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Bis[*O*-propyl *N*′-(2-thienylcarbonyl)thiocarbamato]nickel(II)

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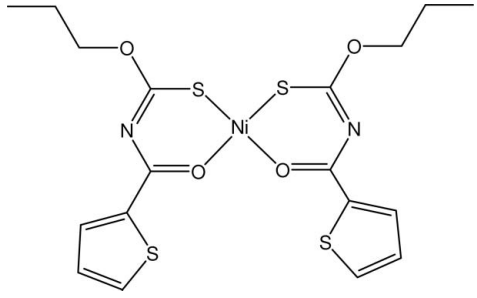
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.041; wR factor = 0.090; data-to-parameter ratio = 15.1.

In the title compound, $[Ni(C_9H_{10}NO_2S_2)_2]$, the Ni^{II} ion adopts a distorted *cis*-NiS_2O_2 square-planar geometry arising from the two *S*,*O*-bidentate ligands. The thiophene rings in each ligand are disordered, with site occupancy ratios of 0.874 (3):0.126 (3) and 0.741 (2):0.259 (2).

Related literature

For related literature, see: Gomes *et al.* (2007); Emen *et al.* (2003); Binzet *et al.* (2003). For the synthesis, see: Ribeiro da Silva *et al.* (2007). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Ni(C_9H_{10}NO_2S_2)_2]$
M_r = 515.31
Triclinic, $P\overline{1}$
a = 7.2627 (3) Å
b = 10.2917 (4) Å
c = 15.6218 (6) Å
α = 72.742 (2)°
β = 80.847 (3)°
γ = 82.978 (3)°
V = 1097.40 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.29 mm^{-1}
T = 100 (2) K
0.26 × 0.12 × 0.02 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.730, T_{max} = 0.975
10984 measured reflections
3845 independent reflections
2975 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.091
S = 1.08
3845 reflections
254 parameters
28 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—O1	1.851 (2)	Ni1—S3	2.1368 (10)
Ni1—O3	1.851 (2)	Ni1—S1	2.1424 (9)

Data collection: *SMART* (Bruker, 2004); cell refinement: *SMART* and *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2545).

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supplementary materials

Acta Cryst. (2007). E**63**, m2588 [**doi:10.1107/S1600536807045850**]

Bis[*O*-propyl *N*'-(2-thienylcarbonyl)thiocarbamato]nickel(II)

L. R. Gomes, J. N. Low, B. Schröder, P. Brandão and L. M. N. B. F. Santos

Comment

The title compound, (I), was synthesized in the course of our studies of the thermochemical properties of thiocarbamate derivates in order to elucidate the binding process in complexes with transition metal ions (Ribeiro da Silva *et al.*, 2007).

The ligand (*N*-2thienylcarbonylthiocarbamic-*O*-propylester) combines with the nickel(II) ion to from a tetra co-ordinated complex with an S_2O_2 co-ordination sphere in a *cis* configuration (Fig. 1, Table 1). The complex shows a slightly distortion to square planar geometry, where the maximum deviation of the atoms from the best plane formed by the five central atoms are: 0.043 (1), 0.053 (1), 0.043 (1), 0.053 (1) and 0.009 (1) Å, for S1, O1, S3 O3 and Ni1, respectively.

Otherwise, the bond lengths involving the ligands are within the range reported for similar complexes, derived from thioureas (Gomes *et al.*, 2007; Emen *et al.*, 2003); Binzet *et al.*, 2003).

Experimental

The preparation of the complex was been described elsewhere (Ribeiro da Silva *et al.*, 2007). Brown plates of (I) were obtained allowing slow vaporization of a methanolic/dichloromethane (1:1) solution of the complex.

Refinement

All the H atoms bonded to C atoms were refined with standard distances: 0.93 Å for aromatic and 0.98, 0.96 and 0.97 Å, for tertiary, secondary and primary aliphatic groups respectively, with *U*iso(H) = 1.5*U*eq(C) for methyl groups and with *U*iso(H) = 1.2*U*eq(C). The thiophene groups are disorded in both ligands by rotation through 180° about the pivot atoms C11 and C31.

The double and single C—C bonds of the thiophene residue were refined with the bond-length restraints 1.424 (1) and 1.362 (1) Å respectively and the S—C bond length value was assigned to be 1.712 (1) Å.

The S atoms in the disordered groups were refined isotropically with the anisotropic temperature factor of the minor component constrained to that of the respective major components by means of the EADP instruction (Sheldrick, 1997). The carbon atoms of the major (parts A) components were refined anisotropically with their anisotropic temperature factors constained to that of the pivot atoms C11 and C31, respectively, for each group by means of the EADP instruction (Sheldrick, 1997). The carbon atoms of the minor components, (parts B), were refined isotropically with U common U values defined by free variables, (Sheldrick, 1997), for each group.

Figures

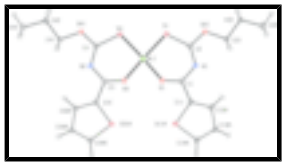


Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level (arbitrary spheres for the H atoms). Only the major disorder components of the thiophene rings are shown.

Bis[*O*-propyl *N*'-(2-thienylcarbonyl)thiocarbamato]nickel(II)

Crystal data

$[Ni(C_9H_{10}N_1O_2S_2)_2]$	$V = 1097.40\ (8)$ Å^3
$M_r = 515.31$	$Z = 2$
Triclinic, $P\overline{1}$	$F_{000} = 532$
Hall symbol: -P 1	$D_x = 1.559$ Mg m^{-3}
$a = 7.2627\ (3)$ Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 10.2917\ (4)$ Å	$\theta = 3.2–38.3°$
$c = 15.6218\ (6)$ Å	$\mu = 1.29$ mm^{-1}
$\alpha = 72.742\ (2)°$	$T = 100\ (2)$ K
$\beta = 80.847\ (3)°$	Plate, brown
$\gamma = 82.978\ (3)°$	0.26 × 0.12 × 0.02 mm

Data collection

Bruker SMART APEX CCD diffractometer	3845 independent reflections
Radiation source: fine-focus sealed tube	2975 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.044$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 25.0°$
$T = 100(2)$ K	$\theta_{min} = 1.4°$
ω scans	$h = -8\rightarrow8$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$k = -12\rightarrow12$
$T_{min} = 0.730$, $T_{max} = 0.975$	$l = -18\rightarrow18$
10984 measured reflections	

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
$wR(F^2) = 0.091$	$w = 1/[\sigma^2(F_o^2) + (0.0354P)^2 + 0.6558P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} = 0.005$

3845 reflections	$\Delta\rho_{max}$ = 0.47 e Å^{-3}
254 parameters	$\Delta\rho_{min}$ = −0.49 e Å^{-3}
28 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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}	Occ. (<1)
Ni1	0.51058 (7)	0.10730 (4)	0.74876 (3)	0.01716 (14)	
S1	0.62325 (14)	0.29040 (8)	0.66089 (6)	0.0231 (2)	
O1	0.5852 (3)	0.0037 (2)	0.66876 (15)	0.0202 (6)	
O21	0.7603 (3)	0.3728 (2)	0.49805 (15)	0.0214 (6)	
C2	0.7036 (5)	0.2589 (3)	0.5591 (2)	0.0190 (8)	
C1	0.6648 (5)	0.0293 (3)	0.5886 (2)	0.0182 (8)	
C22	0.8974 (5)	0.5022 (3)	0.3542 (2)	0.0238 (9)	
H22A	0.9868	0.5291	0.3845	0.029*	
H22B	0.7893	0.5681	0.3509	0.029*	
C23	0.9853 (6)	0.5022 (4)	0.2594 (2)	0.0318 (10)	
H23A	1.0225	0.5917	0.2265	0.048*	
H23B	0.8960	0.4773	0.2291	0.048*	
H23C	1.0930	0.4376	0.2626	0.048*	
C21	0.8384 (5)	0.3631 (3)	0.4076 (2)	0.0199 (8)	
H21A	0.7452	0.3364	0.3794	0.024*	
H21B	0.9451	0.2959	0.4110	0.024*	
C11	0.7005 (5)	−0.08429 (18)	0.54975 (17)	0.0199 (5)	
S11A	0.63615 (19)	−0.24368 (11)	0.61030 (8)	0.0215 (3)	0.874 (3)
C12A	0.7804 (7)	−0.0818 (4)	0.4644 (2)	0.0199 (5)	0.874 (3)
H12A	0.8240	−0.0036	0.4221	0.024*	0.874 (3)
C13A	0.7911 (7)	−0.2100 (3)	0.4457 (3)	0.0199 (5)	0.874 (3)
H13A	0.8414	−0.2261	0.3909	0.024*	0.874 (3)
C14A	0.7169 (7)	−0.3057 (4)	0.51981 (19)	0.0199 (5)	0.874 (3)
H14A	0.7107	−0.3960	0.5211	0.024*	0.874 (3)
S11B	0.8057 (14)	−0.0619 (8)	0.4409 (3)	0.0215 (3)	0.126 (3)
C12B	0.653 (4)	−0.2138 (12)	0.593 (2)	0.025 (6)*	0.126 (3)
H12B	0.5967	−0.2367	0.6527	0.030*	0.126 (3)

C13B	0.693 (5)	−0.313 (3)	0.5443 (17)	0.025 (6)*	0.126 (3)
H13B	0.6715	−0.4051	0.5614	0.030*	0.126 (3)
C14B	0.772 (4)	−0.2315 (11)	0.465 (2)	0.025 (6)*	0.126 (3)
H14B	0.8128	−0.2721	0.4184	0.030*	0.126 (3)
S3	0.40865 (14)	0.22063 (8)	0.84354 (6)	0.0237 (2)	
O3	0.4300 (3)	−0.0572 (2)	0.82358 (14)	0.0200 (6)	
C31	0.3188 (5)	−0.2395 (2)	0.93802 (15)	0.0194 (6)	
S31A	0.3791 (3)	−0.34726 (14)	0.87133 (10)	0.0214 (3)	0.741 (2)
C32A	0.2338 (8)	−0.3073 (4)	1.0208 (2)	0.0194 (6)	0.741 (2)
H32A	0.1934	−0.2651	1.0662	0.023*	0.741 (2)
C33A	0.2111 (10)	−0.4474 (4)	1.0330 (4)	0.0194 (6)	0.741 (2)
H33A	0.1540	−0.5067	1.0850	0.023*	0.741 (2)
C34A	0.2871 (9)	−0.4801 (4)	0.9558 (3)	0.0194 (6)	0.741 (2)
H34A	0.2888	−0.5673	0.9495	0.023*	0.741 (2)
S31B	0.2082 (7)	−0.3039 (4)	1.04503 (19)	0.0214 (3)	0.259 (2)
C32B	0.361 (3)	−0.3334 (13)	0.8907 (10)	0.026 (3)*	0.259 (2)
H32B	0.4224	−0.3112	0.8319	0.031*	0.259 (2)
C33B	0.307 (3)	−0.4676 (17)	0.9362 (9)	0.026 (3)*	0.259 (2)
H33B	0.3228	−0.5442	0.9150	0.031*	0.259 (2)
C34B	0.226 (3)	−0.4553 (11)	1.0185 (11)	0.026 (3)*	0.259 (2)
H34B	0.1793	−0.5315	1.0617	0.031*	0.259 (2)
C41	0.1610 (5)	0.0915 (3)	1.0900 (2)	0.0192 (8)	
H41A	0.2414	0.0125	1.1172	0.023*	
H41B	0.0475	0.0603	1.0802	0.023*	
N1	0.7199 (4)	0.1486 (3)	0.53306 (17)	0.0187 (7)	
C3	0.3537 (5)	−0.0960 (3)	0.9041 (2)	0.0160 (8)	
C42	0.1151 (5)	0.1831 (3)	1.1506 (2)	0.0216 (8)	
H42A	0.0396	0.2638	1.1215	0.026*	
H42B	0.2298	0.2121	1.1609	0.026*	
C4	0.3167 (5)	0.1082 (3)	0.9416 (2)	0.0171 (8)	
O41	0.2562 (3)	0.1712 (2)	1.00466 (14)	0.0190 (6)	
N2	0.2979 (4)	−0.0229 (3)	0.96285 (17)	0.0195 (7)	
C43	0.0080 (5)	0.1084 (4)	1.2414 (2)	0.0241 (8)	
H43A	−0.0199	0.1683	1.2794	0.036*	
H43B	0.0834	0.0291	1.2705	0.036*	
H43C	−0.1065	0.0811	1.2312	0.036*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0219 (3)	0.0141 (2)	0.0156 (2)	−0.00209 (18)	−0.00078 (19)	−0.00487 (17)
S1	0.0335 (6)	0.0172 (4)	0.0190 (4)	−0.0064 (4)	0.0037 (4)	−0.0076 (4)
O1	0.0266 (15)	0.0154 (12)	0.0189 (12)	−0.0022 (10)	0.0002 (11)	−0.0068 (10)
O21	0.0305 (16)	0.0152 (12)	0.0180 (12)	−0.0039 (11)	0.0031 (11)	−0.0062 (10)
C2	0.019 (2)	0.0184 (18)	0.0196 (18)	−0.0020 (15)	−0.0009 (16)	−0.0057 (15)
C1	0.014 (2)	0.0219 (19)	0.0187 (18)	−0.0022 (15)	−0.0032 (15)	−0.0054 (15)
C22	0.030 (2)	0.0208 (19)	0.0189 (18)	−0.0019 (16)	0.0048 (17)	−0.0068 (15)
C23	0.038 (3)	0.030 (2)	0.023 (2)	0.0001 (19)	0.0012 (19)	−0.0043 (17)

C21	0.024 (2)	0.0225 (18)	0.0132 (17)	−0.0017 (16)	−0.0003 (15)	−0.0067 (14)
C11	0.0226 (13)	0.0200 (11)	0.0177 (11)	−0.0006 (9)	−0.0023 (10)	−0.0069 (10)
S11A	0.0269 (7)	0.0161 (5)	0.0221 (7)	−0.0030 (5)	−0.0020 (5)	−0.0064 (5)
C12A	0.0226 (13)	0.0200 (11)	0.0177 (11)	−0.0006 (9)	−0.0023 (10)	−0.0069 (10)
C13A	0.0226 (13)	0.0200 (11)	0.0177 (11)	−0.0006 (9)	−0.0023 (10)	−0.0069 (10)
C14A	0.0226 (13)	0.0200 (11)	0.0177 (11)	−0.0006 (9)	−0.0023 (10)	−0.0069 (10)
S11B	0.0269 (7)	0.0161 (5)	0.0221 (7)	−0.0030 (5)	−0.0020 (5)	−0.0064 (5)
S3	0.0360 (6)	0.0155 (4)	0.0179 (4)	−0.0037 (4)	0.0035 (4)	−0.0051 (4)
O3	0.0262 (15)	0.0160 (12)	0.0172 (12)	−0.0031 (10)	0.0023 (11)	−0.0058 (10)
C31	0.0241 (15)	0.0174 (11)	0.0166 (13)	−0.0034 (9)	−0.0008 (11)	−0.0048 (9)
S31A	0.0275 (8)	0.0163 (6)	0.0212 (7)	−0.0031 (5)	−0.0008 (6)	−0.0070 (5)
C32A	0.0241 (15)	0.0174 (11)	0.0166 (13)	−0.0034 (9)	−0.0008 (11)	−0.0048 (9)
C33A	0.0241 (15)	0.0174 (11)	0.0166 (13)	−0.0034 (9)	−0.0008 (11)	−0.0048 (9)
C34A	0.0241 (15)	0.0174 (11)	0.0166 (13)	−0.0034 (9)	−0.0008 (11)	−0.0048 (9)
S31B	0.0275 (8)	0.0163 (6)	0.0212 (7)	−0.0031 (5)	−0.0008 (6)	−0.0070 (5)
C41	0.021 (2)	0.0180 (17)	0.0182 (18)	−0.0049 (15)	0.0020 (16)	−0.0048 (14)
N1	0.0218 (18)	0.0182 (15)	0.0168 (15)	−0.0011 (13)	−0.0005 (13)	−0.0073 (12)
C3	0.0109 (19)	0.0192 (17)	0.0183 (18)	0.0004 (14)	−0.0053 (15)	−0.0049 (14)
C42	0.023 (2)	0.0211 (18)	0.0221 (19)	−0.0031 (15)	−0.0035 (16)	−0.0067 (15)
C4	0.016 (2)	0.0193 (18)	0.0180 (17)	0.0000 (14)	−0.0014 (15)	−0.0088 (14)
O41	0.0252 (15)	0.0151 (12)	0.0165 (12)	−0.0045 (10)	0.0020 (11)	−0.0054 (10)
N2	0.0259 (19)	0.0161 (15)	0.0175 (15)	−0.0018 (13)	−0.0001 (13)	−0.0077 (12)
C43	0.024 (2)	0.028 (2)	0.0210 (18)	−0.0015 (16)	−0.0015 (16)	−0.0092 (15)

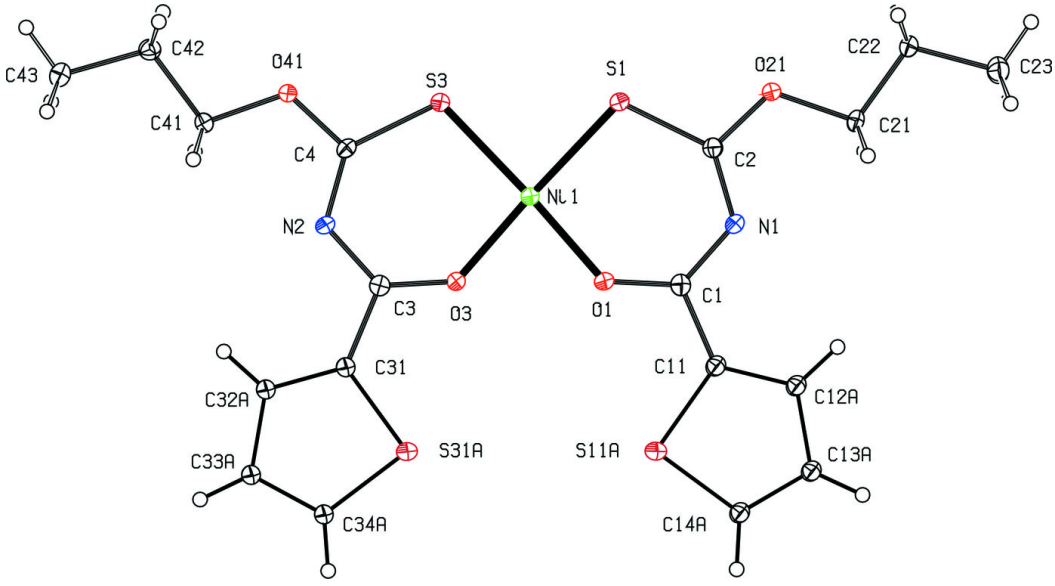
Geometric parameters (Å, °)

Ni1—O1	1.851 (2)	C13B—H13B	0.9300
Ni1—O3	1.851 (2)	C14B—H14B	0.9300
Ni1—S3	2.1368 (10)	S3—C4	1.715 (3)
Ni1—S1	2.1424 (9)	O3—C3	1.259 (4)
S1—C2	1.715 (3)	C31—C32B	1.3619 (10)
O1—C1	1.258 (4)	C31—C32A	1.3623 (10)
O21—C2	1.335 (4)	C31—C3	1.453 (4)
O21—C21	1.464 (4)	C31—S31B	1.7104 (10)
C2—N1	1.302 (4)	C31—S31A	1.7117 (10)
C1—N1	1.341 (4)	S31A—C34A	1.7113 (10)
C1—C11	1.449 (4)	C32A—C33A	1.4237 (10)
C22—C21	1.502 (4)	C32A—H32A	0.9300
C22—C23	1.516 (5)	C33A—C34A	1.3618 (10)
C22—H22A	0.9700	C33A—H33A	0.9300
C22—H22B	0.9700	C34A—H34A	0.9300
C23—H23A	0.9600	S31B—C34B	1.7120 (10)
C23—H23B	0.9600	C32B—C33B	1.4239 (10)
C23—H23C	0.9600	C32B—H32B	0.9300
C21—H21A	0.9700	C33B—C34B	1.3618 (10)
C21—H21B	0.9700	C33B—H33B	0.9300
C11—C12A	1.3617 (10)	C34B—H34B	0.9300
C11—C12B	1.3619 (10)	C41—O41	1.458 (4)
C11—S11B	1.7110 (10)	C41—C42	1.498 (5)

C11—S11A	1.7119 (10)	C41—H41A	0.9700
S11A—C14A	1.7115 (10)	C41—H41B	0.9700
C12A—C13A	1.4236 (10)	C3—N2	1.337 (4)
C12A—H12A	0.9300	C42—C43	1.536 (4)
C13A—C14A	1.3618 (10)	C42—H42A	0.9700
C13A—H13A	0.9300	C42—H42B	0.9700
C14A—H14A	0.9300	C4—N2	1.310 (4)
S11B—C14B	1.7121 (10)	C4—O41	1.325 (4)
C12B—C13B	1.4239 (10)	C43—H43A	0.9600
C12B—H12B	0.9300	C43—H43B	0.9600
C13B—C14B	1.3620 (10)	C43—H43C	0.9600
O1—Ni1—O3	82.18 (9)	C13B—C14B—H14B	116.6
O1—Ni1—S3	176.43 (8)	S11B—C14B—H14B	116.6
O3—Ni1—S3	95.16 (7)	C4—S3—Ni1	107.56 (12)
O1—Ni1—S1	95.46 (7)	C3—O3—Ni1	134.2 (2)
O3—Ni1—S1	175.91 (8)	C32B—C31—C32A	105.8 (8)
S3—Ni1—S1	87.33 (4)	C32B—C31—C3	125.9 (7)
C2—S1—Ni1	106.78 (12)	C32A—C31—C3	128.3 (2)
C1—O1—Ni1	133.9 (2)	C32B—C31—S31B	113.5 (7)
C2—O21—C21	117.4 (2)	C3—C31—S31B	120.5 (2)
N1—C2—O21	117.4 (3)	C32A—C31—S31A	110.4 (2)
N1—C2—S1	132.4 (3)	C3—C31—S31A	121.32 (19)
O21—C2—S1	110.2 (2)	S31B—C31—S31A	118.11 (19)
O1—C1—N1	128.8 (3)	C34A—S31A—C31	91.1 (2)
O1—C1—C11	116.3 (3)	C31—C32A—C33A	115.4 (4)
N1—C1—C11	114.9 (3)	C31—C32A—H32A	122.3
C21—C22—C23	110.7 (3)	C33A—C32A—H32A	122.3
C21—C22—H22A	109.5	C34A—C33A—C32A	108.6 (5)
C23—C22—H22A	109.5	C34A—C33A—H33A	125.7
C21—C22—H22B	109.5	C32A—C33A—H33A	125.7
C23—C22—H22B	109.5	C33A—C34A—S31A	114.4 (4)
H22A—C22—H22B	108.1	C33A—C34A—H34A	122.8
C22—C23—H23A	109.5	S31A—C34A—H34A	122.8
C22—C23—H23B	109.5	C31—S31B—C34B	85.6 (6)
H23A—C23—H23B	109.5	C31—C32B—C33B	116.5 (13)
C22—C23—H23C	109.5	C31—C32B—H32B	121.8
H23A—C23—H23C	109.5	C33B—C32B—H32B	121.8
H23B—C23—H23C	109.5	C34B—C33B—C32B	102.4 (16)
O21—C21—C22	106.6 (3)	C34B—C33B—H33B	128.8
O21—C21—H21A	110.4	C32B—C33B—H33B	128.8
C22—C21—H21A	110.4	C33B—C34B—S31B	122.1 (14)
O21—C21—H21B	110.4	C33B—C34B—H34B	119.0
C22—C21—H21B	110.4	S31B—C34B—H34B	119.0
H21A—C21—H21B	108.6	O41—C41—C42	107.0 (3)
C12A—C11—C12B	107.6 (15)	O41—C41—H41A	110.3
C12A—C11—C1	127.3 (2)	C42—C41—H41A	110.3
C12B—C11—C1	125.0 (15)	O41—C41—H41B	110.3
C12B—C11—S11B	114.3 (15)	C42—C41—H41B	110.3
C1—C11—S11B	120.7 (3)	H41A—C41—H41B	108.6

C12A—C11—S11A	111.4 (2)	C2—N1—C1	122.2 (3)
C1—C11—S11A	121.3 (2)	O3—C3—N2	129.0 (3)
S11B—C11—S11A	118.0 (3)	O3—C3—C31	115.8 (3)
C14A—S11A—C11	91.11 (18)	N2—C3—C31	115.2 (3)
C11—C12A—C13A	113.8 (3)	C41—C42—C43	110.5 (3)
C11—C12A—H12A	123.1	C41—C42—H42A	109.5
C13A—C12A—H12A	123.1	C43—C42—H42A	109.5
C14A—C13A—C12A	110.2 (4)	C41—C42—H42B	109.5
C14A—C13A—H13A	124.9	C43—C42—H42B	109.5
C12A—C13A—H13A	124.9	H42A—C42—H42B	108.1
C13A—C14A—S11A	113.5 (3)	N2—C4—O41	117.5 (3)
C13A—C14A—H14A	123.2	N2—C4—S3	131.7 (3)
S11A—C14A—H14A	123.2	O41—C4—S3	110.7 (2)
C11—S11B—C14B	82.7 (11)	C4—O41—C41	117.4 (2)
C11—C12B—C13B	118 (3)	C4—N2—C3	122.3 (3)
C11—C12B—H12B	121.0	C42—C43—H43A	109.5
C13B—C12B—H12B	121.0	C42—C43—H43B	109.5
C14B—C13B—C12B	98 (3)	H43A—C43—H43B	109.5
C14B—C13B—H13B	131.0	C42—C43—H43C	109.5
C12B—C13B—H13B	131.0	H43A—C43—H43C	109.5
C13B—C14B—S11B	127 (2)	H43B—C43—H43C	109.5

Fig. 1


C43
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C33A
S31A
C34A
C11
C12A
S11A
C13A
C14A