

Bis(1,1,5,5-tetramethyl-2-thiobiuretato)nickel(II)

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Key indicators

Single-crystal X-ray study

T = 150 K

Mean $\sigma(\text{N}-\text{C}) = 0.003 \text{ \AA}$

Disorder in main residue

R factor = 0.030

wR factor = 0.060

Data-to-parameter ratio = 19.1

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

At 150 K, the title compound, $[\text{Ni}(\text{C}_6\text{H}_{12}\text{N}_3\text{OS})_2]$, comprises a *cis* square-planar nickel(II) ion with two anionic bidentate 1,1,5,5-tetramethyl-2-thiobiuretate ligands. All non-H atoms lie on a crystallographic mirror plane.

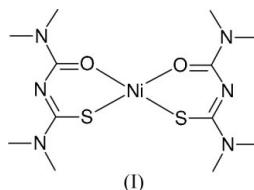
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Comment

The title compound, (I), is the neutral homoleptic nickel(II) complex of the anionic bidentate 1,1,5,5-tetramethyl-2-thiobiuretate ligand. The complex is *cis* square-planar (Table 1) and all non-H atoms lie on a crystallographic mirror plane (Fig. 1).



In both of the ligands, the pattern of bond distances is similar to that observed for the corresponding homoleptic cobalt(III) complex reported by Crane & Whittingham (2004) and indicates that the formal negative charge is predominately localized on the S atom. The relatively long C–S and short C–O average bond lengths [1.747 (4) and 1.261 (3) Å] are consistent with mostly single- and double-bond character, respectively, and this bond localization is also reflected in the average C–N bond distances to the central N atom, *viz.* 1.323 (7) Å in the (iso)thiourea group and 1.348 (7) Å in the urea group.

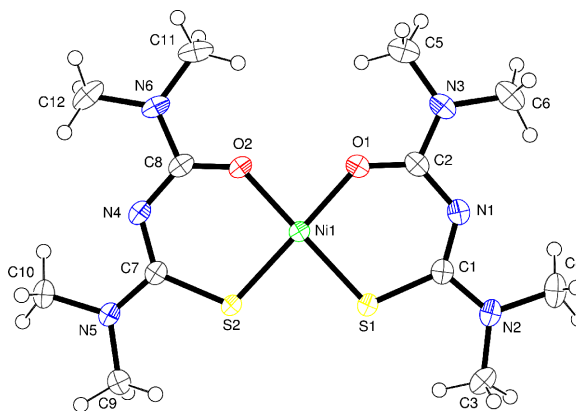


Figure 1

A view of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented by circles of arbitrary size. Only one of the disordered positions for each methyl group is shown.

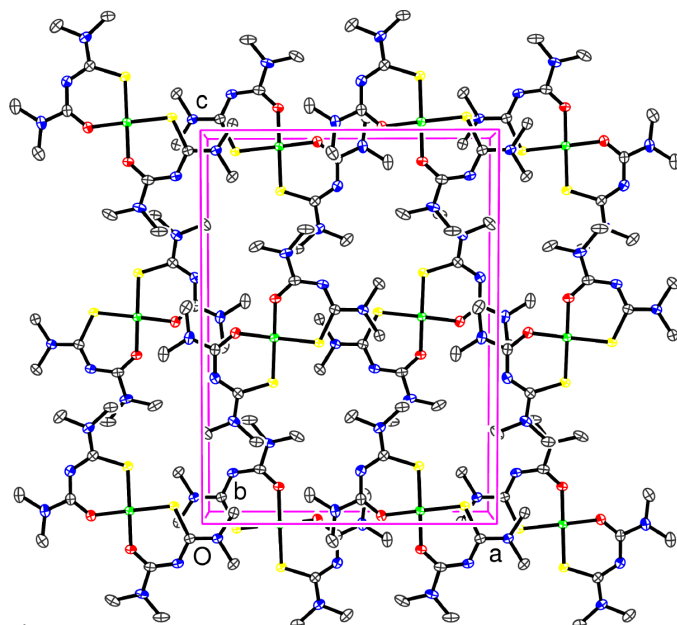


Figure 2
The packing and unit cell of (I), viewed down the *b* axis. H atoms have been omitted.

The molecules are packed in layers (Figs. 3 and 4) perpendicular to the *b* axis, with an interlayer spacing of 3.5062 (3) Å. Of the shortest non-H interatomic contact distance between layers (Table 2), the shortest involving the S atoms is 3.5986 (5) Å for S2 and N5ⁱ [symmetry code: (i) $-x, 1-y, -z$].

Experimental

The title compound, (I), was prepared by a variation of the method of Koenig *et al.* (1987). Dimethylcarbonyl chloride (1.08 g, 10 mmol) and potassium thiocyanate (0.97 g, 10 mmol) in acetonitrile (40 ml) were heated at reflux for 2 h. The solution was allowed to cool to room temperature and excess 40% aqueous dimethylamine (3.4 ml, 30 mmol) was added with stirring, followed after 15 min by nickel(II) acetate tetrahydrate (1.25 g, 5 mmol) and water (5 ml). After stirring for a further 15 min, the crude product was obtained as a purple powder by precipitation with methanol (200 ml), isolation by filtration and washing sequentially with water, methanol and diethyl ether. Suitable crystals were grown by recrystallization from dichloromethane/methanol: yield 1.07 g, 53%. Spectroscopic analysis: IR (KBr disk, cm^{-1}): ν 2921 (*w*), 1540 (*s*), 1481 (*s*), 1389 (*s*), 1357 (*s*), 1266 (*w*), 1198 (*w*), 1115 (*m*), 1031 (*m*), 734 (*m*), 474 (*w*); ¹H NMR (CDCl_3 , p.p.m.): δ 3.18 (*br, s*, 6H), 3.08 (*br, s*, 6H), 2.96 (*s*, 6H), 2.87 (*s*, 6H); ¹³C NMR (CDCl_3 , p.p.m.): δ 171.3, 163.1, 40.1, 39.7, 37.4, 35.9. Analysis calculated for $\text{C}_{12}\text{H}_{24}\text{N}_6\text{NiO}_2\text{S}_2$: C 35.40, H 5.94, N 20.64, S 15.75%; found: C 35.49, H 6.03, N 20.49, S 15.71%.

Crystal data

$[\text{Ni}(\text{C}_6\text{H}_{12}\text{N}_3\text{OS})_2]$	Mo $K\alpha$ radiation
$M_r = 407.20$	Cell parameters from 10003 reflections
Orthorhombic, <i>Pnma</i>	$\theta = 2.2\text{--}30.0^\circ$
$a = 13.9350$ (10) Å	$\mu = 1.32 \text{ mm}^{-1}$
$b = 7.0123$ (5) Å	$T = 150$ (2) K
$c = 18.4739$ (18) Å	Plate, purple
$V = 1805.2$ (3) Å ³	$0.20 \times 0.18 \times 0.02 \text{ mm}$
$Z = 4$	
$D_x = 1.498 \text{ Mg m}^{-3}$	

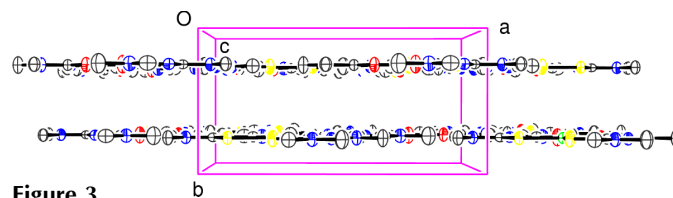


Figure 3
The packing and unit cell of (I), viewed down the *c* axis.

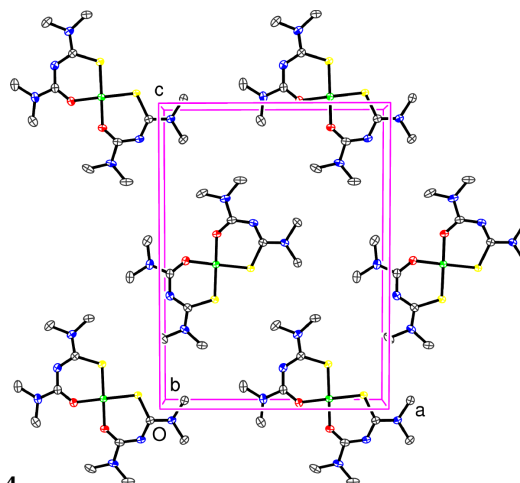


Figure 4
The packing of one layer of molecules of (I), parallel to the *ac* plane. H atoms have been omitted.

Data collection

Stoe IPDS-II area-detector diffractometer	2820 independent reflections
ω scans	1936 reflections with $I > 2\sigma(I)$
Absorption correction: numerical (<i>X-SHAPE</i> ; Stoe & Cie, 2001)	$R_{\text{int}} = 0.065$
$T_{\text{min}} = 0.630$, $T_{\text{max}} = 0.751$	$\theta_{\text{max}} = 30.0^\circ$
18236 measured reflections	$h = -16 \rightarrow 19$
	$k = -9 \rightarrow 9$
	$l = -25 \rightarrow 25$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0271P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.030$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.060$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 0.87$	$\Delta\rho_{\text{max}} = 0.36 \text{ e \AA}^{-3}$
2820 reflections	$\Delta\rho_{\text{min}} = -0.26 \text{ e \AA}^{-3}$
148 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	Extinction coefficient: 0.0017 (3)

Table 1

Selected geometric parameters (Å, °).

Ni1—O1	1.8694 (17)	N1—C1	1.316 (3)
Ni1—O2	1.8634 (15)	N1—C2	1.355 (3)
Ni1—S1	2.1374 (7)	N2—C1	1.353 (3)
Ni1—S2	2.1386 (7)	N3—C2	1.351 (3)
S1—C1	1.743 (2)	N4—C7	1.329 (3)
S2—C7	1.750 (2)	N4—C8	1.341 (3)
O1—C2	1.261 (3)	N5—C7	1.333 (3)
O2—C8	1.260 (3)	N6—C8	1.366 (3)
O1—Ni1—S1	95.16 (6)	C2—O1—Ni1	133.73 (16)
O2—Ni1—S2	94.65 (6)	C8—O2—Ni1	134.24 (17)
O1—Ni1—O2	84.45 (8)	C1—N1—C2	123.6 (2)
S1—Ni1—S2	85.75 (3)	C7—N4—C8	123.39 (19)
O1—Ni1—S2	179.10 (6)	N1—C1—S1	129.24 (18)
O2—Ni1—S1	179.60 (7)	O1—C2—N1	129.2 (2)
C1—S1—Ni1	109.05 (8)	N4—C7—S2	128.39 (18)
C7—S2—Ni1	109.52 (8)	O2—C8—N4	129.8 (2)

Table 2

Interlayer contact distances (Å) less than 3.6 Å for non-H atoms.

S2...N5 ⁱ	3.5986 (5)	N6...C3 ⁱⁱⁱ	3.5470 (6)
C2...C5 ⁱⁱ	3.5161 (4)	N2...C12 ^{iv}	3.5622 (7)

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

All H atoms were initially located in a difference Fourier map. The methyl H atoms were constrained to an ideal geometry, with a C–H distance of 0.98 Å, and $U_{\text{iso}}(\text{H})$ was set to $1.2U_{\text{eq}}(\text{C})$, but each group was allowed to rotate freely about its X–C bond. In their final positions, none of the methyl groups accords with the crystallographic mirror symmetry and hence each methyl group is disordered 50:50 about the mirror plane.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2001); program(s)

used to solve structure: *X-STEP32* (Stoe & Cie, 2001) and *WinGX* (Farrugia, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* and *PLATON* (Spek, 2001).

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supporting information

Acta Cryst. (2004). E60, m449–m451 [https://doi.org/10.1107/S1600536804006294]

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Crystal data[Ni(C₆H₁₂N₃OS)₂] $M_r = 407.20$ Orthorhombic, *Pnma*

Hall symbol: -P 2ac 2n

 $a = 13.935$ (1) Å $b = 7.0123$ (5) Å $c = 18.4739$ (18) Å $V = 1805.2$ (3) Å³ $Z = 4$ $F(000) = 856$ $D_x = 1.498$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 10003 reflections

 $\theta = 2.2$ – 30.0° $\mu = 1.32$ mm⁻¹ $T = 150$ K

Plate, purple

0.20 × 0.18 × 0.02 mm

*Data collection*Stoe IPDS-II area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 ω scans

Absorption correction: numerical

(X-SHAPE; Stoe & Cie, 2001)

 $T_{\min} = 0.630$, $T_{\max} = 0.751$

18236 measured reflections

2820 independent reflections

1936 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.065$ $\theta_{\max} = 30.0^\circ$, $\theta_{\min} = 2.2^\circ$ $h = -16 \rightarrow 19$ $k = -9 \rightarrow 9$ $l = -25 \rightarrow 25$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.030$ $wR(F^2) = 0.060$ $S = 0.87$

2820 reflections

148 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

 $w = 1/[\sigma^2(F_o^2) + (0.0271P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 0.36$ e Å⁻³ $\Delta\rho_{\min} = -0.26$ e Å⁻³

Extinction correction: SHELXL97,

 $F_c^* = kF_c[1 + 0.001 \times F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0017 (3)

Special details

Experimental. The crystal was mounted under the perfluoro-polyether PFO-XR75 (Lancaster Synthesis). A total of 180 frames (6 minute exposure) were collected (ϕ/ω : 45/0–180, $\delta\omega = 1^\circ$.)

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Ni1	0.25640 (2)	0.7500	−0.026041 (15)	0.02336 (8)	
S1	0.26181 (4)	0.7500	−0.14166 (3)	0.03616 (15)	
S2	0.10385 (4)	0.7500	−0.03869 (3)	0.02723 (13)	
O1	0.38951 (12)	0.7500	−0.01340 (9)	0.0346 (4)	
O2	0.25262 (13)	0.7500	0.07478 (8)	0.0401 (4)	
N1	0.45995 (14)	0.7500	−0.12976 (11)	0.0304 (5)	
N2	0.39559 (15)	0.7500	−0.24175 (11)	0.0341 (5)	
N3	0.54773 (15)	0.7500	−0.02573 (13)	0.0376 (5)	
N4	0.09073 (15)	0.7500	0.11138 (9)	0.0262 (4)	
N5	−0.04648 (14)	0.7500	0.04589 (10)	0.0287 (5)	
N6	0.21546 (17)	0.7500	0.19149 (11)	0.0362 (5)	
C1	0.38142 (17)	0.7500	−0.16931 (12)	0.0263 (5)	
C2	0.45972 (17)	0.7500	−0.05643 (13)	0.0287 (5)	
C3	0.3186 (2)	0.7500	−0.29499 (13)	0.0393 (6)	
H3A	0.3352	0.8364	−0.3348	0.047*	0.50
H3B	0.2590	0.7930	−0.2721	0.047*	0.50
H3C	0.3099	0.6206	−0.3140	0.047*	0.50
C4	0.4930 (2)	0.7500	−0.27118 (16)	0.0517 (8)	
H4A	0.5362	0.8144	−0.2372	0.062*	0.50
H4B	0.4935	0.8174	−0.3177	0.062*	0.50
H4C	0.5144	0.6182	−0.2784	0.062*	0.50
C5	0.5585 (2)	0.7500	0.05249 (16)	0.0425 (7)	
H5A	0.6129	0.8311	0.0660	0.051*	0.50
H5B	0.5702	0.6195	0.0694	0.051*	0.50
H5C	0.4998	0.7993	0.0749	0.051*	0.50
C6	0.6360 (2)	0.7500	−0.06748 (18)	0.0501 (8)	
H6A	0.6641	0.6219	−0.0670	0.060*	0.50
H6B	0.6814	0.8407	−0.0461	0.060*	0.50
H6C	0.6221	0.7875	−0.1175	0.060*	0.50
C7	0.04920 (16)	0.7500	0.04660 (12)	0.0229 (4)	
C8	0.18610 (19)	0.7500	0.12095 (12)	0.0276 (5)	
C9	−0.10292 (18)	0.7500	−0.02043 (13)	0.0351 (6)	
H9A	−0.1128	0.8816	−0.0367	0.042*	0.50

H9B	-0.1653	0.6900	-0.0113	0.042*	0.50
H9C	-0.0688	0.6784	-0.0580	0.042*	0.50
C10	-0.10153 (19)	0.7500	0.11318 (12)	0.0348 (6)	
H10A	-0.1191	0.6188	0.1258	0.042*	0.50
H10B	-0.1599	0.8262	0.1068	0.042*	0.50
H10C	-0.0626	0.8050	0.1521	0.042*	0.50
C11	0.3170 (2)	0.7500	0.20903 (15)	0.0553 (9)	
H11A	0.3541	0.7137	0.1661	0.066*	0.50
H11B	0.3292	0.6585	0.2480	0.066*	0.50
H11C	0.3363	0.8778	0.2248	0.066*	0.50
C12	0.1490 (2)	0.7500	0.25251 (15)	0.0445 (7)	
H12A	0.0857	0.7063	0.2362	0.053*	0.50
H12B	0.1435	0.8795	0.2720	0.053*	0.50
H12C	0.1729	0.6642	0.2903	0.053*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.02122 (15)	0.02998 (15)	0.01888 (12)	0.000	-0.00043 (11)	0.000
S1	0.0237 (3)	0.0646 (4)	0.0202 (2)	0.000	0.0022 (2)	0.000
S2	0.0231 (3)	0.0417 (3)	0.0169 (2)	0.000	0.00057 (19)	0.000
O1	0.0233 (8)	0.0532 (12)	0.0272 (8)	0.000	-0.0015 (7)	0.000
O2	0.0283 (9)	0.0740 (13)	0.0180 (8)	0.000	-0.0008 (7)	0.000
N1	0.0253 (10)	0.0366 (12)	0.0293 (10)	0.000	0.0032 (8)	0.000
N2	0.0313 (10)	0.0455 (13)	0.0255 (9)	0.000	0.0070 (9)	0.000
N3	0.0228 (10)	0.0506 (14)	0.0395 (12)	0.000	-0.0029 (9)	0.000
N4	0.0312 (11)	0.0288 (11)	0.0185 (8)	0.000	0.0028 (7)	0.000
N5	0.0268 (10)	0.0392 (13)	0.0202 (9)	0.000	0.0028 (7)	0.000
N6	0.0403 (12)	0.0494 (14)	0.0189 (9)	0.000	-0.0059 (8)	0.000
C1	0.0273 (12)	0.0248 (12)	0.0268 (11)	0.000	0.0029 (8)	0.000
C2	0.0231 (11)	0.0299 (13)	0.0331 (12)	0.000	-0.0008 (9)	0.000
C3	0.0453 (15)	0.0508 (16)	0.0218 (11)	0.000	0.0023 (11)	0.000
C4	0.0396 (16)	0.076 (2)	0.0394 (15)	0.000	0.0175 (12)	0.000
C5	0.0342 (14)	0.0494 (19)	0.0439 (16)	0.000	-0.0106 (12)	0.000
C6	0.0248 (13)	0.070 (2)	0.0558 (18)	0.000	-0.0017 (12)	0.000
C7	0.0277 (11)	0.0186 (10)	0.0225 (10)	0.000	0.0016 (8)	0.000
C8	0.0358 (12)	0.0270 (11)	0.0199 (10)	0.000	-0.0017 (9)	0.000
C9	0.0252 (12)	0.0500 (16)	0.0300 (12)	0.000	0.0016 (10)	0.000
C10	0.0304 (13)	0.0446 (16)	0.0293 (12)	0.000	0.0089 (10)	0.000
C11	0.0518 (18)	0.085 (2)	0.0290 (14)	0.000	-0.0181 (13)	0.000
C12	0.0666 (19)	0.0478 (16)	0.0191 (11)	0.000	0.0009 (11)	0.000

Geometric parameters (Å, °)

Ni1—O1	1.8694 (17)	C3—H3A	0.9800
Ni1—O2	1.8634 (15)	C3—H3B	0.9800
Ni1—S1	2.1374 (7)	C3—H3C	0.9800
Ni1—S2	2.1386 (7)	C4—H4A	0.9800

S1—C1	1.743 (2)	C4—H4B	0.9800
S2—C7	1.750 (2)	C4—H4C	0.9800
O1—C2	1.261 (3)	C5—H5A	0.9800
O2—C8	1.260 (3)	C5—H5B	0.9800
N1—C1	1.316 (3)	C5—H5C	0.9800
N1—C2	1.355 (3)	C6—H6A	0.9800
N2—C1	1.353 (3)	C6—H6B	0.9800
N2—C3	1.455 (3)	C6—H6C	0.9800
N2—C4	1.462 (3)	C9—H9A	0.9800
N3—C2	1.351 (3)	C9—H9B	0.9800
N3—C6	1.452 (4)	C9—H9C	0.9800
N3—C5	1.453 (4)	C10—H10A	0.9800
N4—C7	1.329 (3)	C10—H10B	0.9800
N4—C8	1.341 (3)	C10—H10C	0.9800
N5—C7	1.333 (3)	C11—H11A	0.9800
N5—C9	1.456 (3)	C11—H11B	0.9800
N5—C10	1.461 (3)	C11—H11C	0.9800
N6—C8	1.366 (3)	C12—H12A	0.9800
N6—C11	1.452 (4)	C12—H12B	0.9800
N6—C12	1.459 (4)	C12—H12C	0.9800
S2...N5 ⁱ	3.5986 (5)	N6...C3 ⁱⁱⁱ	3.5470 (6)
C2...C5 ⁱⁱ	3.5161 (4)	N2...C12 ^{iv}	3.5622 (7)
O1—Ni1—S1	95.16 (6)	N3—C5—H5A	109.5
O2—Ni1—S2	94.65 (6)	N3—C5—H5B	109.5
O1—Ni1—O2	84.45 (8)	H5A—C5—H5B	109.5
S1—Ni1—S2	85.75 (3)	N3—C5—H5C	109.5
O1—Ni1—S2	179.10 (6)	H5A—C5—H5C	109.5
O2—Ni1—S1	179.60 (7)	H5B—C5—H5C	109.5
C1—S1—Ni1	109.05 (8)	N3—C6—H6A	109.5
C7—S2—Ni1	109.52 (8)	N3—C6—H6B	109.5
C2—O1—Ni1	133.73 (16)	H6A—C6—H6B	109.5
C8—O2—Ni1	134.24 (17)	N3—C6—H6C	109.5
C1—N1—C2	123.6 (2)	H6A—C6—H6C	109.5
C1—N2—C3	124.1 (2)	H6B—C6—H6C	109.5
C1—N2—C4	120.2 (2)	N4—C7—N5	116.4 (2)
C3—N2—C4	115.6 (2)	N4—C7—S2	128.39 (18)
C2—N3—C6	123.1 (2)	N5—C7—S2	115.23 (17)
C2—N3—C5	120.8 (2)	O2—C8—N4	129.8 (2)
C6—N3—C5	116.1 (2)	O2—C8—N6	115.2 (2)
C7—N4—C8	123.39 (19)	N4—C8—N6	115.0 (2)
C7—N5—C9	123.27 (19)	N5—C9—H9A	109.5
C7—N5—C10	121.1 (2)	N5—C9—H9B	109.5
C9—N5—C10	115.62 (19)	H9A—C9—H9B	109.5
C8—N6—C11	120.3 (2)	N5—C9—H9C	109.5
C8—N6—C12	123.2 (2)	H9A—C9—H9C	109.5
C11—N6—C12	116.5 (2)	H9B—C9—H9C	109.5

N1—C1—N2	115.3 (2)	N5—C10—H10A	109.5
N1—C1—S1	129.24 (18)	N5—C10—H10B	109.5
N2—C1—S1	115.43 (18)	H10A—C10—H10B	109.5
O1—C2—N3	116.1 (2)	N5—C10—H10C	109.5
O1—C2—N1	129.2 (2)	H10A—C10—H10C	109.5
N3—C2—N1	114.7 (2)	H10B—C10—H10C	109.5
N2—C3—H3A	109.5	N6—C11—H11A	109.5
N2—C3—H3B	109.5	N6—C11—H11B	109.5
H3A—C3—H3B	109.5	H11A—C11—H11B	109.5
N2—C3—H3C	109.5	N6—C11—H11C	109.5
H3A—C3—H3C	109.5	H11A—C11—H11C	109.5
H3B—C3—H3C	109.5	H11B—C11—H11C	109.5
N2—C4—H4A	109.5	N6—C12—H12A	109.5
N2—C4—H4B	109.5	N6—C12—H12B	109.5
H4A—C4—H4B	109.5	H12A—C12—H12B	109.5
N2—C4—H4C	109.5	N6—C12—H12C	109.5
H4A—C4—H4C	109.5	H12A—C12—H12C	109.5
H4B—C4—H4C	109.5	H12B—C12—H12C	109.5
O1—Ni1—S1—C1	0.0	C6—N3—C2—N1	0.000 (1)
S2—Ni1—S1—C1	180.0	C5—N3—C2—N1	180.0
O2—Ni1—S2—C7	0.0	C1—N1—C2—O1	0.000 (1)
S1—Ni1—S2—C7	180.0	C1—N1—C2—N3	180.0
O2—Ni1—O1—C2	180.0	C8—N4—C7—N5	180.0
S1—Ni1—O1—C2	0.0	C8—N4—C7—S2	0.0
O1—Ni1—O2—C8	180.0	C9—N5—C7—N4	180.0
S2—Ni1—O2—C8	0.0	C10—N5—C7—N4	0.0
C2—N1—C1—N2	180.0	C9—N5—C7—S2	0.0
C2—N1—C1—S1	0.000 (1)	C10—N5—C7—S2	180.0
C3—N2—C1—N1	180.0	Ni1—S2—C7—N4	0.0
C4—N2—C1—N1	0.0	Ni1—S2—C7—N5	180.0
C3—N2—C1—S1	0.0	Ni1—O2—C8—N4	0.0
C4—N2—C1—S1	180.0	Ni1—O2—C8—N6	180.0
Ni1—S1—C1—N1	0.0	C7—N4—C8—O2	0.0
Ni1—S1—C1—N2	180.0	C7—N4—C8—N6	180.0
Ni1—O1—C2—N3	180.0	C11—N6—C8—O2	0.0
Ni1—O1—C2—N1	0.000 (1)	C12—N6—C8—O2	180.0
C6—N3—C2—O1	180.0	C11—N6—C8—N4	180.0
C5—N3—C2—O1	0.000 (1)	C12—N6—C8—N4	0.0

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $-x+1, -y+1, -z$; (iii) $-x+1/2, -y+1, z+1/2$; (iv) $-x+1/2, -y+1, z-1/2$.