

## Azido{2-[(tri-2-pyridylmethyl)imino-methyl]phenolato}nickel(II)

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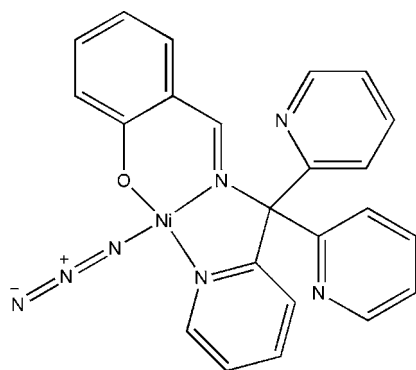
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Key indicators: single-crystal X-ray study;  $T = 295$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.047;  $wR$  factor = 0.097; data-to-parameter ratio = 12.9.

The title compound,  $[\text{Ni}(\text{C}_{23}\text{H}_{17}\text{N}_4\text{O})(\text{N}_3)]$ , was obtained by the reaction of the Schiff base ligand 2-[(tri-2-pyridylmethyl)iminomethyl]phenol with sodium azide and nickel(II) perchlorate in methanol solution. The  $\text{Ni}^{\text{II}}$  atom is four-coordinated by the phenolate O, the imine N and a pyridine N atom of the Schiff base ligand, and by the terminal N atom of an azide ligand, forming a square-planar geometry. The other two pyridyl rings are oriented at an angle of  $72.29$  ( $11$ )° to each other.

### Related literature

For related literature, see: Arnold *et al.* (2003); Borisova *et al.* (2007); Bruckner *et al.* (2000); Li & Gao (2007); Li *et al.* (2007); Mondal *et al.* (2001).



### Experimental

#### Crystal data

 $[\text{Ni}(\text{C}_{23}\text{H}_{17}\text{N}_4\text{O})(\text{N}_3)]$   
 $M_r = 466.15$ 

Monoclinic,  $P2_1/n$   
 $a = 10.7977$  (12) Å  
 $b = 14.9156$  (16) Å  
 $c = 12.7543$  (14) Å  
 $\beta = 103.044$  (2)°

 $V = 2001.1$  (4) Å<sup>3</sup>  
 $Z = 4$ 

Mo  $K\alpha$  radiation  
 $\mu = 1.00$  mm<sup>-1</sup>  
 $T = 295$  (2) K  
 $0.10 \times 0.08 \times 0.04$  mm

#### Data collection

Bruker APEX area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2002)  
 $T_{\text{min}} = 0.906$ ,  $T_{\text{max}} = 0.966$

14754 measured reflections  
 3723 independent reflections  
 2616 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.081$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$   
 $wR(F^2) = 0.097$   
 $S = 0.94$   
 3723 reflections

289 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.48$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.63$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Ni1—O1	1.815 (2)	Ni1—N2	1.850 (2)
Ni1—N1	1.887 (3)	Ni1—N3	1.898 (3)
O1—Ni1—N2	95.71 (10)	O1—Ni1—N3	87.79 (11)
O1—Ni1—N1	178.50 (11)	N2—Ni1—N3	175.69 (13)
N2—Ni1—N1	85.09 (11)	N1—Ni1—N3	91.46 (12)

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); 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: WN2208).

### References

- Arnold, P. J., Davies, S. C., Durrant, M. C., Griffiths, D. V., Hughes, D. L. & Sharpe, P. C. (2003). *Inorg. Chim. Acta*, **348**, 143–149.
- Borisova, N. E., Reshetova, M. D. & Ustynyuk, Y. A. (2007). *Chem. Rev.* **107**, 46–79.
- Bruckner, C., Rettig, S. J. & Dolphin, D. (2000). *Inorg. Chem.* **39**, 6100–6106.
- Bruker (2002). *SADABS*, *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Li, K., Huang, S.-S., Zhang, B.-J., Meng, D.-L. & Diao, Y.-P. (2007). *Acta Cryst. E* **63**, m2291.
- Li, Y.-H. & Gao, J. (2007). *Acta Cryst. E* **63**, o2291–o2292.
- Mondal, N., Mitra, S., Gramlich, V., Ghodsi, S. O. & Malik, K. M. A. (2001). *Polyhedron*, **20**, 135–141.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

**supplementary materials**

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## Azido{2-[(tri-2-pyridylmethyl)iminomethyl]phenolato}nickel(II)

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### Comment

Nickel complexes with Schiff bases have received much attention in recent years due to their pharmacological and catalytic properties (Borisova *et al.*, 2007; Bruckner *et al.*, 2000). 2-(Tri-2-pyridylmethyliminomethyl)phenol is a potential N<sub>4</sub>O pentadentate Schiff base ligand and its complexes with copper(II) have been reported (Arnold *et al.*, 2003; Li & Gao, 2007). We report here the crystal structure of the title compound (Fig. 1).

In the mononuclear nickel complex, the environment around the central nickel atom is essentially square-planar, with a maximum deviation of 0.0529 (32) Å for atom N3. Three of the coordination sites are occupied by the phenolate O1, imine N2 and pyridine N1 atoms of the Schiff base ligand and the fourth site by the terminal N atom of an azide ligand. The other two N atoms of the pyridine rings in the Schiff base are distant from the metal. The Ni1—N1 (pyridine) distance is appreciably longer than that for Ni1—N2 (imine), and the Ni—N3 (azide) distance is almost the same as that found in azido{*N*-[2-(*N,N*-diethylamino)ethyl]salicylideneiminato}nickel(II) [1.901 (2) Å] (Mondal *et al.*, 2001) and azido{2,4-dibromo-6-[(2-diethylaminoethylimino)methyl]phenolato}nickel(II) [1.897 (3) Å] (Li *et al.*, 2007).

### Experimental

2-(Tri-2-pyridylmethyliminomethyl)phenol (0.183 g, 0.5 mmol) and Ni(ClO<sub>4</sub>)<sub>2</sub>·6H<sub>2</sub>O (0.183 g, 0.5 mmol) were stirred in methanol (10 ml) for 20 min. To this solution was added a solution of NaN<sub>3</sub> (0.065 g, 1.0 mmol) in water (2 ml). The mixture was stirred for a further 10 min at room temperature, and then filtered. After keeping the filtrate in air for 3 d, brown plate crystals were formed.

### Refinement

H atoms were placed at calculated positions and refined in the riding-model approximation, with C—H = 0.93 Å and  $U_{iso}(H) = 1.2U_{eq}(C)$ .

### Figures

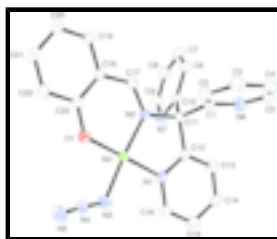


Fig. 1. The structure of the title compound, with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity.

## Azido{2-[(tri-2-pyridylmethyl)iminomethyl]phenolato}nickel(II)

### Crystal data

[Ni(C<sub>23</sub>H<sub>17</sub>N<sub>4</sub>O)(N<sub>3</sub>)]

$M_r = 466.15$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yn

$a = 10.7977$  (12) Å

$b = 14.9156$  (16) Å

$c = 12.7543$  (14) Å

$\beta = 103.044$  (2)°

$V = 2001.1$  (4) Å<sup>3</sup>

$Z = 4$

$F_{000} = 960$

$D_x = 1.547$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 2703 reflections

$\theta = 2.2$ – $25.0$ °

$\mu = 1.00$  mm<sup>-1</sup>

$T = 295$  (2) K

Plate, brown

$0.10 \times 0.08 \times 0.04$  mm

### Data collection

Bruker APEX area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 295$ (2) K

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(SADABS; Bruker, 2002)

$T_{\min} = 0.906$ ,  $T_{\max} = 0.966$

14754 measured reflections

3723 independent reflections

2616 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.081$

$\theta_{\text{max}} = 25.5$ °

$\theta_{\text{min}} = 2.2$ °

$h = -13$ → $12$

$k = -18$ → $17$

$l = -15$ → $15$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.047$

$wR(F^2) = 0.097$

$S = 0.94$

3723 reflections

289 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.48$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.63$  e Å<sup>-3</sup>

Extinction correction: none

*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  $F^2 > 2\sigma(F^2)$  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	0.82925 (4)	0.91145 (3)	0.74918 (3)	0.03162 (15)
N1	1.0057 (2)	0.93353 (17)	0.78930 (19)	0.0319 (6)
N2	0.8733 (2)	0.81489 (16)	0.67416 (19)	0.0292 (6)
N3	0.7952 (3)	1.0088 (2)	0.8344 (3)	0.0571 (9)
N4	0.6969 (3)	1.01342 (19)	0.8625 (2)	0.0430 (8)
N5	0.6054 (3)	1.0224 (2)	0.8930 (2)	0.0580 (9)
N6	1.1723 (3)	0.6869 (2)	0.7657 (2)	0.0490 (8)
N7	1.0587 (3)	0.8768 (2)	0.5391 (2)	0.0439 (7)
O1	0.6589 (2)	0.89314 (15)	0.70908 (18)	0.0417 (6)
C1	1.0501 (3)	0.7098 (2)	0.7556 (2)	0.0336 (8)
C2	0.9695 (4)	0.6632 (2)	0.8061 (3)	0.0430 (9)
H2	0.8847	0.6799	0.7963	0.052*
C3	1.0169 (4)	0.5915 (3)	0.8713 (3)	0.0540 (10)
H3	0.9639	0.5587	0.9051	0.065*
C4	1.1417 (4)	0.5694 (2)	0.8856 (3)	0.0578 (11)
H4	1.1761	0.5222	0.9306	0.069*
C5	1.2157 (4)	0.6183 (3)	0.8320 (3)	0.0586 (11)
H5	1.3011	0.6030	0.8423	0.070*
C6	1.0479 (3)	0.7177 (2)	0.5191 (3)	0.0387 (8)
H6	1.0390	0.6619	0.5492	0.046*
C7	1.0655 (3)	0.7244 (3)	0.4155 (3)	0.0509 (10)
H7	1.0661	0.6734	0.3737	0.061*
C8	1.0819 (4)	0.8081 (3)	0.3753 (3)	0.0545 (11)
H8	1.0963	0.8146	0.3065	0.065*
C9	1.0765 (4)	0.8817 (3)	0.4388 (3)	0.0556 (11)
H9	1.0858	0.9381	0.4105	0.067*
C10	1.0438 (3)	0.7951 (2)	0.5771 (2)	0.0334 (8)
C11	1.0124 (3)	0.7957 (2)	0.6893 (2)	0.0313 (7)
C12	1.0804 (3)	0.8732 (2)	0.7551 (2)	0.0311 (7)
C13	1.2115 (3)	0.8817 (2)	0.7806 (3)	0.0401 (9)
H13	1.2619	0.8394	0.7564	0.048*
C14	1.2667 (3)	0.9531 (2)	0.8417 (3)	0.0443 (9)
H14	1.3547	0.9596	0.8595	0.053*

## supplementary materials

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C15	1.1901 (3)	1.0148 (2)	0.8761 (3)	0.0451 (9)
H15	1.2254	1.0638	0.9173	0.054*
C16	1.0610 (3)	1.0032 (2)	0.8490 (3)	0.0407 (9)
H16	1.0095	1.0450	0.8728	0.049*
C17	0.7940 (3)	0.7606 (2)	0.6136 (2)	0.0324 (8)
H17	0.8282	0.7152	0.5788	0.039*
C18	0.6602 (3)	0.7650 (2)	0.5961 (2)	0.0299 (7)
C19	0.5858 (3)	0.7001 (2)	0.5293 (2)	0.0349 (8)
H19	0.6258	0.6570	0.4958	0.042*
C20	0.4565 (3)	0.6994 (2)	0.5130 (3)	0.0394 (8)
H20	0.4087	0.6560	0.4694	0.047*
C21	0.3973 (3)	0.7644 (2)	0.5625 (3)	0.0430 (9)
H21	0.3091	0.7643	0.5514	0.052*
C22	0.4660 (3)	0.8284 (2)	0.6270 (3)	0.0398 (9)
H22	0.4240	0.8711	0.6595	0.048*
C23	0.5989 (3)	0.8307 (2)	0.6451 (2)	0.0306 (7)

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ni1	0.0290 (2)	0.0333 (2)	0.0331 (2)	0.0004 (2)	0.00817 (17)	-0.0062 (2)
N1	0.0310 (15)	0.0362 (16)	0.0292 (15)	-0.0020 (13)	0.0085 (12)	-0.0003 (12)
N2	0.0279 (15)	0.0329 (15)	0.0278 (14)	0.0004 (12)	0.0084 (12)	-0.0035 (12)
N3	0.0398 (19)	0.058 (2)	0.076 (2)	-0.0026 (17)	0.0191 (18)	-0.0313 (18)
N4	0.044 (2)	0.0416 (18)	0.0398 (18)	0.0105 (16)	0.0026 (16)	-0.0104 (14)
N5	0.050 (2)	0.074 (2)	0.052 (2)	0.0180 (19)	0.0171 (17)	-0.0061 (17)
N6	0.0415 (19)	0.0527 (19)	0.0504 (19)	0.0136 (16)	0.0052 (15)	0.0003 (16)
N7	0.0504 (19)	0.0499 (19)	0.0327 (16)	-0.0009 (15)	0.0122 (14)	0.0014 (14)
O1	0.0330 (13)	0.0443 (15)	0.0483 (14)	-0.0006 (11)	0.0105 (11)	-0.0147 (11)
C1	0.036 (2)	0.037 (2)	0.0279 (18)	-0.0005 (16)	0.0066 (15)	-0.0089 (14)
C2	0.049 (2)	0.044 (2)	0.038 (2)	-0.0021 (18)	0.0119 (17)	-0.0045 (17)
C3	0.079 (3)	0.045 (2)	0.036 (2)	-0.005 (2)	0.011 (2)	0.0035 (19)
C4	0.083 (3)	0.035 (2)	0.048 (2)	0.009 (2)	-0.002 (2)	0.0028 (18)
C5	0.054 (3)	0.055 (3)	0.059 (3)	0.015 (2)	-0.004 (2)	-0.009 (2)
C6	0.033 (2)	0.050 (2)	0.036 (2)	-0.0004 (17)	0.0116 (16)	-0.0067 (16)
C7	0.040 (2)	0.074 (3)	0.040 (2)	-0.002 (2)	0.0112 (18)	-0.020 (2)
C8	0.053 (3)	0.082 (3)	0.030 (2)	-0.003 (2)	0.0112 (18)	-0.001 (2)
C9	0.062 (3)	0.067 (3)	0.039 (2)	-0.003 (2)	0.015 (2)	0.012 (2)
C10	0.0247 (18)	0.046 (2)	0.0292 (18)	-0.0002 (16)	0.0064 (14)	-0.0043 (16)
C11	0.0262 (18)	0.0382 (19)	0.0301 (18)	-0.0003 (15)	0.0077 (14)	-0.0028 (15)
C12	0.0300 (18)	0.0384 (19)	0.0258 (17)	-0.0005 (15)	0.0085 (14)	0.0009 (14)
C13	0.0321 (19)	0.050 (2)	0.043 (2)	-0.0024 (17)	0.0181 (16)	-0.0057 (17)
C14	0.030 (2)	0.056 (2)	0.045 (2)	-0.0094 (18)	0.0048 (16)	-0.0035 (19)
C15	0.042 (2)	0.045 (2)	0.047 (2)	-0.0138 (18)	0.0086 (18)	-0.0084 (17)
C16	0.046 (2)	0.037 (2)	0.039 (2)	-0.0041 (17)	0.0096 (17)	-0.0108 (16)
C17	0.0335 (19)	0.0335 (19)	0.0318 (18)	0.0014 (15)	0.0103 (15)	-0.0045 (15)
C18	0.0290 (18)	0.0352 (19)	0.0244 (16)	0.0012 (15)	0.0037 (14)	0.0044 (14)
C19	0.035 (2)	0.041 (2)	0.0277 (18)	-0.0020 (16)	0.0051 (15)	-0.0006 (15)

C20	0.037 (2)	0.045 (2)	0.0331 (19)	-0.0087 (17)	0.0019 (16)	0.0004 (16)
C21	0.0291 (19)	0.057 (2)	0.040 (2)	-0.0065 (18)	0.0025 (16)	0.0038 (18)
C22	0.031 (2)	0.051 (2)	0.040 (2)	0.0043 (17)	0.0106 (16)	-0.0003 (17)
C23	0.0303 (19)	0.0327 (19)	0.0294 (17)	-0.0007 (15)	0.0082 (14)	0.0030 (15)

*Geometric parameters (Å, °)*

Ni1—O1	1.815 (2)	C7—C8	1.376 (5)
Ni1—N1	1.887 (3)	C7—H7	0.9300
Ni1—N2	1.850 (2)	C8—C9	1.373 (5)
Ni1—N3	1.898 (3)	C8—H8	0.9300
N1—C12	1.345 (4)	C9—H9	0.9300
N1—C16	1.345 (4)	C10—C11	1.543 (4)
N2—C17	1.298 (4)	C11—C12	1.517 (4)
N2—C11	1.498 (4)	C12—C13	1.385 (4)
N3—N4	1.197 (4)	C13—C14	1.374 (4)
N4—N5	1.148 (4)	C13—H13	0.9300
N6—C1	1.340 (4)	C14—C15	1.374 (5)
N6—C5	1.343 (5)	C14—H14	0.9300
N7—C10	1.335 (4)	C15—C16	1.370 (4)
N7—C9	1.339 (4)	C15—H15	0.9300
O1—C23	1.309 (3)	C16—H16	0.9300
C1—C2	1.382 (4)	C17—C18	1.413 (4)
C1—C11	1.540 (4)	C17—H17	0.9300
C2—C3	1.380 (5)	C18—C23	1.407 (4)
C2—H2	0.9300	C18—C19	1.414 (4)
C3—C4	1.360 (5)	C19—C20	1.364 (4)
C3—H3	0.9300	C19—H19	0.9300
C4—C5	1.373 (5)	C20—C21	1.390 (5)
C4—H4	0.9300	C20—H20	0.9300
C5—H5	0.9300	C21—C22	1.366 (4)
C6—C10	1.377 (4)	C21—H21	0.9300
C6—C7	1.381 (4)	C22—C23	1.401 (4)
C6—H6	0.9300	C22—H22	0.9300
O1—Ni1—N2	95.71 (10)	N7—C10—C11	113.6 (3)
O1—Ni1—N1	178.50 (11)	C6—C10—C11	122.9 (3)
N2—Ni1—N1	85.09 (11)	N2—C11—C12	105.8 (2)
O1—Ni1—N3	87.79 (11)	N2—C11—C1	111.3 (2)
N2—Ni1—N3	175.69 (13)	C12—C11—C1	107.1 (2)
N1—Ni1—N3	91.46 (12)	N2—C11—C10	107.8 (2)
C12—N1—C16	118.6 (3)	C12—C11—C10	109.7 (3)
C12—N1—Ni1	116.0 (2)	C1—C11—C10	114.7 (3)
C16—N1—Ni1	125.4 (2)	N1—C12—C13	121.3 (3)
C17—N2—C11	117.7 (3)	N1—C12—C11	116.0 (3)
C17—N2—Ni1	125.6 (2)	C13—C12—C11	122.8 (3)
C11—N2—Ni1	116.70 (19)	C14—C13—C12	119.6 (3)
N4—N3—Ni1	121.0 (2)	C14—C13—H13	120.2
N5—N4—N3	175.9 (4)	C12—C13—H13	120.2
C1—N6—C5	116.8 (3)	C13—C14—C15	119.0 (3)

## supplementary materials

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C10—N7—C9	116.9 (3)	C13—C14—H14	120.5
C23—O1—Ni1	127.6 (2)	C15—C14—H14	120.5
N6—C1—C2	122.5 (3)	C16—C15—C14	119.1 (3)
N6—C1—C11	113.4 (3)	C16—C15—H15	120.5
C2—C1—C11	123.9 (3)	C14—C15—H15	120.5
C3—C2—C1	118.9 (4)	N1—C16—C15	122.5 (3)
C3—C2—H2	120.5	N1—C16—H16	118.8
C1—C2—H2	120.5	C15—C16—H16	118.8
C4—C3—C2	119.4 (4)	N2—C17—C18	125.3 (3)
C4—C3—H3	120.3	N2—C17—H17	117.3
C2—C3—H3	120.3	C18—C17—H17	117.3
C3—C4—C5	118.3 (4)	C23—C18—C17	122.0 (3)
C3—C4—H4	120.8	C23—C18—C19	119.0 (3)
C5—C4—H4	120.8	C17—C18—C19	119.0 (3)
N6—C5—C4	124.0 (4)	C20—C19—C18	121.3 (3)
N6—C5—H5	118.0	C20—C19—H19	119.3
C4—C5—H5	118.0	C18—C19—H19	119.3
C10—C6—C7	118.8 (3)	C19—C20—C21	119.1 (3)
C10—C6—H6	120.6	C19—C20—H20	120.5
C7—C6—H6	120.6	C21—C20—H20	120.5
C8—C7—C6	118.6 (3)	C22—C21—C20	121.2 (3)
C8—C7—H7	120.7	C22—C21—H21	119.4
C6—C7—H7	120.7	C20—C21—H21	119.4
C9—C8—C7	118.7 (3)	C21—C22—C23	120.9 (3)
C9—C8—H8	120.7	C21—C22—H22	119.6
C7—C8—H8	120.7	C23—C22—H22	119.6
N7—C9—C8	123.7 (4)	O1—C23—C22	117.7 (3)
N7—C9—H9	118.2	O1—C23—C18	123.8 (3)
C8—C9—H9	118.2	C22—C23—C18	118.5 (3)
N7—C10—C6	123.3 (3)		
N2—Ni1—N1—C12	-3.4 (2)	N7—C10—C11—N2	80.5 (3)
N3—Ni1—N1—C12	174.0 (2)	C6—C10—C11—N2	-95.5 (3)
N2—Ni1—N1—C16	177.2 (3)	N7—C10—C11—C12	-34.3 (4)
N3—Ni1—N1—C16	-5.4 (3)	C6—C10—C11—C12	149.7 (3)
O1—Ni1—N2—C17	1.9 (3)	N7—C10—C11—C1	-154.9 (3)
N1—Ni1—N2—C17	-176.8 (3)	C6—C10—C11—C1	29.1 (4)
O1—Ni1—N2—C11	-175.1 (2)	C16—N1—C12—C13	0.2 (4)
N1—Ni1—N2—C11	6.2 (2)	Ni1—N1—C12—C13	-179.2 (2)
O1—Ni1—N3—N4	21.3 (3)	C16—N1—C12—C11	179.3 (3)
N1—Ni1—N3—N4	-160.0 (3)	Ni1—N1—C12—C11	-0.1 (3)
N2—Ni1—O1—C23	-1.5 (3)	N2—C11—C12—N1	4.5 (3)
N3—Ni1—O1—C23	-179.0 (3)	C1—C11—C12—N1	-114.3 (3)
C5—N6—C1—C2	-3.0 (5)	C10—C11—C12—N1	120.6 (3)
C5—N6—C1—C11	173.1 (3)	N2—C11—C12—C13	-176.4 (3)
N6—C1—C2—C3	1.4 (5)	C1—C11—C12—C13	64.8 (4)
C11—C1—C2—C3	-174.3 (3)	C10—C11—C12—C13	-60.3 (4)
C1—C2—C3—C4	1.0 (5)	N1—C12—C13—C14	-0.1 (5)
C2—C3—C4—C5	-1.6 (5)	C11—C12—C13—C14	-179.2 (3)
C1—N6—C5—C4	2.5 (5)	C12—C13—C14—C15	-0.1 (5)



C3—C4—C5—N6	-0.2 (6)	C13—C14—C15—C16	0.3 (5)
C10—C6—C7—C8	1.9 (5)	C12—N1—C16—C15	0.0 (5)
C6—C7—C8—C9	-1.8 (6)	Ni1—N1—C16—C15	179.4 (2)
C10—N7—C9—C8	-0.9 (5)	C14—C15—C16—N1	-0.3 (5)
C7—C8—C9—N7	1.4 (6)	C11—N2—C17—C18	175.7 (3)
C9—N7—C10—C6	1.0 (5)	Ni1—N2—C17—C18	-1.3 (4)
C9—N7—C10—C11	-175.0 (3)	N2—C17—C18—C23	-0.3 (5)
C7—C6—C10—N7	-1.5 (5)	N2—C17—C18—C19	-178.9 (3)
C7—C6—C10—C11	174.1 (3)	C23—C18—C19—C20	-1.0 (4)
C17—N2—C11—C12	175.5 (2)	C17—C18—C19—C20	177.6 (3)
Ni1—N2—C11—C12	-7.3 (3)	C18—C19—C20—C21	0.6 (5)
C17—N2—C11—C1	-68.4 (3)	C19—C20—C21—C22	-0.2 (5)
Ni1—N2—C11—C1	108.8 (2)	C20—C21—C22—C23	0.3 (5)
C17—N2—C11—C10	58.2 (3)	Ni1—O1—C23—C22	178.8 (2)
Ni1—N2—C11—C10	-124.6 (2)	Ni1—O1—C23—C18	0.5 (4)
N6—C1—C11—N2	176.2 (2)	C21—C22—C23—O1	-179.0 (3)
C2—C1—C11—N2	-7.8 (4)	C21—C22—C23—C18	-0.7 (5)
N6—C1—C11—C12	-68.6 (3)	C17—C18—C23—O1	0.7 (5)
C2—C1—C11—C12	107.5 (3)	C19—C18—C23—O1	179.3 (3)
N6—C1—C11—C10	53.4 (3)	C17—C18—C23—C22	-177.5 (3)
C2—C1—C11—C10	-130.5 (3)	C19—C18—C23—C22	1.0 (4)

