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# Bis[1,5-bis(1*H*-indol-3-ylmethylene)thiocarbazonato-$\kappa^2N,S$]nickel(II) dimethyl sulfoxide disolvate

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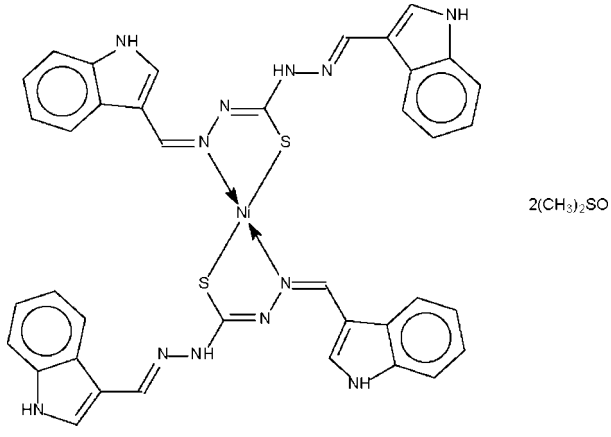
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.049; $wR$ factor = 0.139; data-to-parameter ratio = 18.2.

The Ni atom in the crystal structure of the centrosymmetric title compound, $[Ni(C_{19}H_{15}N_6S)_2]\cdot 2C_2H_6OS$, is *N*,*S*-chelated by the deprotonated Schiff bases in a square-planar geometry. The –CH═N—N═C(S)—NH—N═CH– frament is planar. The two indolyl –NH (donor) sites interact with dimethyl sulfoxide molecules to furnish a layer motif.

## Related literature

For the structure of the unsolvated nickel derivative of 1*H*-indole-3-carboxaldehyde thiosemicarbazone, see: Rizal *et al.* (2008). The ligand is known to be a sensitive complexing agent, see: Ghosh *et al.* (1999).




## Experimental

### Crystal data

$[Ni(C_{19}H_{15}N_6S)_2]\cdot 2C_2H_6OS$
$M_r$ = 933.83
Monoclinic, $C2/c$
$a$ = 19.0340 (5) Å
$b$ = 9.1982 (3) Å
$c$ = 25.1374 (7) Å
$\beta$ = 95.672 (2)°
$V$ = 4379.5 (2) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.69 mm$^{-1}$
$T$ = 100 (2) K
0.30 × 0.03 × 0.03 mm

### Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.821, $T_{max}$ = 0.980
27119 measured reflections
5030 independent reflections
3201 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.092

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.139
$S$ = 1.03
5030 reflections
277 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.60 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.53 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Ni1—N5 | 1.906 (3) | Ni1—S1 | 2.1748 (8) |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1n···O1 | 0.88 | 2.10 | 2.890 (4) | 148 |
| N6—H6n···O1$^{i}$ | 0.88 | 2.03 | 2.855 (4) | 156 |

Symmetry code: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2702).

## References

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# supporting information

*Acta Cryst.* (2008). E**64**, m755 [doi:10.1107/S1600536808011975]

# Bis[1,5-bis(1*H*-indol-3-ylmethylene)thiocarbazonato-$\kappa^2$*N*,*S*]nickel(II) dimethyl sulfoxide disolvate

**Mohd. Razali Rizal, Hapipah M. Ali and Seik Weng Ng**

## S1. Comment

The preceding study reports the nickel derivative of 1*H*-indole-3-carboxaldehyde thiosemicarbazone (Rizal *et al.*, 2008). With bis(1*H*-indole-3-carboxaldehyde thiocarbazone) in place of the thiosemicarbazone, the resulting nickel derivative also has the *N*,*S*-chelated metal center in a square planar coordination geometry. The compound crystallizes from DMSO as a disolvate (Fig. 1). The oxygen atom of the solvent molecule is a hydrogen bond acceptor to the indolyl amino group of two mononuclear molecules; such a hydrogen bonding scheme gives rise to a layer motif.

## S2. Experimental

The Schiff base was synthesized as according to a literature procedure (Ghosh *et al.*, 1999). The Schiff base (2 g, 5.5 mmol) and nickel acetate (0.7 g, 2.8 mmol) were heated in ethanol (50 ml) for 5 h. The brown product was recrystallized from DMSO to give red crystals..

## S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.98 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2–1.5*U*(C). The nitrogen-bound H-atoms were similarly treated [N–H 0.88 Å].

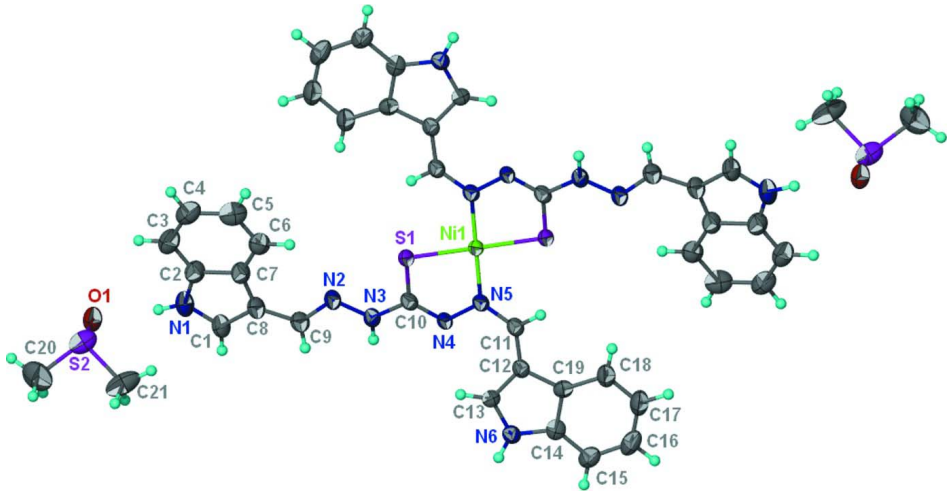


**Figure 1**

Thermal ellipsoid plot (Barbour, 2001) of $Ni(C_{19}H_{15}N_6S)_2{\cdot}2DMSO$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. The molecule lies on a center-of-inversion. Unlabeled atoms are related to the labeled ones by this symmetry element.

**Bis[1,5-bis(1*H*-indol-3-ylmethylene)thiocarbazonato- $\kappa^2N,S$]nickel(II) dimethyl sulfoxide disolvate**

*Crystal data*

$[Ni(C_{19}H_{15}N_6S)_2]{\cdot}2C_2H_6OS$
$M_r = 933.83$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 19.0340\ (5)$ Å
$b = 9.1982\ (3)$ Å
$c = 25.1374\ (7)$ Å
$\beta = 95.672\ (2)°$
$V = 4379.5\ (2)$ Å$^3$
$Z = 4$
$F(000) = 1944$
$D_x = 1.416$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2255 reflections
$\theta = 2.5–23.1°$
$\mu = 0.69$ mm$^{-1}$
$T = 100$ K
Needle, red
0.30 × 0.03 × 0.03 mm

*Data collection*

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.821$, $T_{max} = 0.980$
27119 measured reflections
5030 independent reflections
3201 reflections with $I > 2\sigma(I)$
$R_{int} = 0.092$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.6°$
$h = -24\rightarrow24$
$k = -11\rightarrow9$
$l = -32\rightarrow32$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.139$
$S = 1.04$
5030 reflections
277 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

$w = 1/[\sigma^2(F_o^2) + (0.0695P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.60$ e Å$^{-3}$
$\Delta\rho_{min} = -0.53$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Ni1 | 0.7500 | 0.7500 | 0.5000 | 0.02112 (17) |
| S1 | 0.71406 (4) | 0.69712 (10) | 0.41745 (3) | 0.0248 (2) |
| S2 | 0.54373 (5) | 0.32873 (12) | 0.03925 (4) | 0.0426 (3) |
| N1 | 0.67553 (16) | 0.4672 (4) | 0.14187 (11) | 0.0407 (8) |
| H1N | 0.6749 | 0.4384 | 0.1084 | 0.049* |
| N2 | 0.73446 (14) | 0.5251 (3) | 0.32226 (10) | 0.0275 (6) |
| N3 | 0.77036 (14) | 0.4729 (3) | 0.36844 (10) | 0.0278 (6) |
| H3N | 0.7967 | 0.3945 | 0.3674 | 0.033* |
| N4 | 0.80017 (13) | 0.4836 (3) | 0.45745 (9) | 0.0228 (6) |
| N5 | 0.79004 (13) | 0.5599 (3) | 0.50425 (9) | 0.0219 (6) |
| N6 | 0.87026 (13) | 0.1142 (3) | 0.54254 (10) | 0.0256 (6) |
| H6N | 0.8770 | 0.0305 | 0.5269 | 0.031* |
| O1 | 0.61523 (12) | 0.3930 (3) | 0.03531 (9) | 0.0361 (6) |
| C1 | 0.71111 (19) | 0.3994 (5) | 0.18458 (13) | 0.0366 (9) |
| H1 | 0.7380 | 0.3128 | 0.1830 | 0.044* |
| C2 | 0.64128 (19) | 0.5856 (4) | 0.15846 (13) | 0.0347 (9) |
| C3 | 0.59816 (19) | 0.6863 (5) | 0.13031 (15) | 0.0410 (10) |
| H3 | 0.5891 | 0.6801 | 0.0925 | 0.049* |
| C4 | 0.5688 (2) | 0.7948 (5) | 0.15795 (16) | 0.0437 (10) |
| H4 | 0.5390 | 0.8642 | 0.1390 | 0.052* |
| C5 | 0.5817 (2) | 0.8061 (5) | 0.21364 (16) | 0.0445 (10) |
| H5 | 0.5606 | 0.8827 | 0.2318 | 0.053* |
| C6 | 0.62496 (18) | 0.7069 (4) | 0.24255 (14) | 0.0344 (9) |
| H6 | 0.6332 | 0.7142 | 0.2804 | 0.041* |
| C7 | 0.65623 (18) | 0.5962 (4) | 0.21512 (12) | 0.0314 (8) |
| C8 | 0.70192 (18) | 0.4760 (4) | 0.23012 (12) | 0.0321 (8) |
| C9 | 0.73595 (18) | 0.4385 (4) | 0.28191 (12) | 0.0307 (8) |
| H9 | 0.7600 | 0.3482 | 0.2866 | 0.037* |
| C10 | 0.76516 (16) | 0.5425 (4) | 0.41603 (12) | 0.0237 (7) |
| C11 | 0.80984 (15) | 0.4880 (4) | 0.54786 (12) | 0.0239 (7) |
| H11 | 0.8051 | 0.5388 | 0.5802 | 0.029* |
| C12 | 0.83747 (16) | 0.3449 (4) | 0.55418 (12) | 0.0237 (7) |
| C13 | 0.84099 (16) | 0.2324 (4) | 0.51784 (12) | 0.0235 (7) |
| H13 | 0.8250 | 0.2380 | 0.4809 | 0.028* |
| C14 | 0.88816 (16) | 0.1434 (4) | 0.59618 (13) | 0.0274 (8) |
| C15 | 0.92233 (17) | 0.0566 (4) | 0.63616 (13) | 0.0346 (9) |

| | | | | |
|---|---|---|---|---|
| H15 | 0.9361 | −0.0403 | 0.6293 | 0.042* |
| C16 | 0.93510 (19) | 0.1182 (5) | 0.68610 (14) | 0.0410 (10) |
| H16 | 0.9589 | 0.0626 | 0.7142 | 0.049* |
| C17 | 0.91418 (19) | 0.2594 (5) | 0.69662 (14) | 0.0400 (9) |
| H17 | 0.9234 | 0.2975 | 0.7317 | 0.048* |
| C18 | 0.88050 (17) | 0.3447 (4) | 0.65717 (12) | 0.0330 (9) |
| H18 | 0.8661 | 0.4408 | 0.6647 | 0.040* |
| C19 | 0.86766 (16) | 0.2867 (4) | 0.60527 (13) | 0.0252 (7) |
| C20 | 0.5318 (2) | 0.1994 (5) | −0.01409 (19) | 0.0615 (13) |
| H20A | 0.5247 | 0.2508 | −0.0483 | 0.092* |
| H20B | 0.4904 | 0.1390 | −0.0096 | 0.092* |
| H20C | 0.5737 | 0.1374 | −0.0136 | 0.092* |
| C21 | 0.5542 (2) | 0.2019 (5) | 0.09367 (19) | 0.0580 (13) |
| H21A | 0.5617 | 0.2551 | 0.1275 | 0.087* |
| H21B | 0.5950 | 0.1393 | 0.0897 | 0.087* |
| H21C | 0.5116 | 0.1420 | 0.0935 | 0.087* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ni1 | 0.0294 (3) | 0.0185 (3) | 0.0161 (3) | −0.0020 (3) | 0.0053 (2) | −0.0006 (2) |
| S1 | 0.0359 (4) | 0.0216 (5) | 0.0173 (4) | −0.0002 (4) | 0.0042 (3) | −0.0015 (3) |
| S2 | 0.0332 (5) | 0.0450 (7) | 0.0512 (6) | 0.0053 (5) | 0.0129 (4) | 0.0132 (5) |
| N1 | 0.053 (2) | 0.048 (2) | 0.0219 (15) | 0.0008 (17) | 0.0073 (14) | −0.0063 (14) |
| N2 | 0.0343 (15) | 0.0295 (18) | 0.0192 (13) | −0.0021 (13) | 0.0053 (11) | −0.0032 (12) |
| N3 | 0.0378 (16) | 0.0256 (17) | 0.0202 (13) | 0.0056 (13) | 0.0041 (11) | −0.0039 (12) |
| N4 | 0.0314 (14) | 0.0211 (16) | 0.0166 (12) | −0.0005 (12) | 0.0059 (11) | −0.0036 (11) |
| N5 | 0.0259 (14) | 0.0213 (16) | 0.0192 (12) | −0.0018 (12) | 0.0069 (10) | −0.0026 (11) |
| N6 | 0.0275 (14) | 0.0239 (17) | 0.0255 (14) | 0.0023 (12) | 0.0028 (11) | −0.0027 (12) |
| O1 | 0.0355 (13) | 0.0473 (18) | 0.0255 (12) | −0.0032 (12) | 0.0031 (10) | 0.0014 (11) |
| C1 | 0.049 (2) | 0.039 (2) | 0.0228 (17) | 0.0024 (18) | 0.0068 (16) | −0.0055 (16) |
| C2 | 0.039 (2) | 0.039 (3) | 0.0268 (18) | −0.0054 (18) | 0.0087 (15) | 0.0032 (17) |
| C3 | 0.043 (2) | 0.049 (3) | 0.0314 (19) | −0.002 (2) | 0.0063 (17) | 0.0078 (18) |
| C4 | 0.040 (2) | 0.043 (3) | 0.047 (2) | −0.0003 (19) | −0.0002 (18) | 0.012 (2) |
| C5 | 0.040 (2) | 0.042 (3) | 0.054 (2) | 0.0023 (19) | 0.0148 (19) | 0.004 (2) |
| C6 | 0.0386 (19) | 0.036 (2) | 0.0304 (18) | −0.0014 (17) | 0.0104 (15) | 0.0004 (16) |
| C7 | 0.0352 (19) | 0.037 (2) | 0.0235 (16) | −0.0067 (17) | 0.0086 (14) | 0.0000 (15) |
| C8 | 0.040 (2) | 0.035 (2) | 0.0218 (16) | 0.0003 (17) | 0.0072 (15) | −0.0051 (15) |
| C9 | 0.0378 (19) | 0.030 (2) | 0.0249 (17) | 0.0000 (16) | 0.0079 (14) | −0.0034 (15) |
| C10 | 0.0269 (16) | 0.024 (2) | 0.0214 (15) | −0.0052 (14) | 0.0077 (13) | −0.0041 (14) |
| C11 | 0.0260 (16) | 0.025 (2) | 0.0210 (15) | −0.0025 (14) | 0.0059 (13) | −0.0033 (14) |
| C12 | 0.0243 (16) | 0.025 (2) | 0.0221 (15) | −0.0018 (14) | 0.0040 (12) | −0.0026 (14) |
| C13 | 0.0241 (15) | 0.022 (2) | 0.0241 (16) | 0.0008 (14) | 0.0030 (12) | 0.0015 (14) |
| C14 | 0.0211 (16) | 0.033 (2) | 0.0285 (17) | −0.0031 (14) | 0.0039 (13) | 0.0019 (15) |
| C15 | 0.0316 (19) | 0.034 (2) | 0.0370 (19) | −0.0002 (16) | −0.0006 (15) | 0.0077 (17) |
| C16 | 0.035 (2) | 0.050 (3) | 0.036 (2) | −0.0012 (19) | −0.0063 (16) | 0.0151 (19) |
| C17 | 0.043 (2) | 0.050 (3) | 0.0260 (18) | −0.006 (2) | −0.0013 (15) | 0.0019 (18) |
| C18 | 0.0357 (19) | 0.039 (2) | 0.0247 (17) | −0.0036 (17) | 0.0024 (15) | −0.0016 (16) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C19 | 0.0243 (16) | 0.024 (2) | 0.0280 (17) | −0.0036 (13) | 0.0051 (13) | 0.0024 (14) |
| C20 | 0.042 (2) | 0.064 (3) | 0.077 (3) | −0.018 (2) | −0.005 (2) | −0.012 (3) |
| C21 | 0.049 (2) | 0.053 (3) | 0.076 (3) | 0.010 (2) | 0.026 (2) | 0.031 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Ni1—N5$^{i}$ | 1.906 (3) | C5—C6 | 1.386 (5) |
| Ni1—N5 | 1.906 (3) | C5—H5 | 0.9500 |
| Ni1—S1$^{i}$ | 2.1748 (8) | C6—C7 | 1.396 (5) |
| Ni1—S1 | 2.1748 (8) | C6—H6 | 0.9500 |
| S1—C10 | 1.726 (3) | C7—C8 | 1.434 (5) |
| S2—O1 | 1.496 (2) | C8—C9 | 1.438 (5) |
| S2—C20 | 1.790 (5) | C9—H9 | 0.9500 |
| S2—C21 | 1.794 (4) | C11—C12 | 1.420 (5) |
| N1—C2 | 1.356 (5) | C11—H11 | 0.9500 |
| N1—C1 | 1.362 (4) | C12—C13 | 1.386 (4) |
| N1—H1N | 0.8800 | C12—C19 | 1.456 (4) |
| N2—C9 | 1.293 (4) | C13—H13 | 0.9500 |
| N2—N3 | 1.374 (4) | C14—C15 | 1.394 (5) |
| N3—C10 | 1.369 (4) | C14—C19 | 1.400 (5) |
| N3—H3N | 0.8800 | C15—C16 | 1.377 (5) |
| N4—C10 | 1.298 (4) | C15—H15 | 0.9500 |
| N4—N5 | 1.400 (3) | C16—C17 | 1.392 (6) |
| N5—C11 | 1.304 (4) | C16—H16 | 0.9500 |
| N6—C13 | 1.345 (4) | C17—C18 | 1.372 (5) |
| N6—C14 | 1.384 (4) | C17—H17 | 0.9500 |
| N6—H6N | 0.8800 | C18—C19 | 1.408 (4) |
| C1—C8 | 1.370 (5) | C18—H18 | 0.9500 |
| C1—H1 | 0.9500 | C20—H20A | 0.9800 |
| C2—C3 | 1.385 (5) | C20—H20B | 0.9800 |
| C2—C7 | 1.428 (4) | C20—H20C | 0.9800 |
| C3—C4 | 1.367 (6) | C21—H21A | 0.9800 |
| C3—H3 | 0.9500 | C21—H21B | 0.9800 |
| C4—C5 | 1.401 (5) | C21—H21C | 0.9800 |
| C4—H4 | 0.9500 | | |

| | | | |
|---|---|---|---|
| N5$^{i}$—Ni1—N5 | 180.000 (1) | C7—C8—C9 | 129.1 (3) |
| N5$^{i}$—Ni1—S1$^{i}$ | 86.25 (7) | N2—C9—C8 | 121.3 (3) |
| N5—Ni1—S1$^{i}$ | 93.75 (7) | N2—C9—H9 | 119.3 |
| N5$^{i}$—Ni1—S1 | 93.75 (7) | C8—C9—H9 | 119.3 |
| N5—Ni1—S1 | 86.25 (7) | N4—C10—N3 | 115.5 (3) |
| S1$^{i}$—Ni1—S1 | 180.000 (1) | N4—C10—S1 | 125.0 (2) |
| C10—S1—Ni1 | 94.55 (10) | N3—C10—S1 | 119.5 (2) |
| O1—S2—C20 | 105.20 (18) | N5—C11—C12 | 129.6 (3) |
| O1—S2—C21 | 105.92 (18) | N5—C11—H11 | 115.2 |
| C20—S2—C21 | 97.8 (3) | C12—C11—H11 | 115.2 |
| C2—N1—C1 | 110.0 (3) | C13—C12—C11 | 131.2 (3) |
| C2—N1—H1N | 125.0 | C13—C12—C19 | 105.5 (3) |

| | | | |
|---|---|---|---|
| C1—N1—H1N | 125.0 | C11—C12—C19 | 123.3 (3) |
| C9—N2—N3 | 113.5 (3) | N6—C13—C12 | 110.1 (3) |
| C10—N3—N2 | 120.1 (3) | N6—C13—H13 | 124.9 |
| C10—N3—H3N | 119.9 | C12—C13—H13 | 124.9 |
| N2—N3—H3N | 119.9 | N6—C14—C15 | 130.1 (3) |
| C10—N4—N5 | 111.3 (3) | N6—C14—C19 | 107.2 (3) |
| C11—N5—N4 | 113.6 (3) | C15—C14—C19 | 122.7 (3) |
| C11—N5—Ni1 | 126.4 (2) | C16—C15—C14 | 116.7 (4) |
| N4—N5—Ni1 | 120.03 (19) | C16—C15—H15 | 121.6 |
| C13—N6—C14 | 110.1 (3) | C14—C15—H15 | 121.6 |
| C13—N6—H6N | 125.0 | C15—C16—C17 | 122.0 (3) |
| C14—N6—H6N | 125.0 | C15—C16—H16 | 119.0 |
| N1—C1—C8 | 109.2 (4) | C17—C16—H16 | 119.0 |
| N1—C1—H1 | 125.4 | C18—C17—C16 | 121.2 (3) |
| C8—C1—H1 | 125.4 | C18—C17—H17 | 119.4 |
| N1—C2—C3 | 131.2 (3) | C16—C17—H17 | 119.4 |
| N1—C2—C7 | 107.9 (3) | C17—C18—C19 | 118.6 (4) |
| C3—C2—C7 | 120.9 (4) | C17—C18—H18 | 120.7 |
| C4—C3—C2 | 118.7 (4) | C19—C18—H18 | 120.7 |
| C4—C3—H3 | 120.7 | C14—C19—C18 | 118.8 (3) |
| C2—C3—H3 | 120.7 | C14—C19—C12 | 107.1 (3) |
| C3—C4—C5 | 121.5 (4) | C18—C19—C12 | 134.1 (3) |
| C3—C4—H4 | 119.3 | S2—C20—H20A | 109.5 |
| C5—C4—H4 | 119.3 | S2—C20—H20B | 109.5 |
| C6—C5—C4 | 120.8 (4) | H20A—C20—H20B | 109.5 |
| C6—C5—H5 | 119.6 | S2—C20—H20C | 109.5 |
| C4—C5—H5 | 119.6 | H20A—C20—H20C | 109.5 |
| C5—C6—C7 | 118.8 (3) | H20B—C20—H20C | 109.5 |
| C5—C6—H6 | 120.6 | S2—C21—H21A | 109.5 |
| C7—C6—H6 | 120.6 | S2—C21—H21B | 109.5 |
| C6—C7—C2 | 119.3 (3) | H21A—C21—H21B | 109.5 |
| C6—C7—C8 | 135.2 (3) | S2—C21—H21C | 109.5 |
| C2—C7—C8 | 105.4 (3) | H21A—C21—H21C | 109.5 |
| C1—C8—C7 | 107.5 (3) | H21B—C21—H21C | 109.5 |
| C1—C8—C9 | 123.4 (4) | | |

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| N5$^{i}$—Ni1—S1—C10 | 167.97 (12) | C7—C8—C9—N2 | −8.1 (6) |
| N5—Ni1—S1—C10 | −12.03 (12) | N5—N4—C10—N3 | −178.4 (2) |
| C9—N2—N3—C10 | −170.8 (3) | N5—N4—C10—S1 | 1.3 (4) |
| C10—N4—N5—C11 | 164.8 (3) | N2—N3—C10—N4 | 179.0 (3) |
| C10—N4—N5—Ni1 | −14.8 (3) | N2—N3—C10—S1 | −0.7 (4) |
| S1$^{i}$—Ni1—N5—C11 | 17.7 (3) | Ni1—S1—C10—N4 | 9.5 (3) |
| S1—Ni1—N5—C11 | −162.3 (3) | Ni1—S1—C10—N3 | −170.8 (2) |
| S1$^{i}$—Ni1—N5—N4 | −162.8 (2) | N4—N5—C11—C12 | −2.2 (5) |
| S1—Ni1—N5—N4 | 17.2 (2) | Ni1—N5—C11—C12 | 177.4 (2) |
| C2—N1—C1—C8 | −1.6 (4) | N5—C11—C12—C13 | −12.0 (6) |
| C1—N1—C2—C3 | −179.1 (4) | N5—C11—C12—C19 | 170.0 (3) |
| C1—N1—C2—C7 | 0.7 (4) | C14—N6—C13—C12 | −0.7 (4) |

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|---|---|---|---|
| N1—C2—C3—C4 | 178.5 (4) | C11—C12—C13—N6 | −178.3 (3) |
| C7—C2—C3—C4 | −1.3 (6) | C19—C12—C13—N6 | 0.0 (4) |
| C2—C3—C4—C5 | 0.3 (6) | C13—N6—C14—C15 | −176.7 (3) |
| C3—C4—C5—C6 | 0.0 (6) | C13—N6—C14—C19 | 1.1 (3) |
| C4—C5—C6—C7 | 0.7 (6) | N6—C14—C15—C16 | 177.8 (3) |
| C5—C6—C7—C2 | −1.8 (5) | C19—C14—C15—C16 | 0.4 (5) |
| C5—C6—C7—C8 | −179.1 (4) | C14—C15—C16—C17 | 0.9 (5) |
| N1—C2—C7—C6 | −177.7 (3) | C15—C16—C17—C18 | −0.9 (6) |
| C3—C2—C7—C6 | 2.1 (5) | C16—C17—C18—C19 | −0.4 (5) |
| N1—C2—C7—C8 | 0.3 (4) | N6—C14—C19—C18 | −179.5 (3) |
| C3—C2—C7—C8 | −179.8 (3) | C15—C14—C19—C18 | −1.6 (5) |
| N1—C1—C8—C7 | 1.8 (4) | N6—C14—C19—C12 | −1.1 (3) |
| N1—C1—C8—C9 | −176.2 (3) | C15—C14—C19—C12 | 176.9 (3) |
| C6—C7—C8—C1 | 176.3 (4) | C17—C18—C19—C14 | 1.5 (5) |
| C2—C7—C8—C1 | −1.3 (4) | C17—C18—C19—C12 | −176.4 (3) |
| C6—C7—C8—C9 | −5.9 (7) | C13—C12—C19—C14 | 0.7 (3) |
| C2—C7—C8—C9 | 176.5 (3) | C11—C12—C19—C14 | 179.1 (3) |
| N3—N2—C9—C8 | −179.2 (3) | C13—C12—C19—C18 | 178.8 (3) |
| C1—C8—C9—N2 | 169.4 (3) | C11—C12—C19—C18 | −2.7 (6) |

Symmetry code: (i) −*x*+3/2, −*y*+3/2, −*z*+1.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1n···O1 | 0.88 | 2.10 | 2.890 (4) | 148 |
| N6—H6n···O1$^{ii}$ | 0.88 | 2.03 | 2.855 (4) | 156 |

Symmetry code: (ii) −*x*+3/2, *y*−1/2, −*z*+1/2.