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# Bis(acetato-$\kappa O$)bis(pyridine-2-aldoxime-$\kappa^2 N,N'$)nickel(II)

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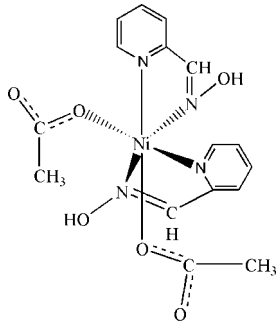
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.044; $wR$ factor = 0.113; data-to-parameter ratio = 17.2.

In the mononuclear title compound, $[Ni(CH_3COO)_2(C_6H_6N_2O)_2]$, 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 O—H···O hydrogen-bonding interactions and intermolecular C—H···O hydrogen-bonding interactions are present in the structure. Adjacent molecules pack along [100] through van der Waals forces.

## Related literature

For $[Ni(PaoH)_2Cl_2]$, see: Krause & Busch (1960); Miyasaka *et al.* (2004).



## Experimental

### Crystal data

$[Ni(C_2H_3O_2)_2(C_6H_6N_2O)_2]$ $M_r$ = 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) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.09 mm$^{-1}$
$T$ = 293 K
0.20 × 0.20 × 0.20 mm

### Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2007)
$T_{min}$ = 0.809, $T_{max}$ = 1.000
14112 measured reflections
4207 independent reflections
3298 reflections with $I > 2\sigma(I)$
$R_{int}$ = 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
$\Delta\rho_{max}$ = 0.35 e Å$^{-3}$
$\Delta\rho_{min}$ = −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, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1$A$···O3 | 0.82 | 1.67 | 2.488 (4) | 176 |
| O2—H2$A$···O5 | 0.82 | 1.65 | 2.463 (3) | 173 |
| C3—H3$A$···O2$^{i}$ | 0.93 | 2.43 | 3.307 (4) | 157 |

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

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: *publCIF* (Westrip, 2010).

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

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# supporting information

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## Bis(acetato-$\kappa O$)bis(pyridine-2-aldoxime-$\kappa^2 N,N'$)nickel(II)

**Youtao Si**

### S1. Comment

$Ni(PaoH)_2Cl_2$ is a good coordination donor building for assembly with transition metal ions, like $Mn^{2+}$. The reaction of $Ni(PaoH)_2Cl_2$ and $Mn(OAc)_2.4H_2O$ 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.

### S2. Experimental

$Ni(PaoH)_2Cl_2$ (0.19 g, 0.5 mmol) and $Mn(OAc)_2.4H_2O$ (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.

### S3. Refinement

Hydrogen atoms were placed at idealized positions and allowed to ride on their parent atoms, with OH, CH and $CH_3$ bonds set equal to 0.82, 0.93 and 0.96 Å, respectively. For H atoms of $CH_3$, $U_{iso}(H) = 1.5U_{eq}(C)$. For other H atoms, $U_{iso}(H) = 1.2U_{eq}$(C or O). The highest residual peak was located at 0.70 Å from H15C.

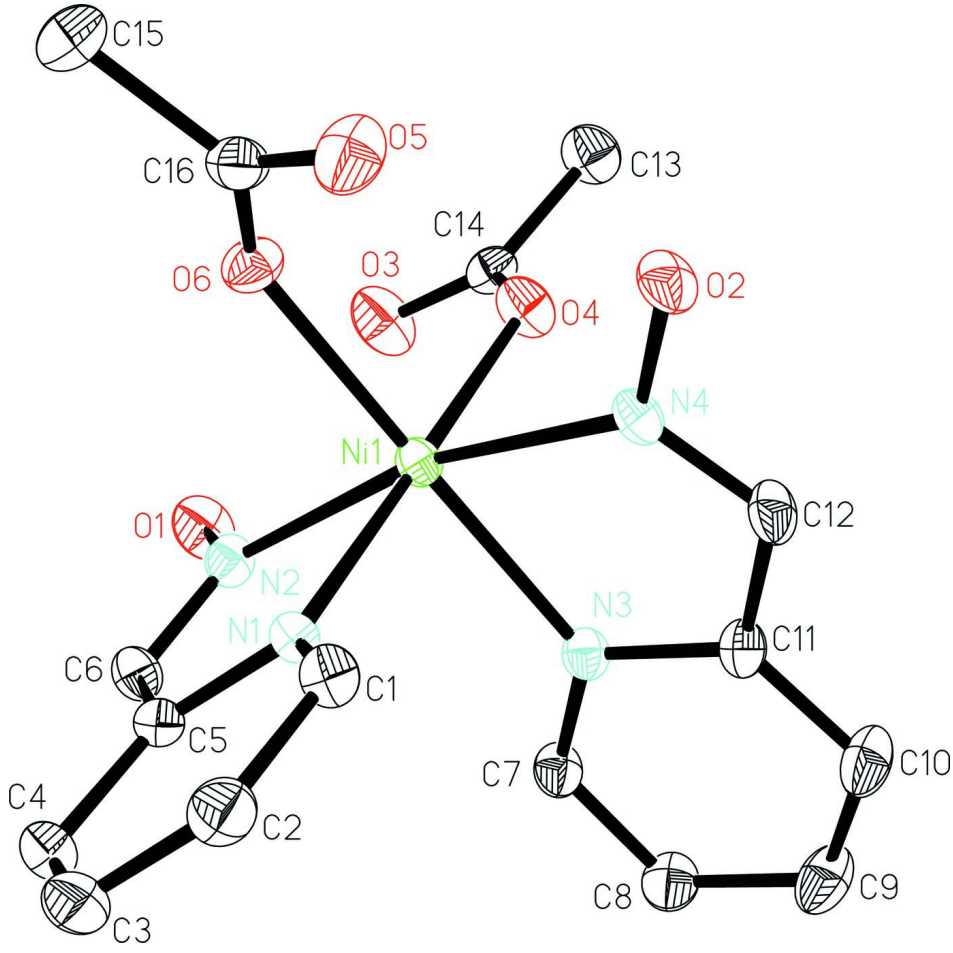


**Figure 1**

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-*κO*)bis(pyridine-2-aldoxime- $\kappa^2N,N'$)nickel(II)**

*Crystal data*

$[Ni(C_2H_3O_2)_2(C_6H_6N_2O)_2]$
$M_r$ = 421.05
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 8.649 (4) Å
$b$ = 13.707 (7) Å
$c$ = 17.775 (7) Å
$\beta$ = 119.051 (17)°
$V$ = 1842.1 (15) Å$^3$
$Z$ = 4
$F(000)$ = 872
$D_x$ = 1.518 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 1810 reflections
$\theta$ = 2.7–27.5°
$\mu$ = 1.09 mm$^{-1}$
$T$ = 293 K
Prism, light purple
0.20 × 0.20 × 0.20 mm

*Data collection*

Rigaku Mercury2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 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 $I > 2\sigma(I)$
$R_{int}$ = 0.035

$\theta_{max}$ = 27.5°, $\theta_{min}$ = 2.6°
$h$ = −9→11
$k$ = −16→17
$l$ = −23→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 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.37 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.

**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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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) | | |

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| 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) |

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| 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, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1*A*···O3 | 0.82 | 1.67 | 2.488 (4) | 176 |
| O2—H2*A*···O5 | 0.82 | 1.65 | 2.463 (3) | 173 |
| C3—H3*A*···O2$^{i}$ | 0.93 | 2.43 | 3.307 (4) | 157 |

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