Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{6,6′-Diethoxy-2,2′-[4,5-dimethyl-*o*-phenylenebis(nitrilomethylidyne)]diphenolato}nickel(II) dihydrate

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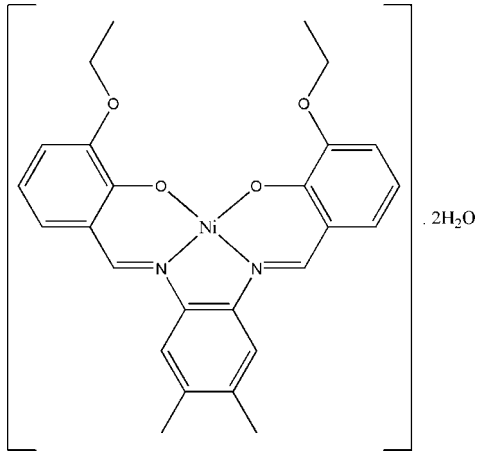
Received 12 March 2009; accepted 3 April 2009

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.122; data-to-parameter ratio = 21.8.

In the title complex, $[Ni(C_{26}H_{26}N_2O_4)]\cdot 2H_2O$, the Ni^{II} ion, lying on a twofold crystallographic rotation axis, has a square-planar geometry, being coordinated by the N_2O_2 unit of the tetradentate Schiff base ligand. The asymmetric unit of the title compound comprises one-half of the complex molecule and one of the water molecules of crystallization. The water H atoms form bifurcated O—H···(O,O) hydrogen bonds with the O atoms of the phenolato and ethoxy groups with $R_1^2(5)$ and $R_1^2(6)$ ring motifs. The dihedral angle between the central benzene ring and the two outer benzene rings are 4.07 (11) and 3.99 (12)°. The dihedral angle between the two O–Ni–N coordination planes is only 0.77 (11)°. In the crystal structure, the molecules are linked together into extended chains along the c axis by intermolecular O—H···O and C—H···O interactions. An interesting feature of the crystal structure is a short intermolecular C ··· C [3.355 (3) Å] contact, which is shorter than the sum of the van der Waals radii. The crystal structure may be further stabilized by intermolecular π–π interactions [centroid–centroid distances in the range 3.5758 (13)–3.6337 (13) Å].

Related literature

For bond-length data, see Allen *et al.* (1987). For related structures see, for example: Clark *et al.* (1968, 1969, 1970). For the applications and bioactivity of Schiff base complexes see, for example: Elmali *et al.* (2000); Blower (1998); Granovski *et al.* (1993); Li & Chang, (1991); Shahrokhian *et al.* (2000). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$[Ni(C_{26}H_{26}N_2O_4)]\cdot 2H_2O$
M_r = 525.23
Orthorhombic, *Pbcn*
a = 12.8706 (4) Å
b = 16.1130 (4) Å
c = 11.8546 (3) Å
V = 2458.45 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.83 mm^{-1}
T = 294 K
0.30 × 0.16 × 0.08 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.790, T_{max} = 0.935
16330 measured reflections
3517 independent reflections
2007 reflections with $I > 2\sigma I$)
R_{int} = 0.065

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.122
S = 1.01
3517 reflections
161 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—O1	1.8447 (15)	Ni1—N1	1.8573 (17)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W1···O1	0.82	2.50	3.087 (2)	129
O1W—H1W1···O2	0.82	2.39	3.145 (3)	152
O1W—H2W1···O1^{i}	0.82	2.47	3.083 (3)	133
O1W—H2W1···O2^{i}	0.82	2.41	3.121 (3)	146
C7—H7A···O1W^{ii}	0.93	2.57	3.383 (3)	146

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used

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to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

HKF and RK thank the Malaysian Government and Universiti Sains Malaysia for the Science Fund grant No. 305/PFIZIK/613312. RK thanks Universiti Sains Malaysia for a post-doctoral research fellowship. HK and AJ thank PNU for financial support. HKF also thanks Universiti Sains Malaysia for the Research University Golden Goose grant No. 1001/PFIZIK/811012.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CS2114).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–S19.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Blower, P. J. (1998). *Transition Met. Chem.* **23**, 109–112.
Bruker (2005). *APEX2* , *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Clark, G. R., Hall, D. & Waters, T. N. (1968). *J. Chem. Soc. A*, pp. 223–226.
Clark, G. R., Hall, D. & Waters, T. N. (1969). *J. Chem. Soc. A*, pp. 823–829.
Clark, G. R., Hall, D. & Waters, T. N. (1970). *J. Chem. Soc. A*, pp. 396–399.
Elmali, A., Elerman, Y. & Svoboda, I. (2000). *Acta Cryst.* C**56**, 423–424.
Granovski, A. D., Nivorozhkin, A. L. & Minkin, V. I. (1993). *Coord. Chem. Rev.* **126**, 1–69.
Li, C. H. & Chang, T. C. (1991). *Eur. Polym. J.* **27**, 35–39.
Shahrokhian, S., Amini, M. K., Kia, R. & Tangestaninejad, S. (2000). *Anal. Chem.* **72**, 956–962.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

Acta Cryst. (2009). E**65**, m498–m499 [doi:10.1107/S1600536809012641]

{6,6′-Diethoxy-2,2′-[4,5-dimethyl-*o*-phenylenebis(nitrilomethylidyne)]diphenolato}nickel(II) dihydrate

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S1. Comment

Schiff base complexes are some of the most important stereochemical models in transition metal coordination chemistry, with their ease of preparation and structural variations (Granovski *et al.*, 1993). Metal derivatives of Schiff bases have been studied extensively, and copper(II) and Ni(II) complexes play a major role in both synthetic and structural research (Elmali *et al.*, 2000; Blower, 1998; Granovski *et al.*, 1993; Li & Chang, 1991; Shahrokhian *et al.*, 2000). Tetradentate Schiff base metal complexes may form *trans* or *cis* planar or tetrahedral structures (Elmali *et al.*, 2000).

The Ni^{II} ion of the title compound (Fig. 1), shows a square planar geometry which is coordinated by two imine N atoms and two phenol O atoms of the tetradentate Schiff base ligand and lies across a crystallographic twofold rotation axis. The bond lengths (Allen *et al.*,, 1987) and angles are within normal ranges and are comparable with the related structures (Clark *et al.*, 1968, 1969, 1970). The water H atoms form bifurcated O—H(O,O) intermolecular hydrogen bonds with the oxygen atoms of the phenolato- and ethoxy groups with $R^2_1(5)$ and $R^2_1(6)$ ring motifs (Bernstein *et al.*, 1995), which may, in part, influence the molecular configuration (Fig. 1). The dihedral angle between the central benzene ring and the two outer benzene rings are 4.07 (11) and 3.99 (12)°. The dihedral angle between the two coordination planes O1—Ni1—N1 and O1A—Ni1—N1A is 0.77 (11)°. In the crystal structure the complex and two water molecules, association of which form the title compound, are linked together into 1-D extended chains by intermolecular O—H···O and C—H···O interactions along the *c* axis (Fig. 2). The interesting feature of the crystal structure is a short intermolecular C1···$C7^{iii}$ [3.355 (3) Å; (iii) 1 - x, -y, 1 - z] contact, shorter than the sum of the van der Waals radius of carbon atoms. The crystal structure is further stabilized by intermolecular π-π [$Cg1\cdots Cg3^{iii}$ = 3.5758 (13) Å; $Cg2\cdots Cg2^{iii}$ = 3.6085 (11) Å; $Cg2\cdots Cg3^{iii}$ = 3.6337 (13) Å, *Cg*1, *Cg*2 and *Cg*3 are the centroid of the Ni1/N1/C8/C8A/N1A, C1–C6, and Ni1/O1/C1/C6/C7/N1 rings, respectively].

S2. Experimental

A chloroform solution (40 ml) of [*N,N*′-Bis(3-ethoxy-salicylidene)- 4,5-dimethyl-phenylenediamine (1 mmol) was added to a ethanol solution (20 mL) of $NiCl_2.6H_2O$ (1.05 mmol, 237 mg). The mixture was refluxed for 30 min and then filtered. After keeping the filtrate in air, deep-red block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent.

S3. Refinement

The water H-atoms were located from the difference Fourier map and constrained to refine with the carrier atom after O—H distance restraint of 0.82 (1) Å. The rest of the hydrogen atoms were positioned geometrically [C—H = 0.95–97 Å] and refined using a riding approximation model. A rotating-group model was used for the methyl groups.

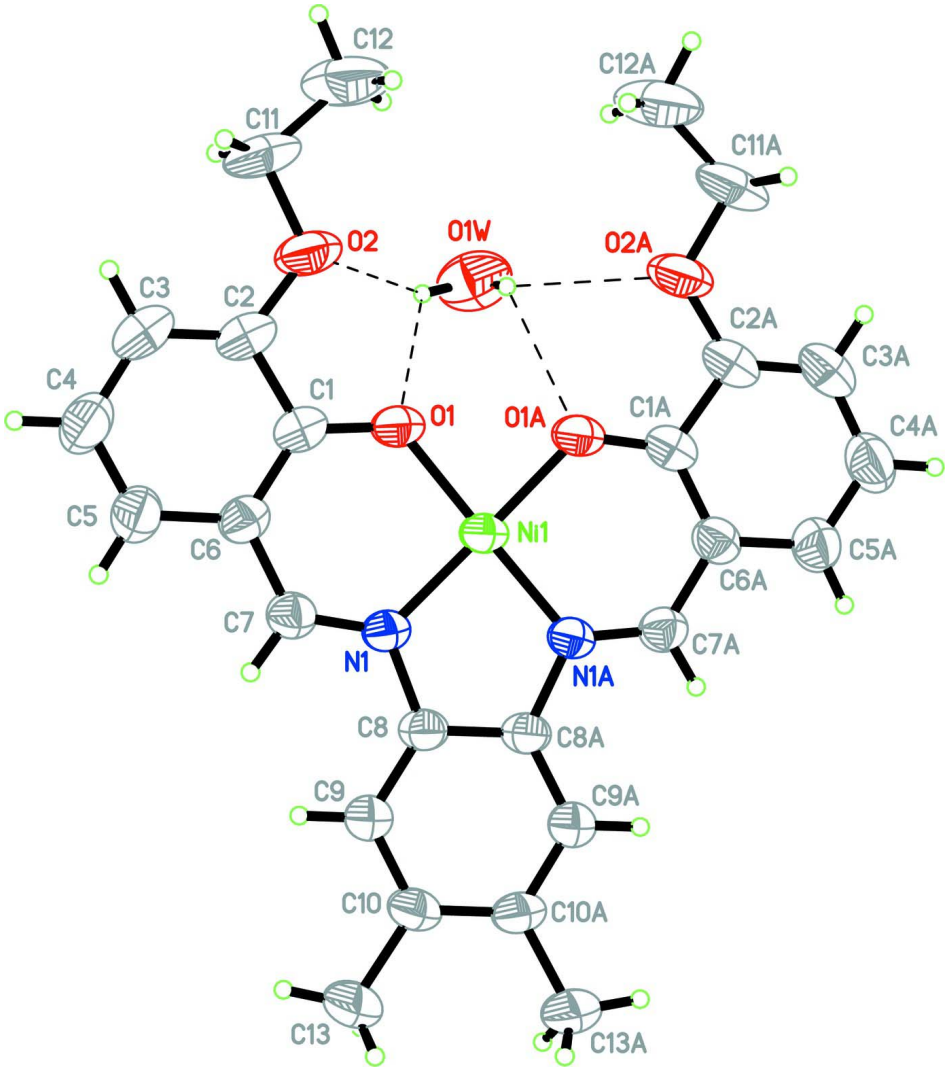

Figure 1

The title molecular compound, showing 50° probability displacement ellipsoids and the atomic numbering, hydrogen bonds are shown as dashed lines. Symmetry code for suffix A: -x + 1, y, -z + 1/2.

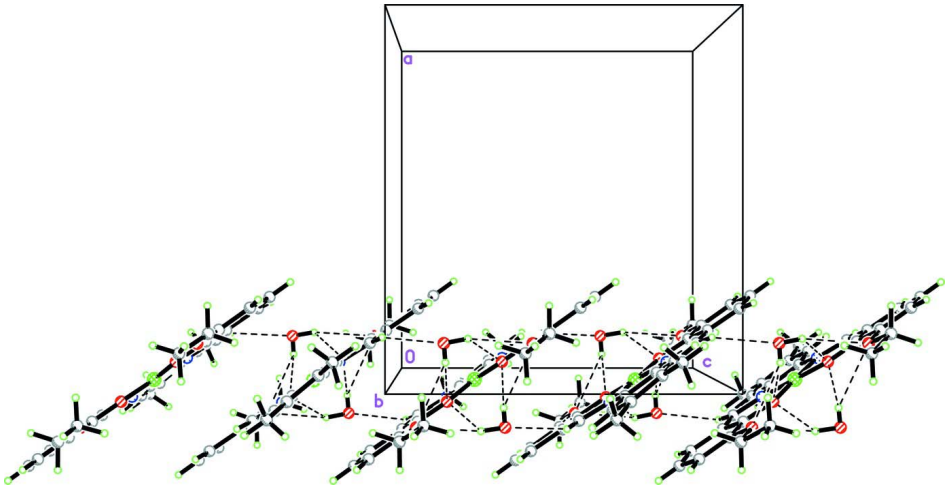

Figure 2

A crystal packing excerpt of the title compound viewed down the *b*-axis, showing 1-D extended chains along the *c*-axis. Intermolecular interactions are drawn as dashed lines.

{6,6′-Diethoxy-2,2′-[4,5-dimethyl-*o*- phenylenebis(nitrilomethylidyne)]diphenolato}nickel(II) dihydrate

Crystal data

$[Ni(C_{26}H_{26}N_2O_4)]\cdot 2H_2O$
$M_r = 525.23$
Orthorhombic, *Pbcn*
Hall symbol: -P 2n 2ab
$a = 12.8706\ (4)$ Å
$b = 16.1130\ (4)$ Å
$c = 11.8546\ (3)$ Å
$V = 2458.45\ (12)$ Å^3
$Z = 4$
$F(000) = 1104$
$D_x = 1.419$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2497 reflections
$\theta = 2.7–22.3°$
$\mu = 0.83$ mm^{-1}
$T = 294$ K
Block, red
0.30 × 0.16 × 0.08 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.790$, $T_{max} = 0.935$
16330 measured reflections
3517 independent reflections
2007 reflections with $I > 2\sigma(I)$
$R_{int} = 0.065$
$\theta_{max} = 29.8°$, $\theta_{min} = 2.5°$
$h = -17\rightarrow17$
$k = -22\rightarrow22$
$l = -16\rightarrow11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.122$
$S = 1.01$
3517 reflections
161 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
$w = 1/[\sigma^2(F_o^2) + (0.0543P)^2 + 0.1108P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.51$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.5000	−0.00935 (2)	0.2500	0.04044 (15)
O1	0.44372 (13)	0.07589 (9)	0.33400 (13)	0.0501 (4)
O2	0.38481 (16)	0.21443 (10)	0.42373 (15)	0.0716 (6)
N1	0.44336 (14)	−0.09376 (10)	0.33719 (15)	0.0398 (4)
C1	0.38667 (17)	0.06930 (14)	0.4246 (2)	0.0441 (5)
C2	0.3505 (2)	0.14350 (15)	0.4772 (2)	0.0524 (6)
C3	0.2894 (2)	0.14174 (16)	0.5706 (2)	0.0605 (7)
H3A	0.2659	0.1912	0.6020	0.073*
C4	0.2614 (2)	0.06548 (19)	0.6203 (2)	0.0660 (8)
H4A	0.2193	0.0646	0.6841	0.079*
C5	0.2961 (2)	−0.00668 (16)	0.5746 (2)	0.0566 (7)
H5A	0.2790	−0.0568	0.6088	0.068*
C6	0.35820 (19)	−0.00679 (13)	0.4755 (2)	0.0451 (6)
C7	0.39054 (17)	−0.08387 (14)	0.42982 (19)	0.0441 (5)
H7A	0.3725	−0.1315	0.4695	0.053*
C8	0.46786 (17)	−0.17483 (13)	0.29740 (18)	0.0412 (5)
C9	0.43332 (19)	−0.24982 (14)	0.3410 (2)	0.0498 (6)
H9A	0.3879	−0.2497	0.4020	0.060*
C10	0.4649 (2)	−0.32468 (14)	0.2957 (2)	0.0519 (6)
C11	0.3545 (2)	0.29234 (15)	0.4698 (3)	0.0759 (9)
H11A	0.3783	0.2974	0.5471	0.091*
H11B	0.2794	0.2979	0.4687	0.091*
C12	0.4041 (3)	0.35795 (18)	0.3968 (3)	0.1078 (13)
H12A	0.3824	0.4119	0.4219	0.162*
H12B	0.3832	0.3500	0.3198	0.162*
H12C	0.4783	0.3537	0.4022	0.162*
C13	0.4247 (3)	−0.40558 (15)	0.3438 (2)	0.0791 (10)
H13A	0.3822	−0.3943	0.4086	0.119*
H13B	0.4823	−0.4399	0.3656	0.119*
H13C	0.3841	−0.4338	0.2877	0.119*
O1W	0.38489 (17)	0.20940 (12)	0.15851 (16)	0.0853 (6)
H1W1	0.3725	0.1955	0.2239	0.128*
H2W1	0.4475	0.2018	0.1648	0.128*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0477 (2)	0.0286 (2)	0.0450 (3)	0.000	0.00116 (19)	0.000
O1	0.0667 (11)	0.0307 (8)	0.0530 (10)	0.0029 (8)	0.0057 (9)	−0.0006 (7)
O2	0.1017 (15)	0.0353 (9)	0.0778 (13)	0.0146 (9)	0.0068 (11)	−0.0068 (9)
N1	0.0447 (11)	0.0313 (9)	0.0434 (11)	0.0007 (8)	0.0005 (9)	−0.0028 (8)
C1	0.0453 (13)	0.0388 (12)	0.0481 (14)	0.0059 (10)	−0.0064 (11)	−0.0071 (11)
C2	0.0561 (15)	0.0429 (14)	0.0582 (16)	0.0118 (12)	−0.0078 (12)	−0.0123 (12)
C3	0.0610 (17)	0.0553 (16)	0.0651 (18)	0.0144 (13)	−0.0023 (14)	−0.0211 (14)
C4	0.0646 (17)	0.0690 (19)	0.0643 (18)	0.0047 (14)	0.0141 (14)	−0.0177 (15)

C5	0.0582 (16)	0.0584 (16)	0.0533 (17)	−0.0020 (12)	0.0091 (13)	−0.0069 (12)
C6	0.0447 (13)	0.0418 (13)	0.0487 (15)	0.0012 (10)	−0.0008 (10)	−0.0074 (11)
C7	0.0470 (13)	0.0392 (12)	0.0461 (14)	−0.0042 (10)	0.0000 (11)	−0.0020 (10)
C8	0.0496 (13)	0.0312 (11)	0.0429 (13)	0.0000 (9)	−0.0010 (10)	−0.0010 (9)
C9	0.0603 (15)	0.0384 (12)	0.0507 (14)	0.0005 (11)	0.0115 (12)	0.0003 (11)
C10	0.0660 (16)	0.0321 (12)	0.0576 (15)	−0.0057 (10)	0.0056 (12)	0.0027 (10)
C11	0.079 (2)	0.0387 (15)	0.111 (2)	0.0179 (14)	−0.0129 (18)	−0.0251 (16)
C12	0.161 (4)	0.0409 (17)	0.122 (3)	0.016 (2)	−0.011 (3)	−0.0029 (18)
C13	0.111 (3)	0.0372 (15)	0.089 (2)	−0.0093 (15)	0.0313 (19)	0.0036 (14)
O1W	0.1029 (16)	0.0723 (14)	0.0809 (14)	0.0234 (12)	−0.0218 (12)	0.0009 (11)

Geometric parameters (Å, º)

Ni1—O1^{i}	1.8447 (15)	C7—H7A	0.9300
Ni1—O1	1.8447 (15)	C8—C9	1.387 (3)
Ni1—N1	1.8573 (17)	C8—C8^{i}	1.396 (4)
Ni1—N1^{i}	1.8573 (17)	C9—C10	1.381 (3)
O1—C1	1.306 (3)	C9—H9A	0.9300
O2—C2	1.380 (3)	C10—C10^{i}	1.410 (5)
O2—C11	1.423 (3)	C10—C13	1.514 (3)
N1—C7	1.301 (3)	C11—C12	1.508 (4)
N1—C8	1.424 (2)	C11—H11A	0.9700
C1—C6	1.415 (3)	C11—H11B	0.9700
C1—C2	1.427 (3)	C12—H12A	0.9600
C2—C3	1.358 (3)	C12—H12B	0.9600
C3—C4	1.410 (4)	C12—H12C	0.9600
C3—H3A	0.9300	C13—H13A	0.9600
C4—C5	1.358 (3)	C13—H13B	0.9600
C4—H4A	0.9300	C13—H13C	0.9600
C5—C6	1.421 (3)	O1W—H1W1	0.8226
C5—H5A	0.9300	O1W—H2W1	0.8179
C6—C7	1.417 (3)		
O1^{i}—Ni1—O1	83.75 (10)	N1—C7—H7A	117.2
O1^{i}—Ni1—N1	178.81 (7)	C6—C7—H7A	117.2
O1—Ni1—N1	95.21 (7)	C9—C8—C8^{i}	119.32 (13)
O1^{i}—Ni1—N1^{i}	95.21 (7)	C9—C8—N1	127.2 (2)
O1—Ni1—N1^{i}	178.81 (7)	C8^{i}—C8—N1	113.45 (11)
N1—Ni1—N1^{i}	85.84 (11)	C10—C9—C8	121.4 (2)
C1—O1—Ni1	127.19 (14)	C10—C9—H9A	119.3
C2—O2—C11	117.8 (2)	C8—C9—H9A	119.3
C7—N1—C8	120.49 (18)	C9—C10—C10^{i}	119.14 (14)
C7—N1—Ni1	125.80 (15)	C9—C10—C13	120.3 (2)
C8—N1—Ni1	113.61 (14)	C10^{i}—C10—C13	120.54 (14)
O1—C1—C6	124.54 (19)	O2—C11—C12	106.4 (2)
O1—C1—C2	118.4 (2)	O2—C11—H11A	110.5
C6—C1—C2	117.1 (2)	C12—C11—H11A	110.5
C3—C2—O2	125.3 (2)	O2—C11—H11B	110.5

C3—C2—C1	121.8 (2)	C12—C11—H11B	110.5
O2—C2—C1	112.9 (2)	H11A—C11—H11B	108.6
C2—C3—C4	120.5 (2)	C11—C12—H12A	109.5
C2—C3—H3A	119.8	C11—C12—H12B	109.5
C4—C3—H3A	119.8	H12A—C12—H12B	109.5
C5—C4—C3	119.7 (3)	C11—C12—H12C	109.5
C5—C4—H4A	120.2	H12A—C12—H12C	109.5
C3—C4—H4A	120.2	H12B—C12—H12C	109.5
C4—C5—C6	121.1 (2)	C10—C13—H13A	109.5
C4—C5—H5A	119.5	C10—C13—H13B	109.5
C6—C5—H5A	119.5	H13A—C13—H13B	109.5
C1—C6—C7	121.4 (2)	C10—C13—H13C	109.5
C1—C6—C5	119.8 (2)	H13A—C13—H13C	109.5
C7—C6—C5	118.8 (2)	H13B—C13—H13C	109.5
N1—C7—C6	125.7 (2)	H1W1—O1W—H2W1	93.7

O1^{i}—Ni1—O1—C1	−177.9 (2)	C2—C1—C6—C7	−179.8 (2)
O1—Ni1—N1—C7	−4.77 (19)	O1—C1—C6—C5	179.7 (2)
N1^{i}—Ni1—N1—C7	175.8 (2)	C2—C1—C6—C5	0.0 (3)
O1—Ni1—N1—C8	178.82 (14)	C4—C5—C6—C1	1.5 (4)
N1^{i}—Ni1—N1—C8	−0.62 (11)	C4—C5—C6—C7	−178.6 (2)
Ni1—O1—C1—C6	0.5 (3)	C8—N1—C7—C6	−177.5 (2)
Ni1—O1—C1—C2	−179.89 (15)	Ni1—N1—C7—C6	6.3 (3)
C11—O2—C2—C3	0.2 (4)	C1—C6—C7—N1	−3.4 (4)
C11—O2—C2—C1	−179.2 (2)	C5—C6—C7—N1	176.7 (2)
O1—C1—C2—C3	178.9 (2)	C7—N1—C8—C9	6.6 (4)
C6—C1—C2—C3	−1.4 (3)	Ni1—N1—C8—C9	−176.77 (19)
O1—C1—C2—O2	−1.6 (3)	C7—N1—C8—C8^{i}	−174.9 (2)
C6—C1—C2—O2	178.1 (2)	Ni1—N1—C8—C8^{i}	1.8 (3)
O2—C2—C3—C4	−178.1 (2)	C8^{i}—C8—C9—C10	3.0 (4)
C1—C2—C3—C4	1.3 (4)	N1—C8—C9—C10	−178.6 (2)
C2—C3—C4—C5	0.3 (4)	C8—C9—C10—C10^{i}	1.0 (5)
C3—C4—C5—C6	−1.7 (4)	C8—C9—C10—C13	−179.1 (2)
O1—C1—C6—C7	−0.2 (4)	C2—O2—C11—C12	178.9 (2)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O1	0.82	2.50	3.087 (2)	129
O1*W*—H1*W*1···O2	0.82	2.39	3.145 (3)	152
O1*W*—H2*W*1···O1^{i}	0.82	2.47	3.083 (3)	133
O1*W*—H2*W*1···O2^{i}	0.82	2.41	3.121 (3)	146
C7—H7*A*···O1*W*^{ii}	0.93	2.57	3.383 (3)	146

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