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[*N*,*N*′-Bis-(*o*-sulfidobenzylidene)-1,3-diaminopropane]nickel(II) 1,4-dioxane solvate

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Key indicators

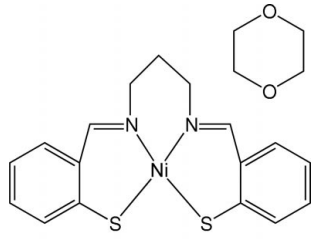
Single-crystal X-ray study
T = 123 K
Mean σ(C–C) = 0.003 Å
R factor = 0.029
wR factor = 0.057
Data-to-parameter ratio = 13.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title tetradentate Schiff base complex (systematic name: {2,2′-[propane-1,3-diylbis(nitrilomethylidyne)]benzenethiolato-κ^4S,N,N',S'}nickel(II) 1,4-dioxane solvate), [Ni($C_{17}H_{16}N_2S_2$)]·$C_4H_8O_2$, contains an Ni atom coordinated within a tetrahedrally distorted planar N_2S_2 environment, with average Ni—N and Ni—S bond lengths of 1.922 (1) and 2.167 (1) Å, respectively.

Comment

As part of our ongoing studies (Reglinski *et al.*, 2002*a*,*b*) on tetradentate Schiff base complexes with N_2X_2 donor sets and varying backbone lengths, the preparation of N_2S_2 complexes of this type was of interest. Eichorn & Goswami (1999) reported the use of a novel Schiff base semi-template for the formation of Ni^{II} complexes with mixed N/S-donating chelates. This method involves the reaction in ethanol of Ni^{II} complexes containing primary amine chelates and 2,2′-dithiodibenzaldehyde (DTDB). In order to assess the applicability of extending this method to the preparation of complexes with longer backbones, the title compound, (I), was prepared by this method. Crystals were obtained and the unit cell was found to be different from that of the previously reported structure of this compound (Gomes *et al.*, 1999), which has two independent nickel complex molecules in the asymmetric unit.



(I)

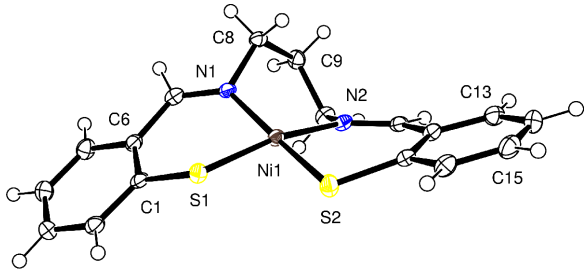


Figure 1
View of (I) (50% probability displacement ellipsoids). The solvent molecule has been omitted.

Experimental

The reaction of tris(propylenediamine)nickel(II)chloride and DTDB (Kasmai & Mischke, 1989) in ethanol produced a brown solid. Analysis found: C 54.28, H 4.58, N 7.04, S 16.62%; calculated for $C_{17}H_{16}N_2NiS_2$: C 55.01, H 4.34, N 7.55, S 17.28%; ^{1}H NMR (270 MHz; solvent $CDCl_3$): δ 7.83 (*s*, 2H, CH═N), 7.69 (*d*, 2H, aromatic), 7.22 (*d*, 2H, aromatic), 7.15 (*t*, 2H, aromatic), 7.00 (*t*, 2H, aromatic), 3.99 (*t*, 4H, ═NCH$_2$—), 2.09 (*p*, 2H, CCH$_2$C). Dark-brown crystals suitable for X-ray analysis were obtained by slow evaporation of a dioxane solution of the brown solid.

Crystal data

$[Ni(C_{17}H_{16}N_2S_2)]\cdot C_4H_8O_2$	$Z = 2$
$M_r = 459.25$	$D_x = 1.489$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 9.2099$ (3) Å	Cell parameters from 4660 reflections
$b = 9.3828$ (2) Å	$\theta = 1.6$–$27.5°$
$c = 13.2522$ (4) Å	$\mu = 1.17$ mm^{-1}
$\alpha = 77.392$ (2)°	$T = 123$ (2) K
$\beta = 88.719$ (2)°	Prism, brown
$\gamma = 66.761$ (2)°	0.25 × 0.25 × 0.20 mm
$V = 1024.30$ (5) Å^3	

Data collection

Nonius KappaCCD diffractometer	$R_{int} = 0.029$
φ and ω scans	$\theta_{max} = 27.5°$
Absorption correction: none	$h = -11 \rightarrow 11$
9186 measured reflections	$k = -11 \rightarrow 12$
4660 independent reflections	$l = -17 \rightarrow 17$
3758 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0146P)^2 + 0.5180P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.029$	
$wR(F^2) = 0.057$	
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.033$
4660 reflections	$\Delta\rho_{max} = 0.36$ e Å^{-3}
349 parameters	$\Delta\rho_{min} = -0.29$ e Å^{-3}
All H-atom parameters refined	

Table 1
Selected geometric parameters (Å, °).

N1—Ni1	1.9140 (14)	S1—Ni1	2.1760 (5)
N2—Ni1	1.9307 (15)	S2—Ni1	2.1574 (5)
N1—Ni1—S2	170.86 (4)	N2—Ni1—S1	169.35 (4)

All H atoms were found in a difference Fourier map and were refined isotropically [C—H = 0.90 (2)–1.02 (2) Å].

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO*; data reduction: *DENZO*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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supporting information

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$Z = 2$
$F(000) = 480$
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Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4660 reflections
$\theta = 1.6$–27.5°
$\mu = 1.17$ mm^{-1}
$T = 123$ K
Prism, brown
0.25 × 0.25 × 0.2 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
9186 measured reflections
4660 independent reflections
3758 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.6°$
$h = -11\rightarrow11$
$k = -11\rightarrow12$
$l = -17\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.057$
$S = 1.03$
4660 reflections
349 parameters
0 restraints
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0146P)^2 + 0.518P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.033$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2710 (2)	0.7389 (2)	0.57855 (14)	0.0159 (4)

C2	0.1408 (2)	0.7676 (2)	0.63999 (15)	0.0189 (4)
C3	0.1601 (2)	0.7008 (2)	0.74544 (15)	0.0216 (4)
C4	0.3099 (2)	0.6008 (2)	0.79286 (16)	0.0235 (4)
C5	0.4386 (2)	0.5709 (2)	0.73374 (15)	0.0209 (4)
C6	0.4231 (2)	0.6404 (2)	0.62742 (14)	0.0163 (4)
C7	0.5667 (2)	0.5992 (2)	0.57264 (14)	0.0173 (4)
C8	0.7439 (2)	0.6049 (2)	0.44351 (15)	0.0169 (4)
C9	0.8365 (2)	0.7036 (2)	0.45712 (16)	0.0193 (4)
C10	0.7314 (2)	0.8817 (2)	0.43429 (15)	0.0192 (4)
C11	0.6252 (2)	1.0193 (2)	0.26429 (14)	0.0165 (4)
C12	0.5229 (2)	1.0864 (2)	0.16979 (14)	0.0178 (4)
C13	0.5847 (2)	1.1463 (2)	0.08023 (16)	0.0224 (4)
C14	0.4958 (2)	1.2121 (2)	−0.01327 (16)	0.0257 (5)
C15	0.3415 (2)	1.2220 (2)	−0.01875 (15)	0.0240 (4)
C16	0.2771 (2)	1.1676 (2)	0.06836 (15)	0.0213 (4)
C17	0.3659 (2)	1.0981 (2)	0.16450 (14)	0.0168 (4)
N1	0.58507 (17)	0.67295 (17)	0.48251 (11)	0.0147 (3)
N2	0.61009 (17)	0.92791 (17)	0.34786 (11)	0.0156 (3)
S1	0.23398 (5)	0.81892 (5)	0.44491 (3)	0.01690 (10)
S2	0.26934 (5)	1.04149 (6)	0.27094 (4)	0.02131 (11)
Ni1	0.44140 (3)	0.85851 (3)	0.387643 (18)	0.01469 (7)
O1	0.87627 (16)	0.38996 (16)	0.74835 (10)	0.0273 (3)
O2	0.91928 (17)	0.23564 (16)	0.96165 (10)	0.0287 (3)
C19	0.9658 (2)	0.2222 (2)	0.78346 (16)	0.0240 (4)
C20	0.9075 (3)	0.1581 (3)	0.88208 (16)	0.0267 (5)
C21	0.8345 (3)	0.4039 (3)	0.92787 (17)	0.0309 (5)
C22	0.8898 (3)	0.4680 (3)	0.82688 (18)	0.0325 (5)
H2	0.041 (2)	0.834 (2)	0.6093 (14)	0.020 (5)*
H3	0.071 (2)	0.725 (2)	0.7839 (15)	0.020 (5)*
H4	0.323 (2)	0.553 (2)	0.8650 (16)	0.028 (6)*
H5	0.544 (2)	0.504 (2)	0.7636 (15)	0.029 (6)*
H7	0.657 (2)	0.506 (2)	0.6091 (13)	0.013 (5)*
H8A	0.799 (2)	0.495 (2)	0.4793 (13)	0.012 (5)*
H8B	0.729 (2)	0.607 (2)	0.3686 (15)	0.021 (5)*
H9A	0.879 (2)	0.674 (2)	0.5288 (15)	0.017 (5)*
H9B	0.919 (2)	0.684 (2)	0.4129 (14)	0.016 (5)*
H10A	0.676 (2)	0.909 (2)	0.4961 (15)	0.016 (5)*
H10B	0.794 (2)	0.944 (2)	0.4160 (14)	0.014 (5)*
H11	0.721 (2)	1.047 (2)	0.2618 (13)	0.015 (5)*
H13	0.688 (2)	1.140 (2)	0.0862 (16)	0.030 (6)*
H14	0.537 (2)	1.248 (2)	−0.0743 (15)	0.022 (5)*
H15	0.281 (2)	1.264 (2)	−0.0846 (15)	0.018 (5)*
H16	0.172 (2)	1.173 (2)	0.0642 (14)	0.019 (5)*
H19A	0.955 (2)	0.172 (2)	0.7274 (15)	0.024 (5)*
H19B	1.079 (2)	0.202 (2)	0.7942 (14)	0.020 (5)*
H20A	0.795 (2)	0.172 (2)	0.8714 (15)	0.027 (6)*
H20B	0.976 (2)	0.040 (2)	0.9083 (15)	0.028 (5)*
H21A	0.853 (2)	0.455 (2)	0.9808 (16)	0.027 (6)*

H21B	0.716 (3)	0.432 (3)	0.9209 (16)	0.036 (6)*
H22A	0.999 (3)	0.455 (2)	0.8372 (15)	0.027 (6)*
H22B	0.824 (2)	0.583 (3)	0.7993 (16)	0.033 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0180 (9)	0.0101 (8)	0.0197 (9)	−0.0052 (7)	0.0012 (7)	−0.0044 (7)
C2	0.0155 (9)	0.0148 (9)	0.0263 (11)	−0.0061 (8)	0.0007 (8)	−0.0046 (8)
C3	0.0217 (10)	0.0197 (10)	0.0237 (10)	−0.0085 (8)	0.0080 (9)	−0.0056 (8)
C4	0.0266 (11)	0.0213 (10)	0.0192 (10)	−0.0085 (9)	0.0033 (9)	−0.0003 (8)
C5	0.0191 (10)	0.0196 (10)	0.0211 (10)	−0.0071 (8)	−0.0028 (8)	0.0003 (8)
C6	0.0170 (9)	0.0126 (9)	0.0185 (9)	−0.0057 (7)	0.0010 (8)	−0.0026 (7)
C7	0.0165 (9)	0.0132 (9)	0.0215 (10)	−0.0051 (8)	−0.0020 (8)	−0.0036 (8)
C8	0.0140 (9)	0.0127 (9)	0.0211 (10)	−0.0025 (7)	0.0018 (8)	−0.0034 (8)
C9	0.0152 (9)	0.0204 (10)	0.0215 (10)	−0.0074 (8)	0.0012 (8)	−0.0023 (8)
C10	0.0197 (10)	0.0187 (10)	0.0213 (10)	−0.0095 (8)	−0.0021 (8)	−0.0052 (8)
C11	0.0143 (9)	0.0129 (9)	0.0227 (10)	−0.0050 (7)	0.0033 (8)	−0.0060 (8)
C12	0.0209 (10)	0.0124 (9)	0.0191 (10)	−0.0059 (7)	0.0017 (8)	−0.0032 (7)
C13	0.0194 (10)	0.0180 (10)	0.0276 (11)	−0.0060 (8)	0.0048 (9)	−0.0037 (8)
C14	0.0300 (11)	0.0215 (11)	0.0201 (11)	−0.0077 (9)	0.0050 (9)	0.0011 (8)
C15	0.0310 (11)	0.0189 (10)	0.0188 (10)	−0.0079 (9)	−0.0034 (9)	−0.0010 (8)
C16	0.0205 (10)	0.0176 (10)	0.0239 (10)	−0.0069 (8)	−0.0033 (8)	−0.0019 (8)
C17	0.0187 (9)	0.0117 (9)	0.0190 (9)	−0.0049 (7)	0.0016 (8)	−0.0037 (7)
N1	0.0134 (7)	0.0115 (7)	0.0190 (8)	−0.0042 (6)	0.0017 (6)	−0.0044 (6)
N2	0.0159 (8)	0.0118 (7)	0.0189 (8)	−0.0049 (6)	−0.0010 (6)	−0.0045 (6)
S1	0.0150 (2)	0.0171 (2)	0.0173 (2)	−0.00633 (18)	−0.00101 (18)	−0.00146 (18)
S2	0.0148 (2)	0.0223 (3)	0.0207 (2)	−0.00485 (19)	0.00009 (19)	0.0028 (2)
Ni1	0.01358 (12)	0.01291 (12)	0.01610 (12)	−0.00437 (9)	0.00019 (9)	−0.00203 (9)
O1	0.0315 (8)	0.0223 (7)	0.0221 (7)	−0.0061 (6)	−0.0015 (6)	−0.0019 (6)
O2	0.0351 (8)	0.0277 (8)	0.0203 (7)	−0.0094 (7)	−0.0020 (6)	−0.0048 (6)
C19	0.0222 (11)	0.0226 (11)	0.0251 (11)	−0.0063 (9)	−0.0007 (9)	−0.0060 (9)
C20	0.0319 (12)	0.0236 (11)	0.0254 (11)	−0.0120 (10)	0.0002 (9)	−0.0053 (9)
C21	0.0341 (13)	0.0282 (12)	0.0280 (12)	−0.0072 (10)	0.0000 (10)	−0.0117 (10)
C22	0.0353 (13)	0.0208 (12)	0.0379 (13)	−0.0082 (10)	−0.0017 (11)	−0.0049 (10)

Geometric parameters (Å, º)

C1—C2	1.404 (3)	C12—C17	1.408 (3)
C1—C6	1.412 (2)	C13—C14	1.378 (3)
C1—S1	1.7495 (18)	C13—H13	0.94 (2)
C2—C3	1.385 (3)	C14—C15	1.390 (3)
C2—H2	0.921 (19)	C14—H14	0.94 (2)
C3—C4	1.392 (3)	C15—C16	1.377 (3)
C3—H3	0.933 (19)	C15—H15	0.963 (18)
C4—C5	1.375 (3)	C16—C17	1.407 (3)
C4—H4	0.95 (2)	C16—H16	0.948 (19)
C5—C6	1.402 (3)	C17—S2	1.7471 (19)

C5—H5	0.96 (2)	N1—Ni1	1.9140 (14)
C6—C7	1.450 (3)	N2—Ni1	1.9307 (15)
C7—N1	1.287 (2)	S1—Ni1	2.1760 (5)
C7—H7	0.973 (18)	S2—Ni1	2.1574 (5)
C8—N1	1.479 (2)	O1—C22	1.430 (2)
C8—C9	1.523 (3)	O1—C19	1.431 (2)
C8—H8A	0.968 (18)	O2—C21	1.427 (2)
C8—H8B	0.999 (19)	O2—C20	1.434 (2)
C9—C10	1.529 (3)	C19—C20	1.496 (3)
C9—H9A	0.975 (18)	C19—H19A	0.990 (19)
C9—H9B	0.937 (19)	C19—H19B	0.990 (19)
C10—N2	1.485 (2)	C20—H20A	1.00 (2)
C10—H10A	0.984 (19)	C20—H20B	1.02 (2)
C10—H10B	0.965 (19)	C21—C22	1.507 (3)
C11—N2	1.286 (2)	C21—H21A	0.98 (2)
C11—C12	1.447 (2)	C21—H21B	1.02 (2)
C11—H11	1.009 (19)	C22—H22A	0.97 (2)
C12—C13	1.407 (3)	C22—H22B	0.99 (2)

C2—C1—C6	118.10 (17)	C15—C14—H14	118.7 (12)
C2—C1—S1	117.96 (13)	C16—C15—C14	120.51 (19)
C6—C1—S1	123.85 (14)	C16—C15—H15	120.1 (12)
C3—C2—C1	121.20 (17)	C14—C15—H15	119.4 (11)
C3—C2—H2	119.9 (12)	C15—C16—C17	121.23 (19)
C1—C2—H2	118.9 (12)	C15—C16—H16	120.4 (12)
C2—C3—C4	120.49 (19)	C17—C16—H16	118.4 (12)
C2—C3—H3	118.6 (12)	C16—C17—C12	118.25 (17)
C4—C3—H3	120.9 (12)	C16—C17—S2	117.24 (14)
C5—C4—C3	119.05 (19)	C12—C17—S2	124.42 (14)
C5—C4—H4	120.2 (12)	C7—N1—C8	115.75 (15)
C3—C4—H4	120.7 (12)	C7—N1—Ni1	131.25 (13)
C4—C5—C6	121.69 (18)	C8—N1—Ni1	113.00 (11)
C4—C5—H5	121.6 (12)	C11—N2—C10	115.91 (16)
C6—C5—H5	116.7 (13)	C11—N2—Ni1	130.86 (12)
C5—C6—C1	119.42 (17)	C10—N2—Ni1	112.78 (12)
C5—C6—C7	116.91 (16)	C1—S1—Ni1	107.57 (6)
C1—C6—C7	123.59 (16)	C17—S2—Ni1	109.63 (6)
N1—C7—C6	126.55 (17)	N1—Ni1—N2	90.94 (6)
N1—C7—H7	118.3 (11)	N1—Ni1—S2	170.86 (4)
C6—C7—H7	115.2 (11)	N2—Ni1—S2	94.62 (5)
N1—C8—C9	109.44 (15)	N1—Ni1—S1	93.17 (5)
N1—C8—H8A	110.1 (11)	N2—Ni1—S1	169.35 (4)
C9—C8—H8A	111.4 (10)	S2—Ni1—S1	82.624 (19)
N1—C8—H8B	107.8 (11)	C22—O1—C19	109.04 (15)
C9—C8—H8B	110.6 (11)	C21—O2—C20	110.24 (15)
H8A—C8—H8B	107.4 (14)	O1—C19—C20	110.75 (16)
C8—C9—C10	111.96 (15)	O1—C19—H19A	107.1 (11)
C8—C9—H9A	109.7 (11)	C20—C19—H19A	111.4 (12)

C10—C9—H9A	106.7 (11)	O1—C19—H19B	108.9 (11)
C8—C9—H9B	109.0 (11)	C20—C19—H19B	110.2 (11)
C10—C9—H9B	109.8 (11)	H19A—C19—H19B	108.4 (15)
H9A—C9—H9B	109.7 (15)	O2—C20—C19	110.81 (17)
N2—C10—C9	111.59 (15)	O2—C20—H20A	109.5 (11)
N2—C10—H10A	107.9 (10)	C19—C20—H20A	111.1 (12)
C9—C10—H10A	109.6 (11)	O2—C20—H20B	106.8 (11)
N2—C10—H10B	108.2 (10)	C19—C20—H20B	109.9 (12)
C9—C10—H10B	110.9 (11)	H20A—C20—H20B	108.6 (16)
H10A—C10—H10B	108.4 (15)	O2—C21—C22	111.31 (18)
N2—C11—C12	127.90 (17)	O2—C21—H21A	108.6 (12)
N2—C11—H11	117.6 (10)	C22—C21—H21A	108.6 (12)
C12—C11—H11	114.4 (10)	O2—C21—H21B	110.3 (12)
C13—C12—C17	119.45 (17)	C22—C21—H21B	110.5 (12)
C13—C12—C11	117.09 (17)	H21A—C21—H21B	107.4 (16)
C17—C12—C11	123.43 (17)	O1—C22—C21	111.26 (18)
C14—C13—C12	121.09 (19)	O1—C22—H22A	110.3 (12)
C14—C13—H13	121.1 (13)	C21—C22—H22A	109.7 (12)
C12—C13—H13	117.9 (13)	O1—C22—H22B	105.5 (12)
C13—C14—C15	119.4 (2)	C21—C22—H22B	111.7 (13)
C13—C14—H14	121.8 (12)	H22A—C22—H22B	108.3 (17)

C6—C1—C2—C3	−0.3 (3)	C9—C8—N1—Ni1	78.07 (16)
S1—C1—C2—C3	176.39 (14)	C12—C11—N2—C10	−177.98 (17)
C1—C2—C3—C4	−1.2 (3)	C12—C11—N2—Ni1	−6.4 (3)
C2—C3—C4—C5	0.8 (3)	C9—C10—N2—C11	−113.05 (19)
C3—C4—C5—C6	1.0 (3)	C9—C10—N2—Ni1	73.81 (18)
C4—C5—C6—C1	−2.5 (3)	C2—C1—S1—Ni1	152.10 (12)
C4—C5—C6—C7	−179.45 (17)	C6—C1—S1—Ni1	−31.40 (16)
C2—C1—C6—C5	2.1 (3)	C16—C17—S2—Ni1	156.60 (12)
S1—C1—C6—C5	−174.40 (14)	C12—C17—S2—Ni1	−26.83 (17)
C2—C1—C6—C7	178.84 (16)	C7—N1—Ni1—N2	142.94 (16)
S1—C1—C6—C7	2.3 (2)	C8—N1—Ni1—N2	−37.06 (12)
C5—C6—C7—N1	−164.25 (17)	C7—N1—Ni1—S1	−27.23 (16)
C1—C6—C7—N1	18.9 (3)	C8—N1—Ni1—S1	152.77 (11)
N1—C8—C9—C10	−38.6 (2)	C11—N2—Ni1—N1	155.57 (16)
C8—C9—C10—N2	−36.3 (2)	C10—N2—Ni1—N1	−32.60 (12)
N2—C11—C12—C13	−163.22 (18)	C11—N2—Ni1—S2	−17.17 (16)
N2—C11—C12—C17	18.7 (3)	C10—N2—Ni1—S2	154.66 (11)
C17—C12—C13—C14	−1.9 (3)	C11—N2—Ni1—S1	−91.7 (3)
C11—C12—C13—C14	179.87 (17)	C10—N2—Ni1—S1	80.1 (3)
C12—C13—C14—C15	1.2 (3)	C17—S2—Ni1—N2	28.01 (8)
C13—C14—C15—C16	0.4 (3)	C17—S2—Ni1—S1	−162.34 (6)
C14—C15—C16—C17	−1.2 (3)	C1—S1—Ni1—N1	35.44 (7)
C15—C16—C17—C12	0.5 (3)	C1—S1—Ni1—N2	−77.1 (3)
C15—C16—C17—S2	177.25 (15)	C1—S1—Ni1—S2	−152.71 (6)
C13—C12—C17—C16	1.1 (3)	C22—O1—C19—C20	58.8 (2)
C11—C12—C17—C16	179.17 (17)	C21—O2—C20—C19	56.4 (2)

C13—C12—C17—S2	−175.45 (14)	O1—C19—C20—O2	−59.1 (2)
C11—C12—C17—S2	2.6 (3)	C20—O2—C21—C22	−55.0 (2)
C6—C7—N1—C8	−179.34 (16)	C19—O1—C22—C21	−57.4 (2)
C6—C7—N1—Ni1	0.7 (3)	O2—C21—C22—O1	56.4 (2)
C9—C8—N1—C7	−101.93 (18)		