

# Diazidobis[4,4,5,5-tetramethyl-2-(1,3-thiazol-2-yl)-2-imidazoline-1-oxyl 3-oxide- $\kappa^2N^1,O^3$ ]nickel(II)

 Jiu Li Chang,<sup>a</sup> Zhi Yong Gao<sup>a\*</sup> and Ning Zhao<sup>b</sup>

<sup>a</sup>College of Chemistry and Environmental Science, Henan Normal University, Xixiang 453002, People's Republic of China, and <sup>b</sup>School of Chemistry and Chemical Engineering, Henan Institute of Science and Technology, Xixiang 453003, People's Republic of China  
Correspondence e-mail: gaozhy201@sohu.com

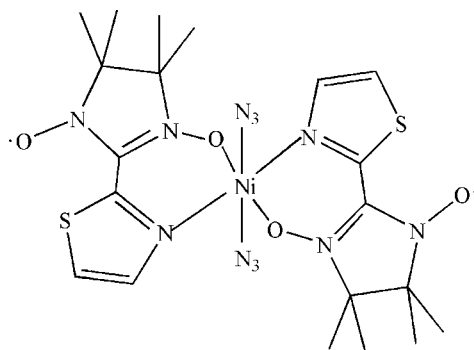
Received 6 October 2010; accepted 19 October 2010

Key indicators: single-crystal X-ray study;  $T = 291$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å; R factor = 0.024;  $wR$  factor = 0.065; data-to-parameter ratio = 16.5.

In the title compound,  $[\text{Ni}(\text{N}_3)_2(\text{C}_{10}\text{H}_{14}\text{N}_3\text{O}_2\text{S})_2]$ , the  $\text{Ni}^{\text{II}}$  atom lies on an inversion center and adopts a distorted *trans*- $\text{NiO}_2\text{N}_4$  octahedral geometry, coordinated by two *N,O*-bidentate 4,4,5,5-tetramethyl-2-(5-methylimidazol-4-yl)-2-imidazoline-1-oxyl 3-oxide nitronyl nitroxide radical ligands and two monodentate azide anions.

## Related literature

For general background to molecular magnetic materials and metal-radical magnetic materials, see: Vostrikova *et al.* (2000); Fegy *et al.* (1998); Kahn *et al.* (2000); Omata *et al.* (2001); Yamamoto *et al.* (2001); Fursova *et al.* (2003); Sroh *et al.* (2003); Chang *et al.* (2009); Schatzschneider *et al.* (2001). For the synthesis of nitronyl nitroxide radical ligands and the title compound, see: Ullman *et al.* (1970, 1972).



## Experimental

### Crystal data

$[\text{Ni}(\text{N}_3)_2(\text{C}_{10}\text{H}_{14}\text{N}_3\text{O}_2\text{S})_2]$   
 $M_r = 623.37$   
Monoclinic,  $P2_1/c$   
 $a = 9.9212$  (7) Å  
 $b = 12.1732$  (8) Å  
 $c = 11.1795$  (8) Å  
 $\beta = 102.695$  (1)°

$V = 1317.17$  (16) Å<sup>3</sup>  
 $Z = 2$   
Mo  $K\alpha$  radiation  
 $\mu = 0.95$  mm<sup>-1</sup>  
 $T = 291$  K  
 $0.40 \times 0.22 \times 0.15$  mm

### Data collection

Bruker SMART APEX CCD diffractometer  
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)  
 $T_{\text{min}} = 0.703$ ,  $T_{\text{max}} = 0.874$

7812 measured reflections  
3005 independent reflections  
2834 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.010$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$   
 $wR(F^2) = 0.065$   
 $S = 1.06$   
3005 reflections

182 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.25$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.27$  e Å<sup>-3</sup>

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

This work was supported by the Natural Science Foundation and Basic Research Program of Henan province (Nos. 092300410195 and 092300410240).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5040).

## References

- Bruker (2002). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Winsconsin, USA.  
Chang, J. L., Gao, Z. Y. & Jiang, K. (2009). *Acta Cryst.* **E65**, m181.  
Fegy, K., Luneau, D., Ohm, T., Paulsen, C. & Rey, P. (1998). *Angew. Chem. Int. Ed.* **37**, 1270–1273.  
Fursova, E. Y., Ovcharenko, V. I., Romanenko, G. V. & Tretyakov, E. V. (2003). *Tetrahedron Lett.* **44**, 6397–6399.  
Kahn, M. L., Sutter, S., Guionneau, P., Ouahab, L., Kahn, O. & Chasseau, D. (2000). *J. Am. Chem. Soc.* **122**, 3413–3421.  
Omata, J., Ishida, T., Hashizume, D., Iwasaki, F. & Nogami, T. (2001). *Inorg. Chem.* **40**, 3954–3958.  
Schatzschneider, U., Weyhermüller, T. & Rentschler, E. (2001). *Eur. J. Inorg. Chem.* pp. 2569–2586.  
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.  
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
Sroh, C., Belorizky, E., Turek, P., Bolvin, H. & Ziessel, R. (2003). *Inorg. Chem.* **42**, 2938–2949.  
Ullman, E. F., Call, L. & Osiecki, J. H. (1970). *J. Org. Chem.* **35**, 3623–3628.  
Ullman, E. F., Osiecki, J. H., Boocock, D. G. B. & Darcy, R. (1972). *J. Am. Chem. Soc.* **94**, 7049–7059.  
Vostrikova, K. E., Luneau, D., Wersdorfer, W., Rey, P. & Verdagner, M. (2000). *J. Am. Chem. Soc.* **122**, 718–719.  
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.  
Yamamoto, Y., Suzuki, T. & Kaizaki, S. (2001). *J. Chem. Soc. Dalton Trans.* pp. 1566–1572.

## supporting information

*Acta Cryst.* (2010). E66, m1481 [https://doi.org/10.1107/S1600536810042455]

## Diazidobis[4,4,5,5-tetramethyl-2-(1,3-thiazol-2-yl)-2-imidazoline-1-oxyl 3-oxide- $\kappa^2N^1,O^3$ ]nickel(II)

Jiu Li Chang, Zhi Yong Gao and Ning Zhao

### S1. Comment

The synthesis and study of transition metal complexes incorporating organic free radicals is a major research focus in the field of molecular magnetism (Vostrikova *et al.*, 2000; Fegy *et al.*, 1998; Kahn *et al.*, 2000; Omata *et al.*, 2001). In this field, nitronyl nitroxides acting as useful paramagnetic building blocks have been extensively used to assemble molecular magnetic materials, because many of them are good stable spin carriers even when coordinated to metal ions (Yamamoto *et al.*, 2001; Fursova *et al.*, 2003; Sroh *et al.*, 2003; Chang *et al.*, 2009; Schatzschneider *et al.*, 2001). We report herein the synthesis and crystal structure of one such nickel complex.

The asymmetric unit of the title compound (Fig. 1) contains half molecule. The Ni<sup>II</sup> atom, lying on an inversion center, is six-coordinated in a distorted octahedral geometry by two N atoms and two O atoms from two 4,4,5,5-tetramethyl-2-(5-methylimidazol-4-yl)-2-imidazoline-1-oxyl-3-oxide nitronyl nitroxide radical ligands and two N atoms from two azide anions.

### S2. Experimental

The nitronyl nitroxide radical(2-(2'-thiazole)-4,4,5,5-tetramethylimidazoline-1-oxyl-3-oxide)was synthesized according to literature procedures (Ullman *et al.* 1970; Ullman *et al.* 1972). A mixed solution of nitronyl nitroxide radical ligands (2.00 mmol) and Ni(Ac)<sub>2</sub>·4H<sub>2</sub>O (1 mmol) in ethanol (10 ml) was added to an aqueous solution(10 mL) of NaN<sub>3</sub>(2 mmol) and the resulting mixed solution was stirred for one hour at room temperature and then filtered off. This filtrate was left to evaporate slowly. After one week, deep purple crystals suitable for X-ray analysis were isolated.

### S3. Refinement

All C—H atoms were positioned geometrically, with C—H = 0.93 or 0.96 Å and constrained to ride on their parent atoms with  $U_{\text{iso}}(\text{H})=1.2\text{U}$  (carrier) or  $U_{\text{iso}}(\text{H})=1.5\text{U}$  (methyl carrier).

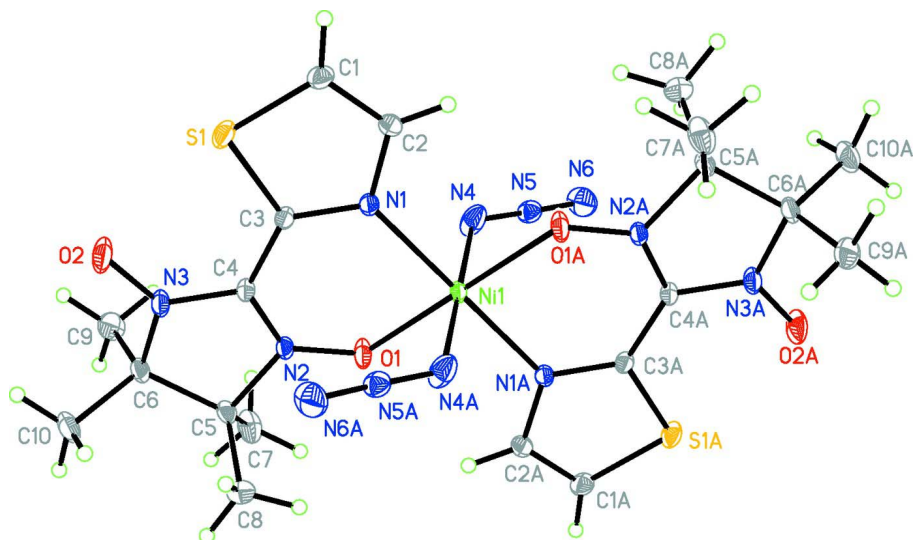


Figure 1

ORTEP drawing of the title compound with atom labeling. The thermal ellipsoids are drawn at 30% probability level [symmetry codes relating the atoms with and without the suffix A:  $-x + 1, -y + 2, -z + 1$ ]

### Diazidobis[4,4,5,5-tetramethyl-2-(1,3-thiazol-2-yl)-2-imidazoline-1-oxyl 3-oxide- $\kappa^2N^1, O^3$ ]nickel(II)

#### Crystal data

$[\text{Ni}(\text{N}_3)_2(\text{C}_{10}\text{H}_{14}\text{N}_3\text{O}_2\text{S})_2]$

$M_r = 623.37$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2_1/c$

$a = 9.9212(7)\ \text{\AA}$

$b = 12.1732(8)\ \text{\AA}$

$c = 11.1795(8)\ \text{\AA}$

$\beta = 102.695(1)^\circ$

$V = 1317.17(16)\ \text{\AA}^3$

$Z = 2$

$F(000) = 648$

$D_x = 1.572\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 5712 reflections

$\theta = 2.7\text{--}29.3^\circ$

$\mu = 0.95\ \text{mm}^{-1}$

$T = 291\ \text{K}$

Block, dark purple

$0.40 \times 0.22 \times 0.15\ \text{mm}$

#### Data collection

Bruker SMART APEX CCD  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.703, T_{\max} = 0.874$

7812 measured reflections

3005 independent reflections

2834 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.010$

$\theta_{\max} = 27.5^\circ, \theta_{\min} = 2.7^\circ$

$h = -12 \rightarrow 9$

$k = -14 \rightarrow 15$

$l = -14 \rightarrow 13$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.024$

$wR(F^2) = 0.065$

$S = 1.06$

3005 reflections

182 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  
 $w = 1/[\sigma^2(F_o^2) + (0.031P)^2 + 0.5195P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.25 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.27 \text{ e } \text{\AA}^{-3}$

*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.

**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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.5000	1.0000	0.5000	0.02603 (8)
S1	0.75033 (4)	1.27825 (3)	0.38125 (4)	0.04133 (11)
O1	0.64775 (12)	0.90740 (9)	0.43831 (12)	0.0486 (3)
O2	0.89398 (15)	1.14747 (11)	0.24875 (14)	0.0611 (4)
N1	0.60808 (11)	1.13921 (9)	0.47330 (10)	0.0272 (2)
N2	0.72751 (11)	0.94577 (9)	0.37164 (10)	0.0285 (2)
N3	0.84655 (12)	1.05745 (10)	0.28101 (11)	0.0360 (3)
N4	0.61887 (17)	0.99070 (14)	0.67735 (14)	0.0568 (4)
N5	0.58855 (14)	0.95757 (10)	0.76655 (12)	0.0380 (3)
N6	0.5618 (2)	0.92594 (14)	0.85593 (15)	0.0652 (5)
C1	0.64979 (16)	1.32436 (12)	0.47626 (15)	0.0391 (3)
H1	0.6423	1.3976	0.4976	0.047*
C2	0.58239 (15)	1.24038 (11)	0.51644 (13)	0.0329 (3)
H2A	0.5231	1.2506	0.5694	0.039*
C3	0.69761 (13)	1.14629 (10)	0.40176 (12)	0.0269 (2)
C4	0.75220 (13)	1.05162 (11)	0.35158 (12)	0.0273 (3)
C5	0.79699 (14)	0.86855 (11)	0.29890 (12)	0.0312 (3)
C6	0.90436 (14)	0.94677 (12)	0.25934 (13)	0.0337 (3)
C7	0.8572 (2)	0.77211 (15)	0.37997 (18)	0.0535 (5)
H7A	0.9144	0.7992	0.4548	0.080*
H7B	0.9117	0.7275	0.3378	0.080*
H7C	0.7834	0.7288	0.3984	0.080*
C8	0.68251 (19)	0.82790 (16)	0.19319 (16)	0.0524 (4)
H8A	0.6110	0.7937	0.2256	0.079*
H8B	0.7201	0.7755	0.1452	0.079*
H8C	0.6447	0.8890	0.1424	0.079*
C9	1.04886 (16)	0.94066 (17)	0.34192 (17)	0.0527 (4)
H9A	1.1050	0.9986	0.3207	0.079*
H9B	1.0898	0.8709	0.3310	0.079*
H9C	1.0427	0.9486	0.4260	0.079*

C10	0.9140 (2)	0.93844 (17)	0.12542 (15)	0.0534 (4)
H10A	0.8244	0.9506	0.0736	0.080*
H10B	0.9463	0.8666	0.1099	0.080*
H10C	0.9772	0.9929	0.1084	0.080*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ni1	0.02752 (13)	0.02314 (12)	0.03225 (13)	-0.00064 (8)	0.01700 (9)	0.00075 (8)
S1	0.0393 (2)	0.02794 (18)	0.0629 (2)	-0.00619 (14)	0.02443 (18)	0.00477 (16)
O1	0.0554 (7)	0.0281 (5)	0.0793 (8)	0.0016 (5)	0.0519 (6)	0.0040 (5)
O2	0.0673 (8)	0.0448 (7)	0.0892 (10)	-0.0049 (6)	0.0564 (8)	0.0112 (6)
N1	0.0276 (5)	0.0250 (5)	0.0319 (5)	0.0002 (4)	0.0125 (4)	0.0003 (4)
N2	0.0263 (5)	0.0278 (5)	0.0360 (6)	0.0008 (4)	0.0166 (4)	-0.0009 (4)
N3	0.0350 (6)	0.0362 (6)	0.0439 (6)	-0.0003 (5)	0.0238 (5)	0.0031 (5)
N4	0.0533 (9)	0.0743 (11)	0.0408 (8)	-0.0261 (8)	0.0058 (7)	0.0125 (7)
N5	0.0436 (7)	0.0299 (6)	0.0405 (7)	-0.0034 (5)	0.0091 (5)	0.0021 (5)
N6	0.1006 (14)	0.0528 (9)	0.0498 (9)	-0.0085 (9)	0.0332 (9)	0.0077 (7)
C1	0.0374 (7)	0.0253 (6)	0.0563 (9)	-0.0016 (5)	0.0136 (7)	-0.0045 (6)
C2	0.0341 (7)	0.0276 (6)	0.0392 (7)	0.0018 (5)	0.0128 (6)	-0.0042 (5)
C3	0.0244 (6)	0.0252 (6)	0.0326 (6)	-0.0015 (5)	0.0098 (5)	0.0023 (5)
C4	0.0242 (6)	0.0302 (6)	0.0300 (6)	-0.0003 (5)	0.0114 (5)	0.0021 (5)
C5	0.0307 (6)	0.0327 (7)	0.0337 (6)	0.0056 (5)	0.0145 (5)	-0.0028 (5)
C6	0.0293 (7)	0.0421 (8)	0.0339 (7)	0.0037 (6)	0.0159 (5)	-0.0027 (6)
C7	0.0550 (10)	0.0485 (10)	0.0647 (11)	0.0239 (8)	0.0300 (9)	0.0160 (8)
C8	0.0515 (10)	0.0551 (10)	0.0507 (9)	-0.0137 (8)	0.0115 (8)	-0.0167 (8)
C9	0.0299 (8)	0.0678 (12)	0.0603 (10)	0.0029 (7)	0.0095 (7)	-0.0120 (9)
C10	0.0586 (11)	0.0703 (12)	0.0397 (8)	0.0009 (9)	0.0288 (8)	-0.0049 (8)

*Geometric parameters (Å, °)*

Ni1—N1	2.0619 (11)	C2—H2A	0.9300
Ni1—N1 <sup>i</sup>	2.0619 (11)	C3—C4	1.4387 (18)
Ni1—N4 <sup>i</sup>	2.0753 (15)	C5—C7	1.523 (2)
Ni1—N4	2.0753 (15)	C5—C8	1.530 (2)
Ni1—O1	2.0831 (10)	C5—C6	1.563 (2)
Ni1—O1 <sup>i</sup>	2.0832 (10)	C6—C10	1.5243 (19)
S1—C1	1.7040 (16)	C6—C9	1.527 (2)
S1—C3	1.7204 (13)	C7—H7A	0.9600
O1—N2	1.2880 (14)	C7—H7B	0.9600
O2—N3	1.2756 (17)	C7—H7C	0.9600
N1—C3	1.3222 (16)	C8—H8A	0.9600
N1—C2	1.3669 (17)	C8—H8B	0.9600
N2—C4	1.3398 (18)	C8—H8C	0.9600
N2—C5	1.5055 (16)	C9—H9A	0.9600
N3—C4	1.3520 (16)	C9—H9B	0.9600
N3—C6	1.5047 (19)	C9—H9C	0.9600
N4—N5	1.1745 (19)	C10—H10A	0.9600

N5—N6	1.1547 (19)	C10—H10B	0.9600
C1—C2	1.351 (2)	C10—H10C	0.9600
C1—H1	0.9300		
N1—Ni1—N1 <sup>i</sup>	180.00 (5)	N2—C4—C3	127.35 (11)
N1—Ni1—N4 <sup>i</sup>	91.22 (5)	N3—C4—C3	123.63 (12)
N1 <sup>i</sup> —Ni1—N4 <sup>i</sup>	88.78 (5)	N2—C5—C7	109.04 (11)
N1—Ni1—N4	88.78 (5)	N2—C5—C8	105.60 (12)
N1 <sup>i</sup> —Ni1—N4	91.22 (5)	C7—C5—C8	109.74 (15)
N4 <sup>i</sup> —Ni1—N4	180.0	N2—C5—C6	101.18 (10)
N1—Ni1—O1	88.32 (4)	C7—C5—C6	115.82 (12)
N1 <sup>i</sup> —Ni1—O1	91.68 (4)	C8—C5—C6	114.50 (12)
N4 <sup>i</sup> —Ni1—O1	90.39 (7)	N3—C6—C10	109.03 (13)
N4—Ni1—O1	89.61 (7)	N3—C6—C9	106.66 (13)
N1—Ni1—O1 <sup>i</sup>	91.68 (4)	C10—C6—C9	109.73 (13)
N1 <sup>i</sup> —Ni1—O1 <sup>i</sup>	88.32 (4)	N3—C6—C5	101.08 (10)
N4 <sup>i</sup> —Ni1—O1 <sup>i</sup>	89.61 (7)	C10—C6—C5	115.53 (13)
N4—Ni1—O1 <sup>i</sup>	90.38 (7)	C9—C6—C5	114.01 (13)
O1—Ni1—O1 <sup>i</sup>	180.0	C5—C7—H7A	109.5
C1—S1—C3	89.29 (7)	C5—C7—H7B	109.5
N2—O1—Ni1	124.18 (8)	H7A—C7—H7B	109.5
C3—N1—C2	110.91 (11)	C5—C7—H7C	109.5
C3—N1—Ni1	125.52 (9)	H7A—C7—H7C	109.5
C2—N1—Ni1	123.11 (9)	H7B—C7—H7C	109.5
O1—N2—C4	127.15 (11)	C5—C8—H8A	109.5
O1—N2—C5	119.91 (11)	C5—C8—H8B	109.5
C4—N2—C5	112.82 (10)	H8A—C8—H8B	109.5
O2—N3—C4	123.76 (12)	C5—C8—H8C	109.5
O2—N3—C6	123.12 (11)	H8A—C8—H8C	109.5
C4—N3—C6	112.60 (11)	H8B—C8—H8C	109.5
N5—N4—Ni1	129.20 (13)	C6—C9—H9A	109.5
N6—N5—N4	178.30 (19)	C6—C9—H9B	109.5
C2—C1—S1	110.99 (11)	H9A—C9—H9B	109.5
C2—C1—H1	124.5	C6—C9—H9C	109.5
S1—C1—H1	124.5	H9A—C9—H9C	109.5
C1—C2—N1	114.84 (12)	H9B—C9—H9C	109.5
C1—C2—H2A	122.6	C6—C10—H10A	109.5
N1—C2—H2A	122.6	C6—C10—H10B	109.5
N1—C3—C4	122.97 (11)	H10A—C10—H10B	109.5
N1—C3—S1	113.94 (10)	C6—C10—H10C	109.5
C4—C3—S1	122.99 (9)	H10A—C10—H10C	109.5
N2—C4—N3	108.88 (11)	H10B—C10—H10C	109.5
N1—Ni1—O1—N2	-21.29 (12)	O1—N2—C4—N3	177.25 (14)
N1 <sup>i</sup> —Ni1—O1—N2	158.71 (12)	C5—N2—C4—N3	-6.89 (15)
N4 <sup>i</sup> —Ni1—O1—N2	69.92 (13)	O1—N2—C4—C3	1.4 (2)
N4—Ni1—O1—N2	-110.08 (13)	C5—N2—C4—C3	177.22 (13)
O1 <sup>i</sup> —Ni1—O1—N2	-114 (16)	O2—N3—C4—N2	-178.14 (14)

---

N1 <sup>i</sup> —Ni1—N1—C3	177 (16)	C6—N3—C4—N2	-6.19 (16)
N4 <sup>i</sup> —Ni1—N1—C3	-70.05 (12)	O2—N3—C4—C3	-2.1 (2)
N4—Ni1—N1—C3	109.95 (12)	C6—N3—C4—C3	169.88 (12)
O1—Ni1—N1—C3	20.30 (11)	N1—C3—C4—N2	-2.8 (2)
O1 <sup>i</sup> —Ni1—N1—C3	-159.70 (11)	S1—C3—C4—N2	173.34 (11)
N1 <sup>i</sup> —Ni1—N1—C2	-11 (16)	N1—C3—C4—N3	-178.16 (13)
N4 <sup>i</sup> —Ni1—N1—C2	101.39 (12)	S1—C3—C4—N3	-1.98 (19)
N4—Ni1—N1—C2	-78.61 (12)	O1—N2—C5—C7	-45.32 (18)
O1—Ni1—N1—C2	-168.26 (11)	C4—N2—C5—C7	138.49 (14)
O1 <sup>i</sup> —Ni1—N1—C2	11.74 (11)	O1—N2—C5—C8	72.54 (16)
Ni1—O1—N2—C4	15.2 (2)	C4—N2—C5—C8	-103.65 (14)
Ni1—O1—N2—C5	-160.42 (9)	O1—N2—C5—C6	-167.85 (12)
N1—Ni1—N4—N5	148.00 (19)	C4—N2—C5—C6	15.96 (14)
N1 <sup>i</sup> —Ni1—N4—N5	-32.00 (19)	O2—N3—C6—C10	-50.34 (19)
N4 <sup>i</sup> —Ni1—N4—N5	21 (16)	C4—N3—C6—C10	137.65 (14)
O1—Ni1—N4—N5	-123.68 (18)	O2—N3—C6—C9	68.08 (18)
O1 <sup>i</sup> —Ni1—N4—N5	56.32 (18)	C4—N3—C6—C9	-103.93 (14)
Ni1—N4—N5—N6	-172 (100)	O2—N3—C6—C5	-172.49 (14)
C3—S1—C1—C2	-0.63 (12)	C4—N3—C6—C5	15.50 (15)
S1—C1—C2—N1	-0.18 (17)	N2—C5—C6—N3	-17.26 (12)
C3—N1—C2—C1	1.19 (18)	C7—C5—C6—N3	-134.97 (13)
Ni1—N1—C2—C1	-171.36 (10)	C8—C5—C6—N3	95.77 (14)
C2—N1—C3—C4	174.82 (12)	N2—C5—C6—C10	-134.76 (13)
Ni1—N1—C3—C4	-12.85 (18)	C7—C5—C6—C10	107.53 (16)
C2—N1—C3—S1	-1.67 (15)	C8—C5—C6—C10	-21.73 (19)
Ni1—N1—C3—S1	170.66 (6)	N2—C5—C6—C9	96.76 (13)
C1—S1—C3—N1	1.34 (11)	C7—C5—C6—C9	-20.95 (18)
C1—S1—C3—C4	-175.14 (12)	C8—C5—C6—C9	-150.21 (14)

---

Symmetry code: (i)  $-x+1, -y+2, -z+1$ .