	−0.0047 (7)	−0.0030 (6)
C1	0.0266 (10)	0.0241 (9)	0.0258 (10)	−0.0070 (7)	−0.0046 (7)	−0.0053 (7)
C2	0.0362 (11)	0.0285 (10)	0.0250 (10)	−0.0103 (8)	−0.0045 (8)	−0.0035 (8)
C3	0.0355 (11)	0.0258 (10)	0.0318 (11)	−0.0118 (8)	−0.0018 (9)	−0.0034 (8)
C4	0.0287 (10)	0.0251 (9)	0.0335 (11)	−0.0070 (8)	−0.0077 (8)	−0.0075 (8)
C5	0.0517 (14)	0.0316 (11)	0.0266 (10)	−0.0142 (10)	−0.0113 (10)	−0.0037 (8)
C6	0.0444 (13)	0.0281 (10)	0.0256 (10)	−0.0148 (9)	−0.0067 (9)	−0.0015 (8)
C7	0.0493 (14)	0.0314 (11)	0.0456 (14)	−0.0196 (10)	−0.0076 (11)	−0.0095 (10)
C8	0.0305 (10)	0.0280 (10)	0.0227 (9)	−0.0097 (8)	−0.0047 (8)	−0.0032 (7)
C9	0.0258 (10)	0.0268 (10)	0.0211 (9)	−0.0056 (7)	−0.0027 (7)	−0.0050 (7)
C10	0.0336 (11)	0.0297 (10)	0.0235 (10)	−0.0096 (8)	−0.0085 (8)	−0.0024 (8)
C11	0.0310 (11)	0.0335 (11)	0.0261 (10)	−0.0119 (8)	−0.0043 (8)	−0.0060 (8)
C12	0.0304 (11)	0.0364 (11)	0.0251 (10)	−0.0133 (9)	−0.0042 (8)	−0.0059 (8)
C13	0.0309 (11)	0.0374 (11)	0.0291 (10)	−0.0108 (9)	−0.0048 (8)	−0.0083 (9)
C14	0.0330 (11)	0.0353 (11)	0.0272 (10)	−0.0130 (9)	−0.0047 (8)	−0.0057 (8)
C15	0.0350 (11)	0.0316 (10)	0.0277 (10)	−0.0118 (9)	−0.0050 (8)	−0.0041 (8)
C16	0.0396 (12)	0.0345 (11)	0.0300 (11)	−0.0125 (9)	−0.0078 (9)	−0.0057 (9)
C17	0.0534 (15)	0.0356 (12)	0.0375 (13)	−0.0065 (11)	−0.0114 (11)	−0.0104 (10)

Geometric parameters (Å, º)

Ni—S1	2.1796 (6)	C2—H1	0.950
Ni—S1^{i}	2.1796 (6)	C3—H2	0.950
Ni—N1	1.9310 (19)	C5—H3	0.950
Ni—N1^{i}	1.9310 (19)	C6—H4	0.950
S1—C9	1.726 (3)	C7—H5	0.980
S2—C9	1.7514 (19)	C7—H6	0.980
S2—C10	1.813 (3)	C7—H7	0.980

O1—C4	1.359 (3)	C8—H8	0.950
O1—C7	1.430 (3)	C10—H9	0.990
N1—N2	1.413 (3)	C10—H10	0.990
N1—C8	1.295 (3)	C11—H11	0.990
N2—C9	1.285 (3)	C11—H12	0.990
C1—C2	1.397 (3)	C12—H13	0.990
C1—C6	1.408 (3)	C12—H14	0.990
C1—C8	1.461 (4)	C13—H15	0.990
C2—C3	1.387 (4)	C13—H16	0.990
C3—C4	1.394 (3)	C14—H17	0.990
C4—C5	1.391 (4)	C14—H18	0.990
C5—C6	1.381 (4)	C15—H19	0.990
C10—C11	1.520 (3)	C15—H20	0.990
C11—C12	1.530 (4)	C16—H21	0.990
C12—C13	1.523 (3)	C16—H22	0.990
C13—C14	1.524 (4)	C17—H23	0.980
C14—C15	1.521 (3)	C17—H24	0.980
C15—C16	1.523 (4)	C17—H25	0.980
C16—C17	1.523 (4)		

S1—Ni—S1^{i}	180	H5—C7—H7	109.469
S1—Ni—N1	85.67 (5)	H6—C7—H7	109.468
S1—Ni—N1^{i}	94.33 (5)	N1—C8—H8	113.566
S1^{i}—Ni—N1	94.33 (5)	C1—C8—H8	113.564
S1^{i}—Ni—N1^{i}	85.67 (5)	S2—C10—H9	108.878
N1—Ni—N1^{i}	180	S2—C10—H10	108.867
Ni—S1—C9	96.01 (7)	C11—C10—H9	108.875
C9—S2—C10	102.83 (10)	C11—C10—H10	108.870
C4—O1—C7	117.90 (18)	H9—C10—H10	107.715
Ni—N1—N2	120.42 (14)	C10—C11—H11	109.150
Ni—N1—C8	125.18 (14)	C10—C11—H12	109.154
N2—N1—C8	114.39 (18)	C12—C11—H11	109.156
N1—N2—C9	111.78 (18)	C12—C11—H12	109.148
C2—C1—C6	117.6 (2)	H11—C11—H12	107.871
C2—C1—C8	114.61 (18)	C11—C12—H13	108.897
C6—C1—C8	127.8 (2)	C11—C12—H14	108.908
C1—C2—C3	122.6 (2)	C13—C12—H13	108.898
C2—C3—C4	118.7 (2)	C13—C12—H14	108.904
O1—C4—C3	124.3 (2)	H13—C12—H14	107.731
O1—C4—C5	116.1 (2)	C12—C13—H15	108.904
C3—C4—C5	119.7 (3)	C12—C13—H16	108.898
C4—C5—C6	121.2 (2)	C14—C13—H15	108.903
C1—C6—C5	120.2 (2)	C14—C13—H16	108.909
N1—C8—C1	132.87 (18)	H15—C13—H16	107.731
S1—C9—S2	114.13 (12)	C13—C14—H17	108.794
S1—C9—N2	124.92 (15)	C13—C14—H18	108.791
S2—C9—N2	120.93 (17)	C15—C14—H17	108.796
S2—C10—C11	113.48 (16)	C15—C14—H18	108.799

C10—C11—C12	112.26 (18)	H17—C14—H18	107.675
C11—C12—C13	113.35 (18)	C14—C15—H19	108.797
C12—C13—C14	113.35 (19)	C14—C15—H20	108.794
C13—C14—C15	113.81 (19)	C16—C15—H19	108.799
C14—C15—C16	113.81 (19)	C16—C15—H20	108.804
C15—C16—C17	113.3 (2)	H19—C15—H20	107.669
C1—C2—H1	118.691	C15—C16—H21	108.921
C3—C2—H1	118.690	C15—C16—H22	108.918
C2—C3—H2	120.632	C17—C16—H21	108.926
C4—C3—H2	120.627	C17—C16—H22	108.913
C4—C5—H3	119.383	H21—C16—H22	107.738
C6—C5—H3	119.378	C16—C17—H23	109.473
C1—C6—H4	119.926	C16—C17—H24	109.467
C5—C6—H4	119.914	C16—C17—H25	109.462
O1—C7—H5	109.474	H23—C17—H24	109.479
O1—C7—H6	109.474	H23—C17—H25	109.474
O1—C7—H7	109.472	H24—C17—H25	109.472
H5—C7—H6	109.470		

S1—Ni—N1—N2	−11.14 (10)	C8—N1—N2—C9	−167.88 (15)
S1—Ni—N1—C8	167.80 (12)	N1—N2—C9—S1	−3.7 (3)
N1—Ni—S1—C9	6.77 (5)	N1—N2—C9—S2	174.53 (13)
S1—Ni—N1^{i}—N2^{i}	−168.86 (10)	C2—C1—C6—C5	1.2 (3)
S1—Ni—N1^{i}—C8^{i}	12.20 (12)	C6—C1—C2—C3	−0.9 (3)
N1^{i}—Ni—S1—C9	−173.23 (5)	C2—C1—C8—N1	176.14 (18)
S1^{i}—Ni—N1—N2	168.86 (10)	C8—C1—C2—C3	177.33 (15)
S1^{i}—Ni—N1—C8	−12.20 (12)	C6—C1—C8—N1	−5.8 (4)
N1—Ni—S1^{i}—C9^{i}	173.23 (5)	C8—C1—C6—C5	−176.73 (17)
S1^{i}—Ni—N1^{i}—N2^{i}	11.14 (10)	C1—C2—C3—C4	−0.3 (3)
S1^{i}—Ni—N1^{i}—C8^{i}	−167.80 (12)	C2—C3—C4—O1	−178.68 (17)
N1^{i}—Ni—S1^{i}—C9^{i}	−6.77 (5)	C2—C3—C4—C5	1.2 (3)
Ni—S1—C9—S2	177.99 (9)	O1—C4—C5—C6	179.01 (17)
Ni—S1—C9—N2	−3.64 (16)	C3—C4—C5—C6	−0.9 (3)
C9—S2—C10—C11	84.61 (13)	C4—C5—C6—C1	−0.4 (3)
C10—S2—C9—S1	178.65 (11)	S2—C10—C11—C12	175.43 (11)
C10—S2—C9—N2	0.21 (17)	C10—C11—C12—C13	−174.38 (15)
C7—O1—C4—C3	6.1 (3)	C11—C12—C13—C14	177.19 (15)
C7—O1—C4—C5	−173.77 (16)	C12—C13—C14—C15	−179.74 (15)
Ni—N1—N2—C9	11.17 (19)	C13—C14—C15—C16	−176.95 (15)
Ni—N1—C8—C1	176.31 (13)	C14—C15—C16—C17	177.52 (15)
N2—N1—C8—C1	−4.7 (3)		

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