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# Bis(2,2'-bipyridine- $\kappa^2N,N'$ )(croconato- $\kappa^2O,O'$ )nickel(II)

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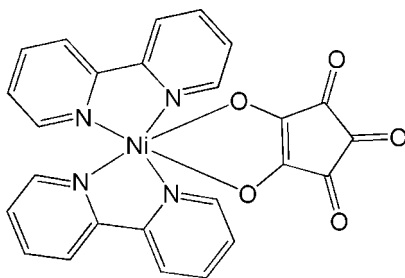
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 Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(C-C) = 0.004$  Å;  $R$  factor = 0.044;  $wR$  factor = 0.102; data-to-parameter ratio = 15.4.

The title compound,  $[Ni(C_5O_5)(C_{10}H_8N_2)_2]$ , lies across a crystallographic twofold axis, around which two 2,2'-bipyridine (2,2'-bipy) ligands are arranged in a propeller manner. The local geometry of the  $NiN_4O_2$  coordination core basically adopts an octahedral geometry. The molecular twofold axis is along the direction of the molecular dipole moment, and the complex is packed with its dipole moment alternately along the  $+b$  and  $-b$  directions. The crystal structure is stabilized by intermolecular  $C-H \cdots O$  hydrogen bonds.

## Related literature

For the synthesis, see: Chen *et al.* (2008). For related structures, see: Chen *et al.* (2005, 2007). For other related literature, see: Coronado *et al.* (2007); Wang *et al.* (2002).



## Experimental

### Crystal data

 $[Ni(C_5O_5)(C_{10}H_8N_2)_2]$   
 $M_r = 511.13$ 

 Orthorhombic,  $Pbcn$   
 $a = 12.725$  (5) Å

 $b = 10.752$  (5) Å  
 $c = 15.733$  (5) Å  
 $V = 2152.6$  (15) Å<sup>3</sup>  
 $Z = 4$ 

 Mo  $K\alpha$  radiation  
 $\mu = 0.95$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 $0.20 \times 0.19 \times 0.10$  mm

### Data collection

 Bruker APEXII CCD diffractometer  
 Absorption correction: multi-scan (*APEX2*; Bruker, 2005)  
 $T_{min} = 0.821$ ,  $T_{max} = 0.902$ 

 10055 measured reflections  
 2466 independent reflections  
 1536 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.089$ 

### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.044$   
 $wR(F^2) = 0.102$   
 $S = 1.02$   
 2466 reflections

 160 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{max} = 0.26$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.38$  e Å<sup>-3</sup>

**Table 1**  
Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$C4-H4 \cdots O1^i$	0.93	2.57	3.340 (4)	141
$C8-H8 \cdots O2^{ii}$	0.93	2.24	3.114 (4)	156
$C9-H9 \cdots O3^{iii}$	0.93	2.57	3.222 (4)	127

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; 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: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2071).

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## supporting information

*Acta Cryst.* (2008). E64, m1459 [doi:10.1107/S1600536808033771]

**Bis(2,2'-bipyridine- $\kappa^2N,N'$ )(croconato- $\kappa^2O,O'$ )nickel(II)****Hong-Feng Chen, Qi Fang and Wen-Tao Yu****S1. Comment**

The croconate  $C_5O_5^{2-}$  anion has attracted increasing attention in recent years because this polydentate ligand gave rise to a variety of interesting complexes (Chen *et al.*, 2008; Coronado *et al.*, 2007; Chen *et al.*, 2005; Wang *et al.*, 2002;). Typically, the  $C_5O_5^{2-}$  anion serves as a terminal bidentate chelate ligand or a bridging ligand utilizing more than two O atoms for coordination. We previously reported a mixing-coordinated complex  $[Ni(C_5O_5)(phen)_2]$  with 1,10-phenanthroline (phen) as the first ligand and the  $C_5O_5^{2-}$  anion as the second ligand (Chen *et al.*, 2007). The similar chelating behavior of 2,2'-bipy and 1,10-phen prompted us to replace phen ligand by 2,2'-bipy. In this report, the structure of this mixing-coordinated complex is reported.

The title compound crystallizes to the same space group as  $[Ni(C_5O_5)(phen)_2]$ . Both crystals have very similar cell parameters and show many common features. The chiral molecule lies across twofold axis which is along the direction of the molecular dipole moment. Around the molecular axis, two 2,2'-bipy ligands are arranged in a propeller manner. The  $Ni^{2+}$  is coordinated by four N atoms of the two 2,2'-bipy ligands and two O atoms of a croconate ligand to furnish a slightly distorted octahedral  $NiN_4O_2$  coordination core. The dihedral angle between the croconate plane and a 2,2'-bipy plane is  $88.7(1)^\circ$ , and that between the two 2,2'-bipy planes is  $81.9(1)^\circ$  in  $[Ni(C_5O_5)(2,2'-bipy)_2]$ . These are close to the corresponding dihedral angles ( $86.9(1)^\circ$  and  $86.6(1)^\circ$ ) in  $[Ni(C_5O_5)(phen)_2]$ . The C—O bond lengths involving coordinated O atoms are longer than those of other C—O bonds. In both crystals, molecules packed alternately along +b and -b directions.

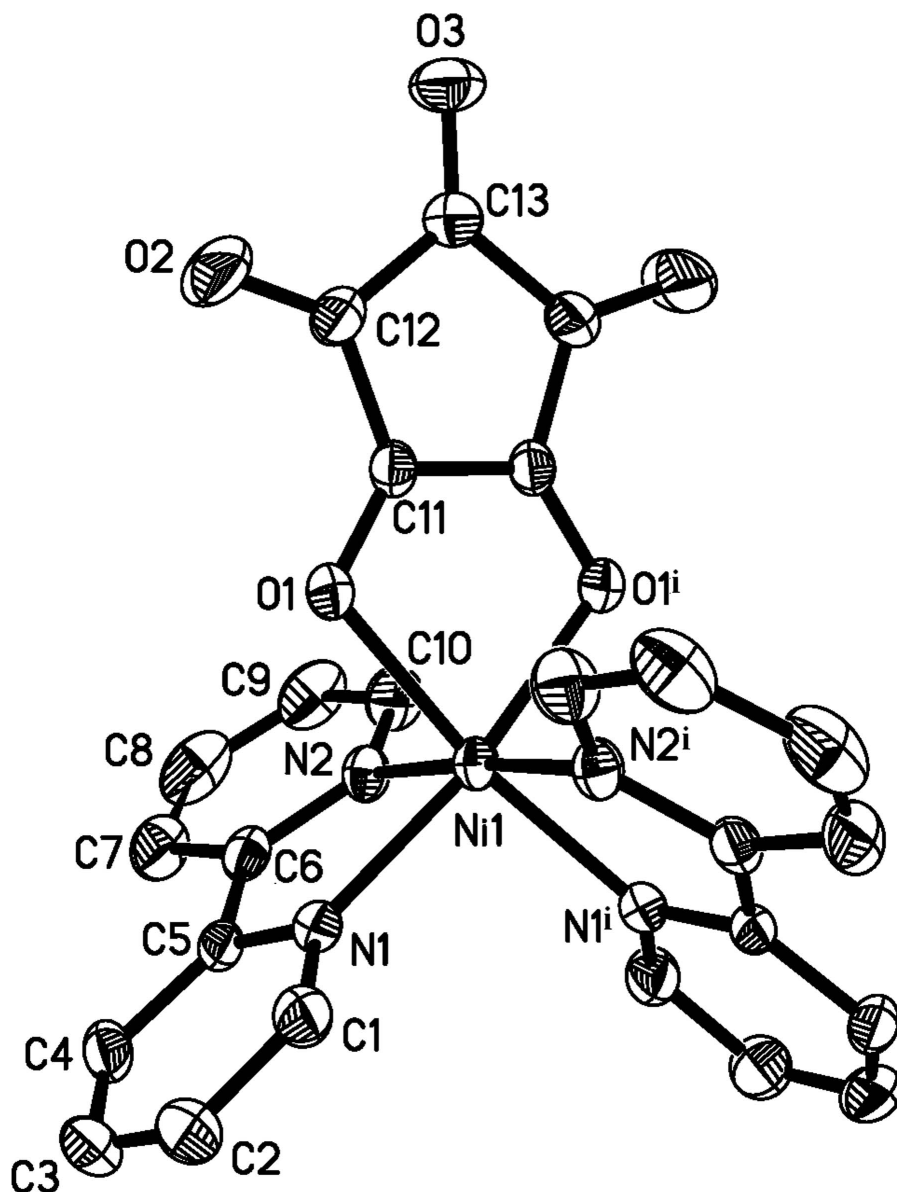
However, we can not fail to notice some differences between the two crystals. The Ni—O bond length of  $[Ni(C_5O_5)(2,2'-bipy)_2]$  {2.102 (2) Å} is longer than that {2.098 (3) Å} of  $[Ni(C_5O_5)(phen)_2]$ . Meanwhile, the Ni—N bond lengths of  $[Ni(C_5O_5)(2,2'-bipy)_2]$  {2.059 (2), 2.066 (2) Å} is considerably shorter than those {2.071 (3), 2.088 (3) Å} of  $[Ni(C_5O_5)(phen)_2]$ . It seems that 2,2'-bipyridine is a stronger ligand to  $Ni^{2+}$  in comparison with 1,10-phenanthroline. The crystal structure is stabilized by intermolecular C—H $\cdots$ O hydrogen bonds (Table 1).

**S2. Experimental**

$[K_2(C_5O_5)]$  (0.050 g, 0.23 mmol) and  $NiCl_2 \cdot 6H_2O$  (0.060 g, 0.25 mmol) were dissolved in mixed solvent of water (15 ml) and dimethylformamide (10 ml). Then 2,2'-bipy (0.080 g, 0.51 mmol) was added. The mixture was heated to 340–350 K under continuous stirring for 20 min and then filtered. The green-yellow prisms crystals were obtained by slow evaporation at 313 K.

**S3. Refinement**

All H atoms were positioned geometrically and allowed to ride on their attached atom. The C—H bond lengths for aromatic groups were set to 0.93 Å.



**Figure 1**

The molecular structure of  $[\text{Ni}(\text{C}_5\text{O}_5)(2,2'\text{-bipy})_2]$ . Displacement ellipsoids are drawn at the 30% probability level and H atoms have been omitted. [symmetry code: (i)  $-x + 1, y, -z + 3/2.$ ]

**Bis(2,2'-bipyridine- $\kappa^2\text{N},\text{N}'$ )(croconato- $\kappa^2\text{O},\text{O}'$ )nickel(II)**

*Crystal data*

$[\text{Ni}(\text{C}_5\text{O}_5)(\text{C}_{10}\text{H}_8\text{N}_2)_2]$

$M_r = 511.13$

Orthorhombic, *Pbcn*

Hall symbol:  $-\text{P } 2_n 2ab$

$a = 12.725 (5) \text{ \AA}$

$b = 10.752 (5) \text{ \AA}$

$c = 15.733 (5) \text{ \AA}$

$V = 2152.6 (15) \text{ \AA}^3$

$Z = 4$

$F(000) = 1048$

$D_x = 1.577 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71069 \text{ \AA}$

Cell parameters from 2518 reflections

$\theta = 2.5\text{--}23.4^\circ$

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

$T = 293 \text{ K}$

Prism, green-yellow

$0.20 \times 0.19 \times 0.10 \text{ mm}$

*Data collection*

Bruker APEXII CCD diffractometer	10055 measured reflections
Radiation source: fine-focus sealed tube	2466 independent reflections
Graphite monochromator	1536 reflections with $I > 2\sigma(I)$
Detector resolution: 10.0 pixels $\text{mm}^{-1}$	$R_{\text{int}} = 0.089$
$\varphi$ and $\omega$ scans	$\theta_{\text{max}} = 27.5^\circ$ , $\theta_{\text{min}} = 2.5^\circ$
Absorption correction: multi-scan (APEX2; Bruker, 2005)	$h = -15 \rightarrow 16$
$T_{\text{min}} = 0.821$ , $T_{\text{max}} = 0.902$	$k = -13 \rightarrow 10$
	$l = -20 \rightarrow 19$

*Refinement*

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.044$	H-atom parameters constrained
$wR(F^2) = 0.102$	$w = 1/[\sigma^2(F_o^2) + (0.0372P)^2 + 0.0108P]$
$S = 1.02$	where $P = (F_o^2 + 2F_c^2)/3$
2466 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
160 parameters	$\Delta\rho_{\text{max}} = 0.26 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.38 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

*Special details*

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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	0.5000	0.46011 (4)	0.2500	0.03546 (17)
O1	0.56048 (15)	0.31353 (15)	0.17633 (10)	0.0439 (5)
O2	0.6016 (2)	0.0512 (2)	0.12408 (16)	0.1053 (10)
O3	0.5000	-0.1097 (3)	0.2500	0.0700 (9)
N1	0.45364 (18)	0.58822 (19)	0.34037 (12)	0.0397 (5)
N2	0.63184 (17)	0.46676 (19)	0.32573 (12)	0.0419 (6)
C1	0.3650 (3)	0.6535 (3)	0.34092 (17)	0.0531 (8)
H1	0.3173	0.6410	0.2970	0.064*
C2	0.3402 (3)	0.7384 (3)	0.4029 (2)	0.0717 (10)
H2	0.2774	0.7824	0.4013	0.086*
C3	0.4114 (4)	0.7561 (3)	0.4673 (2)	0.0742 (11)
H3	0.3977	0.8142	0.5097	0.089*
C4	0.5025 (3)	0.6888 (3)	0.46926 (18)	0.0570 (9)
H4	0.5502	0.6989	0.5135	0.068*
C5	0.5226 (2)	0.6052 (2)	0.40425 (15)	0.0406 (7)
C6	0.6200 (2)	0.5320 (2)	0.39824 (16)	0.0431 (7)

C7	0.6964 (3)	0.5264 (3)	0.4613 (2)	0.0638 (9)
H7	0.6872	0.5696	0.5119	0.077*
C8	0.7854 (3)	0.4569 (4)	0.4486 (2)	0.0770 (12)
H8	0.8367	0.4526	0.4906	0.092*
C9	0.7982 (2)	0.3940 (3)	0.3737 (2)	0.0679 (10)
H9	0.8587	0.3479	0.3633	0.081*
C10	0.7195 (2)	0.4008 (3)	0.31437 (19)	0.0575 (8)
H10	0.7276	0.3572	0.2637	0.069*
C11	0.5300 (2)	0.2129 (3)	0.21214 (15)	0.0393 (6)
C12	0.5511 (3)	0.0864 (3)	0.18605 (18)	0.0530 (8)
C13	0.5000	0.0035 (4)	0.2500	0.0487 (10)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ni1	0.0404 (3)	0.0388 (3)	0.0271 (2)	0.000	-0.0053 (2)	0.000
O1	0.0587 (13)	0.0418 (11)	0.0310 (9)	-0.0040 (10)	0.0083 (9)	0.0013 (8)
O2	0.167 (3)	0.0586 (15)	0.0903 (17)	-0.0026 (15)	0.0769 (19)	-0.0177 (13)
O3	0.086 (2)	0.0405 (17)	0.084 (2)	0.000	0.0118 (18)	0.000
N1	0.0510 (14)	0.0360 (12)	0.0322 (11)	-0.0008 (12)	-0.0020 (11)	0.0015 (10)
N2	0.0437 (14)	0.0480 (14)	0.0340 (12)	0.0003 (12)	-0.0082 (10)	0.0017 (10)
C1	0.064 (2)	0.0507 (18)	0.0443 (16)	0.0138 (17)	0.0003 (16)	0.0011 (14)
C2	0.098 (3)	0.057 (2)	0.060 (2)	0.024 (2)	0.022 (2)	-0.0018 (17)
C3	0.119 (3)	0.048 (2)	0.056 (2)	-0.002 (2)	0.028 (2)	-0.0121 (16)
C4	0.084 (2)	0.0514 (17)	0.0359 (15)	-0.022 (2)	0.0095 (16)	-0.0076 (13)
C5	0.0582 (19)	0.0341 (14)	0.0295 (13)	-0.0130 (14)	0.0012 (12)	0.0026 (11)
C6	0.0535 (18)	0.0442 (16)	0.0317 (14)	-0.0198 (15)	-0.0080 (13)	0.0070 (13)
C7	0.076 (2)	0.068 (2)	0.0482 (18)	-0.023 (2)	-0.0272 (17)	0.0038 (15)
C8	0.065 (2)	0.090 (3)	0.076 (3)	-0.023 (2)	-0.041 (2)	0.033 (2)
C9	0.0442 (18)	0.080 (3)	0.079 (2)	0.0036 (19)	-0.0144 (18)	0.026 (2)
C10	0.0494 (19)	0.067 (2)	0.0555 (19)	0.0078 (18)	-0.0081 (15)	0.0055 (16)
C11	0.0431 (17)	0.0439 (16)	0.0309 (13)	-0.0025 (14)	-0.0005 (11)	-0.0019 (12)
C12	0.066 (2)	0.0462 (17)	0.0463 (17)	-0.0038 (17)	0.0129 (16)	-0.0085 (14)
C13	0.052 (2)	0.042 (2)	0.052 (2)	0.000	0.000 (2)	0.000

*Geometric parameters (Å, °)*

Ni1—N2	2.059 (2)	C3—C4	1.367 (4)
Ni1—N2 <sup>i</sup>	2.059 (2)	C3—H3	0.9300
Ni1—N1	2.066 (2)	C4—C5	1.385 (4)
Ni1—N1 <sup>i</sup>	2.066 (2)	C4—H4	0.9300
Ni1—O1 <sup>i</sup>	2.1022 (18)	C5—C6	1.472 (4)
Ni1—O1	2.1022 (18)	C6—C7	1.389 (4)
O1—C11	1.280 (3)	C7—C8	1.371 (5)
O2—C12	1.227 (3)	C7—H7	0.9300
O3—C13	1.217 (5)	C8—C9	1.369 (5)
N1—C1	1.328 (3)	C8—H8	0.9300
N1—C5	1.347 (3)	C9—C10	1.370 (4)

N2—C10	1.334 (3)	C9—H9	0.9300
N2—C6	1.347 (3)	C10—H10	0.9300
C1—C2	1.372 (4)	C11—C11 <sup>i</sup>	1.415 (5)
C1—H1	0.9300	C11—C12	1.446 (4)
C2—C3	1.373 (5)	C12—C13	1.493 (4)
C2—H2	0.9300	C13—C12 <sup>i</sup>	1.493 (4)
N2—Ni1—N2 <sup>i</sup>	176.02 (12)	C3—C4—C5	118.9 (3)
N2—Ni1—N1	79.12 (9)	C3—C4—H4	120.6
N2 <sup>i</sup> —Ni1—N1	98.19 (8)	C5—C4—H4	120.6
N2—Ni1—N1 <sup>i</sup>	98.19 (8)	N1—C5—C4	121.3 (3)
N2 <sup>i</sup> —Ni1—N1 <sup>i</sup>	79.12 (9)	N1—C5—C6	115.4 (2)
N1—Ni1—N1 <sup>i</sup>	96.35 (11)	C4—C5—C6	123.3 (3)
N2—Ni1—O1 <sup>i</sup>	90.30 (8)	N2—C6—C7	120.2 (3)
N2 <sup>i</sup> —Ni1—O1 <sup>i</sup>	92.68 (8)	N2—C6—C5	115.3 (2)
N1—Ni1—O1 <sup>i</sup>	90.91 (8)	C7—C6—C5	124.5 (3)
N1 <sup>i</sup> —Ni1—O1 <sup>i</sup>	169.72 (7)	C8—C7—C6	119.8 (3)
N2—Ni1—O1	92.68 (8)	C8—C7—H7	120.1
N2 <sup>i</sup> —Ni1—O1	90.30 (8)	C6—C7—H7	120.1
N1—Ni1—O1	169.72 (7)	C9—C8—C7	119.5 (3)
N1 <sup>i</sup> —Ni1—O1	90.91 (8)	C9—C8—H8	120.2
O1 <sup>i</sup> —Ni1—O1	82.88 (10)	C7—C8—H8	120.2
C11—O1—Ni1	106.29 (15)	C8—C9—C10	118.2 (3)
C1—N1—C5	118.5 (2)	C8—C9—H9	120.9
C1—N1—Ni1	126.82 (19)	C10—C9—H9	120.9
C5—N1—Ni1	114.72 (18)	N2—C10—C9	123.2 (3)
C10—N2—C6	118.9 (2)	N2—C10—H10	118.4
C10—N2—Ni1	125.83 (19)	C9—C10—H10	118.4
C6—N2—Ni1	114.66 (19)	O1—C11—C11 <sup>i</sup>	122.26 (14)
N1—C1—C2	123.5 (3)	O1—C11—C12	127.9 (2)
N1—C1—H1	118.3	C11 <sup>i</sup> —C11—C12	109.83 (15)
C2—C1—H1	118.3	O2—C12—C11	127.8 (3)
C1—C2—C3	117.7 (3)	O2—C12—C13	125.4 (3)
C1—C2—H2	121.1	C11—C12—C13	106.8 (2)
C3—C2—H2	121.1	O3—C13—C12 <sup>i</sup>	126.64 (17)
C4—C3—C2	120.2 (3)	O3—C13—C12	126.64 (17)
C4—C3—H3	119.9	C12 <sup>i</sup> —C13—C12	106.7 (3)
C2—C3—H3	119.9		
N2—Ni1—O1—C11	90.49 (17)	C1—N1—C5—C6	-178.6 (2)
N2 <sup>i</sup> —Ni1—O1—C11	-92.14 (18)	Ni1—N1—C5—C6	1.2 (3)
N1—Ni1—O1—C11	53.7 (5)	C3—C4—C5—N1	-1.0 (4)
N1 <sup>i</sup> —Ni1—O1—C11	-171.27 (17)	C3—C4—C5—C6	177.3 (3)
O1 <sup>i</sup> —Ni1—O1—C11	0.52 (13)	C10—N2—C6—C7	-2.5 (4)
N2—Ni1—N1—C1	174.7 (2)	Ni1—N2—C6—C7	169.1 (2)
N2 <sup>i</sup> —Ni1—N1—C1	-2.3 (2)	C10—N2—C6—C5	178.1 (2)
N1 <sup>i</sup> —Ni1—N1—C1	77.5 (2)	Ni1—N2—C6—C5	-10.3 (3)
O1 <sup>i</sup> —Ni1—N1—C1	-95.2 (2)	N1—C5—C6—N2	6.1 (3)

O1—Ni1—N1—C1	-147.8 (4)	C4—C5—C6—N2	-172.3 (2)
N2—Ni1—N1—C5	-5.04 (17)	N1—C5—C6—C7	-173.3 (2)
N2 <sup>i</sup> —Ni1—N1—C5	177.93 (18)	C4—C5—C6—C7	8.3 (4)
N1 <sup>i</sup> —Ni1—N1—C5	-102.20 (19)	N2—C6—C7—C8	1.8 (4)
O1 <sup>i</sup> —Ni1—N1—C5	85.09 (18)	C5—C6—C7—C8	-178.8 (3)
O1—Ni1—N1—C5	32.5 (5)	C6—C7—C8—C9	0.2 (5)
N1—Ni1—N2—C10	179.3 (2)	C7—C8—C9—C10	-1.5 (5)
N1 <sup>i</sup> —Ni1—N2—C10	-85.7 (2)	C6—N2—C10—C9	1.2 (4)
O1 <sup>i</sup> —Ni1—N2—C10	88.5 (2)	Ni1—N2—C10—C9	-169.4 (2)
O1—Ni1—N2—C10	5.6 (2)	C8—C9—C10—N2	0.8 (5)
N1—Ni1—N2—C6	8.43 (17)	Ni1—O1—C11—C11 <sup>i</sup>	-1.5 (4)
N1 <sup>i</sup> —Ni1—N2—C6	103.37 (17)	Ni1—O1—C11—C12	-179.9 (2)
O1 <sup>i</sup> —Ni1—N2—C6	-82.44 (17)	O1—C11—C12—O2	-0.7 (5)
O1—Ni1—N2—C6	-165.32 (17)	C11 <sup>i</sup> —C11—C12—O2	-179.3 (3)
C5—N1—C1—C2	0.6 (4)	O1—C11—C12—C13	178.9 (2)
Ni1—N1—C1—C2	-179.1 (2)	C11 <sup>i</sup> —C11—C12—C13	0.3 (4)
N1—C1—C2—C3	0.1 (5)	O2—C12—C13—O3	-0.6 (4)
C1—C2—C3—C4	-1.2 (5)	C11—C12—C13—O3	179.89 (13)
C2—C3—C4—C5	1.7 (5)	O2—C12—C13—C12 <sup>i</sup>	179.4 (4)
C1—N1—C5—C4	-0.1 (4)	C11—C12—C13—C12 <sup>i</sup>	-0.11 (13)
Ni1—N1—C5—C4	179.63 (19)		

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

*Hydrogen-bond geometry (Å, °)*

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
C4—H4...O1 <sup>ii</sup>	0.93	2.57	3.340 (4)	141
C8—H8...O2 <sup>iii</sup>	0.93	2.24	3.114 (4)	156
C9—H9...O3 <sup>iv</sup>	0.93	2.57	3.222 (4)	127

Symmetry codes: (ii)  $x, -y+1, z+1/2$ ; (iii)  $-x+3/2, -y+1/2, z+1/2$ ; (iv)  $x+1/2, y+1/2, -z+1/2$ .