

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Bis(acetato- κ O)bis(pyridine-2-aldoxime- κ^2 N,N')nickel(II)

Youtao Si

Universite de Europeenne de Bretagne, Universite de Bretagne Occidentale, CS 93837, 29238 Brest Cedex 3, France
Correspondence e-mail: siyoutao@hotmail.com

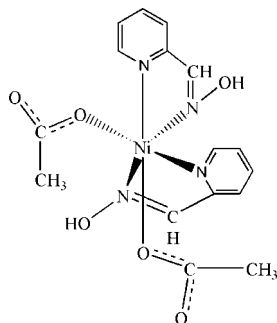
Received 26 March 2012; accepted 3 April 2012

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.044; wR factor = 0.113; data-to-parameter ratio = 17.2.

In the mononuclear title compound, $[\text{Ni}(\text{CH}_3\text{COO})_2(\text{C}_6\text{H}_6\text{N}_2\text{O})_2]$, the Ni^{II} atom is coordinated by two pyridine-2-aldoxime (PaoH) ligands and two acetate groups, with *cis* coordination for the pairs of identical ligands. While each acetate group binds to the Ni^{II} atom by one O atom, each PaoH chelates the Ni^{II} atom through two N atoms. The O atom on PaoH is not deprotonated and does not participate in bonding to the Ni^{II} atom. Thus, the Ni^{II} atom exhibits an octahedral environment. Intramolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen-bonding interactions and intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen-bonding interactions are present in the structure. Adjacent molecules pack along $[100]$ through van der Waals forces.

Related literature

For $[\text{Ni}(\text{PaoH})_2\text{Cl}_2]$, see: Krause & Busch (1960); Miyasaka *et al.* (2004).



Experimental

Crystal data

 $[\text{Ni}(\text{C}_2\text{H}_3\text{O}_2)_2(\text{C}_6\text{H}_6\text{N}_2\text{O})_2]$ $M_r = 421.05$

Monoclinic, $P2_1/c$
 $a = 8.649$ (4) Å
 $b = 13.707$ (7) Å
 $c = 17.775$ (7) Å
 $\beta = 119.051$ (17)°
 $V = 1842.1$ (15) Å³

$Z = 4$
Mo $K\alpha$ radiation
 $\mu = 1.09$ mm⁻¹
 $T = 293$ K
 $0.20 \times 0.20 \times 0.20$ mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan
(*CrystalClear*; Rigaku, 2007)
 $T_{\text{min}} = 0.809$, $T_{\text{max}} = 1.000$

14112 measured reflections
4207 independent reflections
3298 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.035$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.113$
 $S = 1.08$
4207 reflections

244 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.35$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.37$ e Å⁻³

Table 1

Selected bond lengths (Å).

Ni1—O4	2.059 (2)	Ni1—N2	2.084 (2)
Ni1—O6	2.061 (2)	Ni1—N1	2.096 (2)
Ni1—N4	2.081 (2)	Ni1—N3	2.122 (2)

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O1—H1A \cdots O3	0.82	1.67	2.488 (4)	176
O2—H2A \cdots O5	0.82	1.65	2.463 (3)	173
C3—H3A \cdots O2'	0.93	2.43	3.307 (4)	157

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

Data collection: *CrystalClear* (Rigaku, 2007); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *WinGX* (Farrugia, 1999); software used to prepare material for publication: *pubCIF* (Westrip, 2010).

We thank the Centre Nationale de la Recherche Scientifique (CNRS) and the Université de Bretagne Occidentale (UBO) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RU2032).

References

- Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Krause, R. A. & Busch, D. H. (1960). *J. Am. Chem. Soc.* **82**, 4830–4834.
Miyasaka, H., Furukawa, S., Yanagida, S., Sugiura, K. & Yamashita, M. (2004). *Inorg. Chim. Acta*, **357**, 1619–1626.
Rigaku (2007). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supplementary materials

Acta Cryst. (2012). E68, m554 [doi:10.1107/S1600536812014377]

Bis(acetato- κ O)bis(pyridine-2-aldoxime- κ^2 N,N')nickel(II)

Youtao Si

Comment

Ni(PaoH)₂Cl₂ is a good coordination donor building for assembly with transition metal ions, like Mn²⁺. The reaction of Ni(PaoH)₂Cl₂ and Mn(OAc)₂·4H₂O afforded, unexpectedly, the title compound, in which AcO⁻ is substituted for Cl⁻.

Cis coordination fashion was found for the identical ligands. The average Ni—N bond length is 2.095 (18) Å, and the average Fe—O bond length is 2.060 (1) Å. The O atoms on PaoH remain protonated, and intramolecular O—H···O hydrogen-bonds are present, with the acceptor O atom from acetate.

Experimental

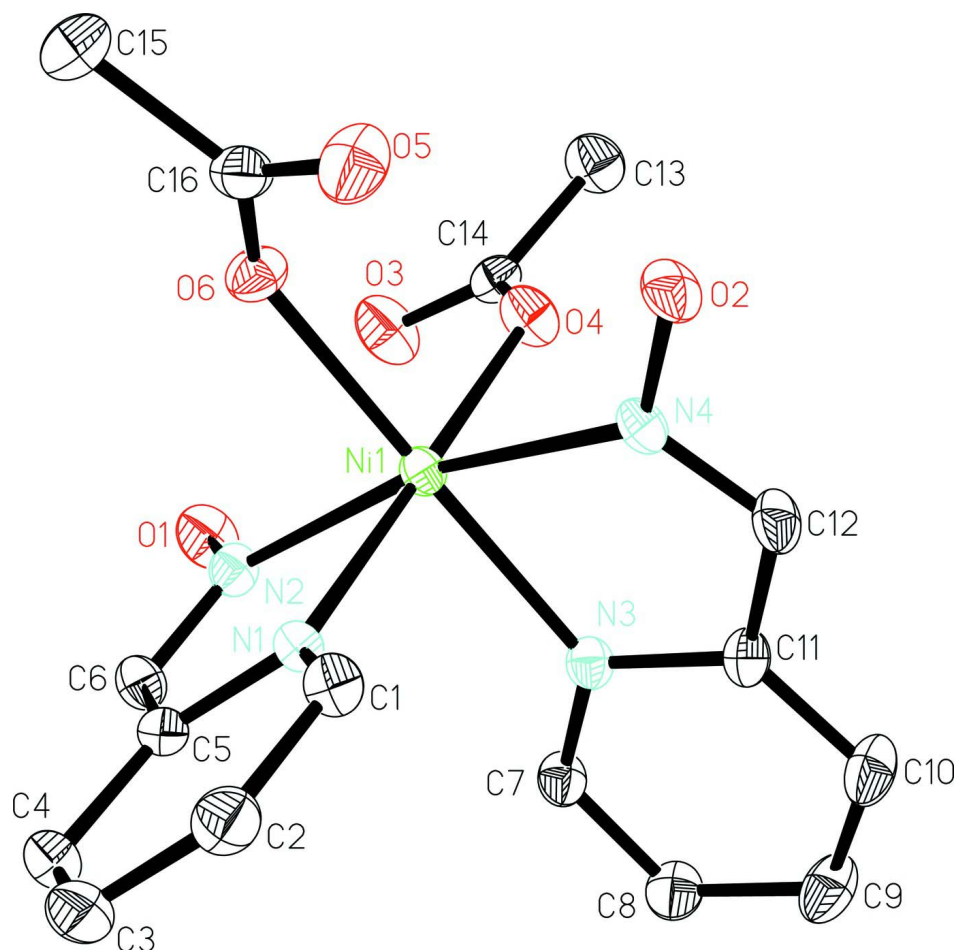
Ni(PaoH)₂Cl₂ (0.19 g, 0.5 mmol) and Mn(OAc)₂·4H₂O (0.24 g, 1 mmol) were dissolved in DMF (1 mL) and MeOH (15 mL), then the mixture was stirred for 1 h, followed by filtration. After standing in air for 3 days, well shaped light purple crystals were obtained from the solution.

Refinement

Hydrogen atoms were placed at idealized positions and allowed to ride on their parent atoms, with OH, CH and CH₃ bonds set equal to 0.82, 0.93 and 0.96 Å, respectively. For H atoms of CH₃, $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$. For other H atoms, $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C or O})$. The highest residual peak was located at 0.70 Å from H15C.

Computing details

Data collection: *CrystalClear* (Rigaku, 2007); cell refinement: *CrystalClear* (Rigaku, 2007); data reduction: *CrystalClear* (Rigaku, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *WinGX* (Farrugia, 1999); software used to prepare material for publication: *publCIF* (Westrip, 2010).


Figure 1

The molecular structure of the title compound, with atom labels and 20% probability displacement ellipsoids for all non-H atoms (H atoms omitted).

Bis(acetato- κ O)bis(pyridine-2-aldoxime- κ^2 N,N')nickel(II)
Crystal data

$[\text{Ni}(\text{C}_2\text{H}_3\text{O}_2)_2(\text{C}_6\text{H}_6\text{N}_2\text{O})_2]$

$M_r = 421.05$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 8.649\ (4)\ \text{\AA}$

$b = 13.707\ (7)\ \text{\AA}$

$c = 17.775\ (7)\ \text{\AA}$

$\beta = 119.051\ (17)^\circ$

$V = 1842.1\ (15)\ \text{\AA}^3$

$Z = 4$

$F(000) = 872$

$D_x = 1.518\ \text{Mg m}^{-3}$

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

Cell parameters from 1810 reflections

$\theta = 2.7\text{--}27.5^\circ$

$\mu = 1.09\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Prism, light purple

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

Data collection

Rigaku Mercury2
diffractometer

Radiation source: fine-focus sealed tube
Graphite monochromator

Detector resolution: $13.6612\ \text{pixels mm}^{-1}$

CCD_Profile_fitting scans

Absorption correction: multi-scan
(*CrystalClear*; Rigaku, 2007)

$T_{\min} = 0.809$, $T_{\max} = 1.000$
 14112 measured reflections
 4207 independent reflections
 3298 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.035$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 2.6^\circ$
 $h = -9 \rightarrow 11$
 $k = -16 \rightarrow 17$
 $l = -23 \rightarrow 23$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.113$
 $S = 1.08$
 4207 reflections
 244 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
 $w = 1/[\sigma^2(F_o^2) + (0.0526P)^2 + 0.2764P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.35 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.37 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.00171 (4)	0.80019 (2)	0.15100 (2)	0.03476 (13)
O3	0.3495 (3)	0.88769 (19)	0.33957 (15)	0.0740 (7)
O5	-0.4089 (3)	0.87646 (17)	0.10176 (16)	0.0686 (7)
O6	-0.1317 (2)	0.92515 (14)	0.14997 (13)	0.0499 (5)
O1	0.3372 (3)	0.92561 (17)	0.19987 (14)	0.0627 (6)
H1A	0.3453	0.9146	0.2470	0.094*
O4	0.1120 (3)	0.79396 (15)	0.28287 (12)	0.0531 (5)
O2	-0.3346 (2)	0.70350 (14)	0.13957 (13)	0.0493 (5)
H2A	-0.3671	0.7602	0.1271	0.074*
N3	0.1359 (3)	0.67005 (16)	0.15232 (14)	0.0391 (5)
N2	0.1841 (3)	0.88691 (16)	0.13709 (15)	0.0408 (5)
N1	-0.1082 (3)	0.80866 (15)	0.01696 (14)	0.0370 (5)
N4	-0.1728 (3)	0.69206 (16)	0.14512 (14)	0.0385 (5)
C15	-0.3523 (4)	1.0447 (2)	0.1205 (2)	0.0618 (8)
H15A	-0.4773	1.0458	0.1004	0.093*
H15B	-0.3272	1.0807	0.0813	0.093*
H15C	-0.2909	1.0738	0.1766	0.093*
C3	-0.2199 (5)	0.8366 (3)	-0.1565 (2)	0.0603 (8)
H3A	-0.2570	0.8451	-0.2147	0.072*
C16	-0.2919 (4)	0.9406 (2)	0.12523 (19)	0.0482 (7)
C7	0.2866 (3)	0.6588 (2)	0.14993 (18)	0.0443 (6)

H7A	0.3472	0.7145	0.1490	0.053*
C4	-0.0615 (4)	0.8770 (2)	-0.0945 (2)	0.0558 (8)
H4A	0.0081	0.9139	-0.1104	0.067*
C11	0.0493 (3)	0.5883 (2)	0.15438 (18)	0.0428 (6)
C2	-0.3204 (4)	0.7842 (2)	-0.1307 (2)	0.0547 (8)
H2B	-0.4277	0.7574	-0.1711	0.066*
C14	0.2413 (4)	0.8323 (2)	0.34460 (18)	0.0436 (6)
C1	-0.2604 (3)	0.7717 (2)	-0.04356 (18)	0.0450 (6)
H1B	-0.3294	0.7358	-0.0266	0.054*
C13	0.2694 (4)	0.8122 (2)	0.4337 (2)	0.0619 (9)
H13A	0.1793	0.7685	0.4302	0.093*
H13B	0.2633	0.8723	0.4599	0.093*
H13C	0.3835	0.7829	0.4679	0.093*
C5	-0.0093 (4)	0.86133 (19)	-0.00854 (18)	0.0413 (6)
C12	-0.1192 (4)	0.6044 (2)	0.15257 (19)	0.0478 (7)
H12A	-0.1846	0.5528	0.1567	0.057*
C6	0.1540 (4)	0.9011 (2)	0.06049 (19)	0.0463 (7)
H6A	0.2330	0.9355	0.0491	0.056*
C9	0.2713 (4)	0.4870 (2)	0.1523 (2)	0.0652 (9)
H9A	0.3170	0.4256	0.1522	0.078*
C8	0.3571 (4)	0.5693 (2)	0.1487 (2)	0.0549 (8)
H8A	0.4611	0.5648	0.1456	0.066*
C10	0.1161 (4)	0.4964 (2)	0.1560 (2)	0.0607 (9)
H10A	0.0572	0.4413	0.1595	0.073*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.03189 (19)	0.0365 (2)	0.0371 (2)	-0.00362 (13)	0.01775 (15)	0.00059 (14)
O3	0.0659 (14)	0.0939 (19)	0.0554 (14)	-0.0353 (14)	0.0241 (11)	-0.0081 (13)
O5	0.0434 (12)	0.0570 (14)	0.1006 (19)	0.0026 (10)	0.0311 (12)	0.0034 (13)
O6	0.0412 (10)	0.0474 (11)	0.0631 (13)	0.0031 (8)	0.0270 (9)	-0.0046 (10)
O1	0.0501 (12)	0.0747 (15)	0.0596 (14)	-0.0285 (11)	0.0237 (10)	-0.0104 (11)
O4	0.0481 (11)	0.0691 (14)	0.0347 (11)	-0.0148 (10)	0.0142 (9)	-0.0021 (9)
O2	0.0356 (10)	0.0568 (13)	0.0626 (13)	-0.0030 (8)	0.0294 (9)	0.0071 (10)
N3	0.0350 (11)	0.0385 (12)	0.0424 (13)	-0.0019 (9)	0.0177 (9)	0.0026 (10)
N2	0.0339 (11)	0.0389 (12)	0.0492 (14)	-0.0081 (9)	0.0197 (10)	-0.0029 (10)
N1	0.0394 (11)	0.0374 (12)	0.0374 (12)	-0.0007 (9)	0.0212 (9)	0.0016 (9)
N4	0.0326 (11)	0.0460 (13)	0.0390 (12)	-0.0071 (9)	0.0190 (9)	0.0030 (10)
C15	0.0566 (18)	0.0544 (19)	0.069 (2)	0.0126 (15)	0.0265 (16)	-0.0026 (16)
C3	0.078 (2)	0.064 (2)	0.0404 (17)	0.0078 (17)	0.0296 (16)	0.0033 (15)
C16	0.0484 (16)	0.0555 (18)	0.0450 (16)	0.0083 (14)	0.0262 (13)	0.0021 (13)
C7	0.0359 (13)	0.0438 (15)	0.0555 (18)	0.0003 (12)	0.0239 (12)	0.0057 (13)
C4	0.074 (2)	0.0536 (19)	0.0545 (19)	0.0053 (15)	0.0422 (17)	0.0089 (15)
C11	0.0411 (14)	0.0374 (14)	0.0460 (16)	-0.0049 (11)	0.0181 (12)	0.0027 (12)
C2	0.0577 (18)	0.0531 (18)	0.0430 (17)	0.0019 (14)	0.0163 (14)	-0.0033 (14)
C14	0.0427 (14)	0.0414 (15)	0.0425 (16)	0.0054 (12)	0.0174 (12)	-0.0025 (12)
C1	0.0414 (14)	0.0475 (16)	0.0422 (16)	-0.0017 (12)	0.0173 (12)	0.0017 (13)
C13	0.064 (2)	0.073 (2)	0.0407 (17)	-0.0059 (16)	0.0194 (15)	-0.0016 (15)
C5	0.0504 (15)	0.0373 (14)	0.0450 (16)	0.0023 (12)	0.0301 (13)	0.0005 (12)

C12	0.0435 (15)	0.0425 (16)	0.0609 (19)	-0.0096 (12)	0.0280 (13)	0.0055 (13)
C6	0.0483 (15)	0.0457 (16)	0.0550 (18)	-0.0081 (12)	0.0331 (14)	0.0019 (13)
C9	0.0530 (18)	0.0430 (17)	0.093 (3)	0.0070 (14)	0.0307 (18)	-0.0010 (17)
C8	0.0417 (15)	0.0550 (18)	0.071 (2)	0.0072 (13)	0.0297 (15)	0.0049 (16)
C10	0.0506 (17)	0.0384 (16)	0.089 (3)	-0.0057 (13)	0.0307 (17)	-0.0003 (16)

Geometric parameters (Å, °)

Ni1—O4	2.059 (2)	C3—C2	1.367 (5)
Ni1—O6	2.061 (2)	C3—C4	1.390 (5)
Ni1—N4	2.081 (2)	C3—H3A	0.9300
Ni1—N2	2.084 (2)	C7—C8	1.375 (4)
Ni1—N1	2.096 (2)	C7—H7A	0.9300
Ni1—N3	2.122 (2)	C4—C5	1.383 (4)
O3—C14	1.241 (3)	C4—H4A	0.9300
O5—C16	1.249 (4)	C11—C10	1.380 (4)
O6—C16	1.252 (3)	C11—C12	1.459 (4)
O1—N2	1.358 (3)	C2—C1	1.384 (4)
O1—H1A	0.8200	C2—H2B	0.9300
O4—C14	1.241 (3)	C14—C13	1.507 (4)
O2—N4	1.364 (3)	C1—H1B	0.9300
O2—H2A	0.8200	C13—H13A	0.9600
N3—C7	1.333 (3)	C13—H13B	0.9600
N3—C11	1.358 (3)	C13—H13C	0.9600
N2—C6	1.271 (3)	C5—C6	1.454 (4)
N1—C1	1.331 (3)	C12—H12A	0.9300
N1—C5	1.355 (3)	C6—H6A	0.9300
N4—C12	1.272 (3)	C9—C8	1.368 (4)
C15—C16	1.507 (4)	C9—C10	1.381 (4)
C15—H15A	0.9600	C9—H9A	0.9300
C15—H15B	0.9600	C8—H8A	0.9300
C15—H15C	0.9600	C10—H10A	0.9300
O4—Ni1—O6	89.56 (9)	N3—C7—C8	123.4 (3)
O4—Ni1—N4	87.21 (8)	N3—C7—H7A	118.3
O6—Ni1—N4	101.66 (9)	C8—C7—H7A	118.3
O4—Ni1—N2	101.53 (8)	C5—C4—C3	118.8 (3)
O6—Ni1—N2	88.73 (9)	C5—C4—H4A	120.6
N4—Ni1—N2	166.55 (9)	C3—C4—H4A	120.6
O4—Ni1—N1	179.06 (8)	N3—C11—C10	121.5 (3)
O6—Ni1—N1	90.05 (8)	N3—C11—C12	115.7 (2)
N4—Ni1—N1	93.71 (8)	C10—C11—C12	122.8 (3)
N2—Ni1—N1	77.60 (9)	C3—C2—C1	119.1 (3)
O4—Ni1—N3	90.23 (9)	C3—C2—H2B	120.4
O6—Ni1—N3	179.02 (8)	C1—C2—H2B	120.4
N4—Ni1—N3	77.37 (9)	O4—C14—O3	125.7 (3)
N2—Ni1—N3	92.24 (9)	O4—C14—C13	117.9 (3)
N1—Ni1—N3	90.17 (8)	O3—C14—C13	116.4 (3)
C16—O6—Ni1	131.6 (2)	N1—C1—C2	122.9 (3)
N2—O1—H1A	109.5	N1—C1—H1B	118.5

C14—O4—Ni1	135.2 (2)	C2—C1—H1B	118.5
N4—O2—H2A	109.5	C14—C13—H13A	109.5
C7—N3—C11	117.8 (2)	C14—C13—H13B	109.5
C7—N3—Ni1	129.37 (19)	H13A—C13—H13B	109.5
C11—N3—Ni1	112.80 (17)	C14—C13—H13C	109.5
C6—N2—O1	115.6 (2)	H13A—C13—H13C	109.5
C6—N2—Ni1	116.18 (18)	H13B—C13—H13C	109.5
O1—N2—Ni1	128.13 (18)	N1—C5—C4	122.1 (3)
C1—N1—C5	118.0 (2)	N1—C5—C6	115.5 (2)
C1—N1—Ni1	128.49 (18)	C4—C5—C6	122.4 (3)
C5—N1—Ni1	113.46 (17)	N4—C12—C11	117.0 (2)
C12—N4—O2	115.2 (2)	N4—C12—H12A	121.5
C12—N4—Ni1	116.72 (18)	C11—C12—H12A	121.5
O2—N4—Ni1	127.99 (16)	N2—C6—C5	117.2 (2)
C16—C15—H15A	109.5	N2—C6—H6A	121.4
C16—C15—H15B	109.5	C5—C6—H6A	121.4
H15A—C15—H15B	109.5	C8—C9—C10	119.1 (3)
C16—C15—H15C	109.5	C8—C9—H9A	120.4
H15A—C15—H15C	109.5	C10—C9—H9A	120.4
H15B—C15—H15C	109.5	C9—C8—C7	118.7 (3)
C2—C3—C4	119.0 (3)	C9—C8—H8A	120.6
C2—C3—H3A	120.5	C7—C8—H8A	120.6
C4—C3—H3A	120.5	C11—C10—C9	119.4 (3)
O5—C16—O6	125.2 (3)	C11—C10—H10A	120.3
O5—C16—C15	116.4 (3)	C9—C10—H10A	120.3
O6—C16—C15	118.3 (3)		
O4—Ni1—O6—C16	-108.2 (3)	N2—Ni1—N4—C12	46.2 (5)
N4—Ni1—O6—C16	-21.1 (3)	N1—Ni1—N4—C12	95.3 (2)
N2—Ni1—O6—C16	150.2 (3)	N3—Ni1—N4—C12	6.0 (2)
N1—Ni1—O6—C16	72.6 (3)	O4—Ni1—N4—O2	90.6 (2)
N3—Ni1—O6—C16	-30 (5)	O6—Ni1—N4—O2	1.7 (2)
O6—Ni1—O4—C14	-83.6 (3)	N2—Ni1—N4—O2	-138.3 (3)
N4—Ni1—O4—C14	174.7 (3)	N1—Ni1—N4—O2	-89.1 (2)
N2—Ni1—O4—C14	5.0 (3)	N3—Ni1—N4—O2	-178.5 (2)
N1—Ni1—O4—C14	-18 (5)	Ni1—O6—C16—O5	7.5 (5)
N3—Ni1—O4—C14	97.3 (3)	Ni1—O6—C16—C15	-170.6 (2)
O4—Ni1—N3—C7	-98.1 (2)	C11—N3—C7—C8	0.6 (4)
O6—Ni1—N3—C7	-176 (100)	Ni1—N3—C7—C8	-178.1 (2)
N4—Ni1—N3—C7	174.8 (3)	C2—C3—C4—C5	1.1 (5)
N2—Ni1—N3—C7	3.4 (2)	C7—N3—C11—C10	1.5 (4)
N1—Ni1—N3—C7	81.0 (2)	Ni1—N3—C11—C10	-179.7 (2)
O4—Ni1—N3—C11	83.15 (19)	C7—N3—C11—C12	-177.0 (2)
O6—Ni1—N3—C11	5 (5)	Ni1—N3—C11—C12	1.8 (3)
N4—Ni1—N3—C11	-3.93 (17)	C4—C3—C2—C1	-1.0 (5)
N2—Ni1—N3—C11	-175.29 (19)	Ni1—O4—C14—O3	-2.7 (5)
N1—Ni1—N3—C11	-97.69 (19)	Ni1—O4—C14—C13	176.1 (2)
O4—Ni1—N2—C6	177.5 (2)	C5—N1—C1—C2	0.4 (4)
O6—Ni1—N2—C6	-93.2 (2)	Ni1—N1—C1—C2	178.6 (2)

N4—Ni1—N2—C6	47.8 (5)	C3—C2—C1—N1	0.2 (5)
N1—Ni1—N2—C6	-2.9 (2)	C1—N1—C5—C4	-0.2 (4)
N3—Ni1—N2—C6	86.8 (2)	Ni1—N1—C5—C4	-178.6 (2)
O4—Ni1—N2—O1	1.8 (2)	C1—N1—C5—C6	179.1 (2)
O6—Ni1—N2—O1	91.1 (2)	Ni1—N1—C5—C6	0.6 (3)
N4—Ni1—N2—O1	-128.0 (4)	C3—C4—C5—N1	-0.6 (4)
N1—Ni1—N2—O1	-178.6 (2)	C3—C4—C5—C6	-179.8 (3)
N3—Ni1—N2—O1	-88.9 (2)	O2—N4—C12—C11	177.0 (2)
O4—Ni1—N1—C1	-154 (5)	Ni1—N4—C12—C11	-6.9 (3)
O6—Ni1—N1—C1	-88.5 (2)	N3—C11—C12—N4	3.3 (4)
N4—Ni1—N1—C1	13.2 (2)	C10—C11—C12—N4	-175.2 (3)
N2—Ni1—N1—C1	-177.2 (2)	O1—N2—C6—C5	-179.6 (2)
N3—Ni1—N1—C1	90.6 (2)	Ni1—N2—C6—C5	4.1 (3)
O4—Ni1—N1—C5	24 (5)	N1—C5—C6—N2	-3.2 (4)
O6—Ni1—N1—C5	89.74 (18)	C4—C5—C6—N2	176.1 (3)
N4—Ni1—N1—C5	-168.57 (18)	C10—C9—C8—C7	0.7 (5)
N2—Ni1—N1—C5	1.04 (17)	N3—C7—C8—C9	-1.7 (5)
N3—Ni1—N1—C5	-91.21 (18)	N3—C11—C10—C9	-2.3 (5)
O4—Ni1—N4—C12	-84.9 (2)	C12—C11—C10—C9	176.1 (3)
O6—Ni1—N4—C12	-173.8 (2)	C8—C9—C10—C11	1.2 (5)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1—H1A \cdots O3	0.82	1.67	2.488 (4)	176
O2—H2A \cdots O5	0.82	1.65	2.463 (3)	173
C3—H3A \cdots O2 ⁱ	0.93	2.43	3.307 (4)	157

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