Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Triaqua(5-formyl-*N*-salicylidene-DL-alaninato-κ^3N,O,O')nickel(II) monohydrate

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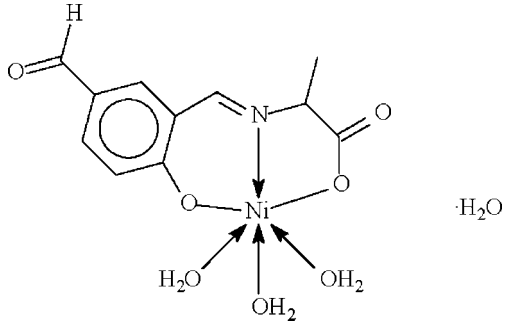
Received 17 May 2007; accepted 18 May 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.036; wR factor = 0.099; data-to-parameter ratio = 12.3.

The deprotonated Schiff-base dianion in the title compound, $[Ni(C_{11}H_9NO_4)(H_2O)_3]\cdot H_2O$, occupies the meridional sites of the NiO_5N octahedron. The neutral complex molecule interacts with the uncoordinated water molecule by way of O—H···O hydrogen bonds to give rise to a three-dimensional network. The ethylidene part of the molecule is disordered over two positions in a 0.74:0.26 ratio.

Related literature

For the structures of salicylidene–glycine–nickel complexes, see Cui *et al.* (1992, 1993); Rodríguez *et al.* (1990).



Experimental

Crystal data

$[Ni(C_{11}H_9NO_4)(H_2O)_3].H_2O$
M_r = 349.97
Triclinic, $P\overline{1}$
a = 6.861 (2) Å
b = 8.664 (2) Å
c = 12.363 (3) Å
α = 82.967 (3)°
β = 80.639 (3)°
γ = 77.706 (3)°
V = 705.5 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.41 mm^{-1}
T = 295 (2) K
0.20 × 0.10 × 0.05 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan *SADABS* (Sheldrick, 1996)
T_{min} = 0.870, T_{max} = 0.933
4072 measured reflections
2966 independent reflections
2635 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.099
S = 1.04
2966 reflections
241 parameters
35 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—N1	1.999 (2)	Ni1—O1	2.0455 (16)
Ni1—O3	2.0149 (16)	Ni1—O3*W*	2.053 (2)
Ni1—O2*W*	2.0450 (19)	Ni1—O1*W*	2.1063 (19)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···O1^{i}	0.85 (1)	1.95 (1)	2.784 (2)	170 (3)
O1*w*—H1*w*2···O4^{ii}	0.84 (1)	1.97 (2)	2.786 (3)	162 (4)
O2*w*—H2*w*1···O3^{iii}	0.85 (1)	1.93 (1)	2.769 (2)	173 (4)
O2*w*—H2*w*2···O2^{i}	0.85 (1)	2.19 (2)	2.937 (3)	147 (3)
O3*w*—H3*w*1···O2^{iv}	0.84 (1)	1.95 (1)	2.753 (3)	161 (3)
O3*w*—H3*w*2···O4*w*^{v}	0.85 (1)	1.85 (1)	2.689 (3)	171 (4)
O4*w*—H4*w*1···O2	0.84 (1)	1.92 (1)	2.741 (3)	166 (3)
O4*w*—H4*w*2···O3^{vi}	0.84 (1)	2.11 (2)	2.929 (3)	165 (4)

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, -y+2, -z$; (iii) $-x+1, -y+2, -z+1$; (iv) $-x+2, -y+1, -z+1$; (v) $x, y+1, z$; (vi) $x+1, y-1, z$.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

We are grateful to the Ministry of Education Foundation of the Guangxi Zhuang Autonomous Region for funding this study. We thank Hechi University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2419).

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supplementary materials

Acta Cryst. (2007). E**63**, m1715-m1716 [**doi:10.1107/S1600536807024518**]

Triaqua(5-formyl-*N*-salicylidene-DL-alaninato-κ^3*N*,*O*,*O*')nickel(II) monohydrate

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Comment

The salicylidene-glycine carboxylic acid when doubly deprotonated generally chelates to metal centers through its *N*,*O*,*O*' atoms. The planar ligand chelates to nickel in this manner in, for example, the tripyridinenickel complex for which it occupies the meridional sites (Cui *et al.*, 1992). The 3-methoxy analog also affords a six-coordinate tripyridine complex, but it also contains ethanol as the solvate molecule (Cui *et al.*, 1993). The *N*-(5-bromosalicylidene)tryptophanate complex is a triaqua complex that crystallizes with two uncoordinated water molecules (Rodríguez *et al.*, 1990).

This chelating feature is also found in the title compound, (I), (Table 1) which has a formyl group as substituent in the aromatic ring. The formyl substitutent in involved in hydrogen bonding interactions with the water molecules to give rise to a three-dimenional network architecture (Table 2).

Experimental

5-Formylsalicylaldehyde (0.2 mmol, 0.27 g), D,*L*-alanine (0.2 mmol, 0.18 g) and potassium hydroxide (0.2 mmol, 0.11 g) were dissolved in 80% aqueous methanol (15 ml). The mixture was stirred for 1 h to give a clear yellow solution. To the solution was added an aqueous solution (15 ml) of nickel(II) acetate hexahydrate (0.2 mmol, 0.57 g). The mixture heated at 323 K for 3 h. Green crystals of (I) were obtained in about 50% yield.

Refinement

The ethylidene part of the molecule is disordered over two positions; the disorder refined to a 0.737 (11):0.263 (11) ratio. Pairs of equivalent carbon-carbon distances were restrained to within 0.01 Å of each other, and the disordered atoms were restrained to vibrate in a nearly isotropic manner.

The carbon-bound H atoms were placed in calculated positions (C—H 0.93 Å), and were included in the refinement in the riding model approximation, with U_{iso}(H) = 1.2U_{eq}(C).

The water H-atoms were located in a difference Fourier map, and were refined with a distance restraint of O–H = 0.85±0.01 Å; U_{iso} was freely varied for each H atom.

Figures

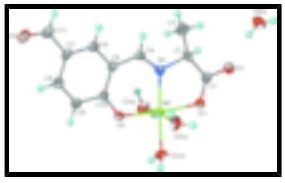

Fig. 1. **Figure 1**. View of (I) as a displacement ellipsoid plot (50% probability). Hydrogen atoms are drawn as spheres of arbitrary radii; the minor disorder component is not shown.

Triaqua(5-formyl-*N*-salicylidene-D,*L*-alaninato-κ^3*N*,\ *O*,*O*$^{\prime}$)nickel(II) monohydrate

Crystal data

$[Ni(C_{11}H_9NO_4)(H_2O)_3].H_2O$	$Z = 2$
$M_r = 349.97$	$F_{000} = 364$
Triclinic, $P\overline{1}$	$D_x = 1.647$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.861$ (2) Å	Cell parameters from 2418 reflections
$b = 8.664$ (2) Å	$\theta = 2.3$–27.1°
$c = 12.363$ (3) Å	$\mu = 1.41$ mm^{-1}
$\alpha = 82.967$ (3)°	$T = 295$ (2) K
$\beta = 80.639$ (3)°	Block, green
$\gamma = 77.706$ (3)°	0.20 × 0.10 × 0.05 mm
$V = 705.5$ (3) Å^3	

Data collection

Bruker SMART CCD diffractometer	2966 independent reflections
Radiation source: fine-focus sealed tube	2635 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.020$
$T = 295$(2) K	$\theta_{max} = 27.1^\circ$
φ and ω scans	$\theta_{min} = 1.7^\circ$
Absorption correction: Multi-scan SADABS (Sheldrick, 1996)	$h = -5 \rightarrow 8$
$T_{min} = 0.870$, $T_{max} = 0.933$	$k = -9 \rightarrow 11$
4072 measured reflections	$l = -14 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.036$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.099$	$w = 1/[\sigma^2(F_o^2) + (0.059P)^2 + 0.1949P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
2966 reflections	$\Delta\rho_{max} = 0.55$ e Å^{-3}
241 parameters	$\Delta\rho_{min} = -0.43$ e Å^{-3}
35 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ni1	0.62546 (4)	0.75271 (3)	0.39426 (2)	0.02769 (12)	
O1	0.7525 (3)	0.52716 (18)	0.44937 (13)	0.0347 (4)	
O2	0.9267 (3)	0.3003 (2)	0.39286 (16)	0.0463 (5)	
O3	0.5195 (3)	0.96942 (18)	0.32259 (13)	0.0315 (4)	
O4	0.6313 (4)	1.3584 (2)	−0.14612 (15)	0.0495 (5)	
O1W	0.3722 (3)	0.6685 (2)	0.36805 (15)	0.0396 (4)	
O2W	0.4613 (3)	0.8013 (2)	0.54397 (15)	0.0382 (4)	
O3W	0.8478 (3)	0.8416 (2)	0.44387 (17)	0.0445 (5)	
O4W	1.0881 (3)	0.0138 (2)	0.31021 (19)	0.0474 (5)	
N1	0.7874 (3)	0.6852 (2)	0.25235 (17)	0.0356 (5)	
C1	0.8554 (4)	0.4445 (3)	0.3764 (2)	0.0355 (5)	
C2	0.9180 (6)	0.5251 (4)	0.2619 (3)	0.0302 (10)	0.737 (11)
H2	1.0598	0.5342	0.2535	0.036*	0.737 (11)
C3	0.8859 (14)	0.4276 (7)	0.1736 (6)	0.065 (2)	0.737 (11)
H3A	0.9225	0.3167	0.1967	0.097*	0.737 (11)
H3B	0.9684	0.4520	0.1058	0.097*	0.737 (11)
H3C	0.7468	0.4529	0.1630	0.097*	0.737 (11)
C2'	0.817 (2)	0.5062 (9)	0.2564 (6)	0.045 (4)	0.263 (11)
H2'	0.6895	0.4803	0.2457	0.054*	0.263 (11)
C3'	0.980 (2)	0.430 (2)	0.1702 (14)	0.049 (4)	0.263 (11)
H3'1	0.9542	0.4786	0.0985	0.073*	0.263 (11)
H3'2	0.9805	0.3190	0.1744	0.073*	0.263 (11)
H3'3	1.1085	0.4456	0.1831	0.073*	0.263 (11)
C4	0.8019 (4)	0.7699 (3)	0.1609 (2)	0.0361 (5)	
H4	0.8834	0.7222	0.1015	0.043*	
C5	0.7030 (3)	0.9339 (3)	0.14088 (18)	0.0284 (5)	
C6	0.7401 (4)	1.0054 (3)	0.03400 (19)	0.0320 (5)	
H6	0.8249	0.9459	−0.0190	0.038*	
C7	0.6553 (4)	1.1611 (3)	0.00411 (19)	0.0326 (5)	
C8	0.5282 (4)	1.2502 (3)	0.0832 (2)	0.0372 (5)	
H8	0.4712	1.3555	0.0643	0.045*	
C9	0.4865 (4)	1.1843 (3)	0.1885 (2)	0.0375 (6)	
H9	0.4005	1.2458	0.2400	0.045*	
C10	0.5710 (3)	1.0242 (3)	0.22144 (18)	0.0279 (4)	
C11	0.6961 (4)	1.2240 (3)	−0.1101 (2)	0.0386 (6)	
H11	0.7779	1.1560	−0.1590	0.046*	
H1W1	0.336 (5)	0.601 (3)	0.418 (2)	0.058 (10)*	
H1W2	0.369 (6)	0.640 (4)	0.3058 (16)	0.066 (11)*	
H2W1	0.473 (6)	0.875 (3)	0.580 (3)	0.065 (11)*	
H2W2	0.3354 (18)	0.810 (4)	0.548 (3)	0.069 (12)*	
H3W1	0.933 (4)	0.787 (3)	0.482 (2)	0.046 (9)*	
H3W2	0.930 (4)	0.886 (4)	0.399 (2)	0.061 (11)*	
H4W1	1.048 (5)	0.1082 (18)	0.326 (3)	0.052 (9)*	
H4W2	1.207 (3)	−0.009 (4)	0.325 (3)	0.071 (12)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.03501 (19)	0.02257 (17)	0.02212 (17)	−0.00216 (12)	−0.00137 (12)	0.00139 (11)
O1	0.0449 (10)	0.0265 (8)	0.0270 (8)	−0.0007 (7)	0.0002 (7)	0.0024 (6)
O2	0.0660 (13)	0.0256 (8)	0.0379 (10)	0.0062 (8)	−0.0041 (9)	0.0025 (7)
O3	0.0409 (9)	0.0247 (7)	0.0234 (8)	−0.0008 (7)	0.0009 (7)	0.0012 (6)
O4	0.0741 (14)	0.0393 (10)	0.0324 (10)	−0.0108 (9)	−0.0107 (9)	0.0109 (8)
O1W	0.0515 (11)	0.0420 (10)	0.0285 (9)	−0.0172 (8)	−0.0077 (8)	0.0020 (8)
O2W	0.0443 (11)	0.0399 (10)	0.0305 (9)	−0.0111 (8)	0.0032 (8)	−0.0105 (7)
O3W	0.0438 (11)	0.0461 (11)	0.0454 (11)	−0.0136 (9)	−0.0159 (9)	0.0105 (9)
O4W	0.0417 (11)	0.0376 (10)	0.0598 (13)	−0.0030 (9)	−0.0008 (10)	−0.0093 (9)
N1	0.0460 (12)	0.0244 (9)	0.0283 (10)	0.0029 (8)	0.0019 (9)	0.0024 (7)
C1	0.0442 (14)	0.0258 (11)	0.0322 (13)	−0.0020 (10)	−0.0042 (10)	0.0034 (9)
C2	0.0248 (19)	0.0265 (16)	0.0328 (18)	0.0014 (13)	0.0023 (14)	0.0028 (12)
C3	0.112 (6)	0.033 (2)	0.042 (3)	0.013 (3)	−0.020 (4)	−0.0076 (19)
C2'	0.049 (7)	0.036 (5)	0.038 (5)	0.004 (5)	0.011 (5)	0.004 (4)
C3'	0.057 (7)	0.037 (6)	0.036 (6)	0.007 (6)	0.007 (6)	0.010 (4)
C4	0.0437 (14)	0.0333 (12)	0.0236 (11)	0.0018 (10)	0.0034 (10)	−0.0006 (9)
C5	0.0312 (11)	0.0268 (10)	0.0257 (11)	−0.0058 (9)	−0.0038 (9)	0.0032 (8)
C6	0.0356 (12)	0.0342 (12)	0.0249 (11)	−0.0065 (10)	−0.0016 (9)	−0.0012 (9)
C7	0.0414 (13)	0.0326 (12)	0.0241 (11)	−0.0100 (10)	−0.0075 (10)	0.0047 (9)
C8	0.0507 (15)	0.0253 (11)	0.0326 (13)	−0.0046 (10)	−0.0068 (11)	0.0051 (9)
C9	0.0520 (15)	0.0263 (11)	0.0288 (12)	−0.0002 (10)	−0.0018 (11)	−0.0005 (9)
C10	0.0313 (11)	0.0268 (10)	0.0248 (11)	−0.0050 (9)	−0.0052 (9)	0.0008 (8)
C11	0.0500 (15)	0.0383 (13)	0.0281 (12)	−0.0132 (11)	−0.0068 (10)	0.0045 (10)

Geometric parameters (Å, °)

Ni1—N1	1.999 (2)	C2—C3	1.528 (6)
Ni1—O3	2.0149 (16)	C2—H2	0.9800
Ni1—O2W	2.0450 (19)	C3—H3A	0.9600
Ni1—O1	2.0455 (16)	C3—H3B	0.9600
Ni1—O3W	2.053 (2)	C3—H3C	0.9600
Ni1—O1W	2.1063 (19)	C2'—C3'	1.512 (9)
C1—O1	1.250 (3)	C2'—H2'	0.9800
C1—O2	1.245 (3)	C3'—H3'1	0.9600
O3—C10	1.302 (3)	C3'—H3'2	0.9600
O4—C11	1.212 (3)	C3'—H3'3	0.9600
O1W—H1W1	0.845 (10)	C4—C5	1.449 (3)
O1W—H1W2	0.842 (10)	C4—H4	0.9300
O2W—H2W1	0.845 (10)	C5—C6	1.397 (3)
O2W—H2W2	0.845 (10)	C5—C10	1.421 (3)
O3W—H3W1	0.840 (10)	C6—C7	1.382 (3)
O3W—H3W2	0.847 (10)	C6—H6	0.9300
O4W—H4W1	0.841 (10)	C7—C8	1.390 (4)
O4W—H4W2	0.844 (10)	C7—C11	1.454 (3)
N1—C4	1.272 (3)	C8—C9	1.368 (3)

N1—C2	1.485 (4)	C8—H8	0.9300
N1—C2'	1.516 (8)	C9—C10	1.422 (3)
C1—C2	1.538 (4)	C9—H9	0.9300
C1—C2'	1.558 (8)	C11—H11	0.9300
N1—Ni1—O3	91.55 (7)	C1—C2—H2	110.1
N1—Ni1—O2W	175.02 (7)	C2—C3—H3A	109.5
O3—Ni1—O2W	93.10 (7)	C2—C3—H3B	109.5
N1—Ni1—O1	81.70 (7)	H3A—C3—H3B	109.5
O3—Ni1—O1	173.25 (6)	C2—C3—H3C	109.5
O2W—Ni1—O1	93.65 (7)	H3A—C3—H3C	109.5
N1—Ni1—O3W	95.22 (9)	H3B—C3—H3C	109.5
O3—Ni1—O3W	89.33 (8)	C3'—C2'—N1	114.9 (11)
O2W—Ni1—O3W	86.63 (8)	C3'—C2'—C1	113.1 (11)
O1—Ni1—O3W	91.04 (8)	N1—C2'—C1	105.0 (6)
N1—Ni1—O1W	93.73 (9)	C3'—C2'—H2'	107.8
O3—Ni1—O1W	91.45 (7)	N1—C2'—H2'	107.8
O2W—Ni1—O1W	84.37 (8)	C1—C2'—H2'	107.8
O1—Ni1—O1W	89.24 (7)	C2'—C3'—H3'1	109.5
O3W—Ni1—O1W	170.99 (8)	C2'—C3'—H3'2	109.5
C1—O1—Ni1	114.98 (14)	H3'1—C3'—H3'2	109.5
C10—O3—Ni1	126.69 (14)	C2'—C3'—H3'3	109.5
Ni1—O1W—H1W1	114 (2)	H3'1—C3'—H3'3	109.5
Ni1—O1W—H1W2	119 (3)	H3'2—C3'—H3'3	109.5
H1W1—O1W—H1W2	110 (3)	N1—C4—C5	125.9 (2)
Ni1—O2W—H2W1	124 (3)	N1—C4—H4	117.0
Ni1—O2W—H2W2	116 (3)	C5—C4—H4	117.0
H2W1—O2W—H2W2	104 (4)	C6—C5—C10	118.8 (2)
Ni1—O3W—H3W1	123 (2)	C6—C5—C4	116.7 (2)
Ni1—O3W—H3W2	122 (2)	C10—C5—C4	124.6 (2)
H3W1—O3W—H3W2	96 (3)	C7—C6—C5	122.4 (2)
H4W1—O4W—H4W2	103 (3)	C7—C6—H6	118.8
C4—N1—C2	118.8 (2)	C5—C6—H6	118.8
C4—N1—C2'	121.0 (3)	C6—C7—C8	118.9 (2)
C2—N1—C2'	29.3 (5)	C6—C7—C11	118.7 (2)
C4—N1—Ni1	126.63 (17)	C8—C7—C11	122.3 (2)
C2—N1—Ni1	114.18 (17)	C9—C8—C7	120.5 (2)
C2'—N1—Ni1	107.9 (4)	C9—C8—H8	119.8
O2—C1—O1	123.8 (2)	C7—C8—H8	119.8
O2—C1—C2	116.6 (2)	C8—C9—C10	121.8 (2)
O1—C1—C2	119.3 (2)	C8—C9—H9	119.1
O2—C1—C2'	116.3 (3)	C10—C9—H9	119.1
O1—C1—C2'	115.2 (4)	O3—C10—C5	124.49 (19)
C2—C1—C2'	28.4 (5)	O3—C10—C9	117.9 (2)
N1—C2—C3	109.6 (4)	C5—C10—C9	117.6 (2)
N1—C2—C1	107.6 (2)	O4—C11—C7	124.9 (3)
C3—C2—C1	109.3 (4)	O4—C11—H11	117.6
N1—C2—H2	110.1	C7—C11—H11	117.6
C3—C2—H2	110.1		

N1—Ni1—O1—C1	−5.22 (18)	C4—N1—C2'—C3'	37.6 (17)
O2W—Ni1—O1—C1	172.96 (19)	C2—N1—C2'—C3'	−57.0 (15)
O3W—Ni1—O1—C1	−100.35 (19)	Ni1—N1—C2'—C3'	−164.6 (12)
O1W—Ni1—O1—C1	88.66 (19)	C4—N1—C2'—C1	162.6 (5)
N1—Ni1—O3—C10	−4.48 (19)	C2—N1—C2'—C1	68.0 (8)
O2W—Ni1—O3—C10	177.31 (19)	Ni1—N1—C2'—C1	−39.7 (9)
O3W—Ni1—O3—C10	90.72 (19)	O2—C1—C2'—C3'	−38.8 (16)
O1W—Ni1—O3—C10	−98.26 (19)	O1—C1—C2'—C3'	164.5 (11)
O3—Ni1—N1—C4	2.1 (2)	C2—C1—C2'—C3'	58.9 (15)
O1—Ni1—N1—C4	−177.6 (3)	O2—C1—C2'—N1	−164.9 (5)
O3W—Ni1—N1—C4	−87.3 (2)	O1—C1—C2'—N1	38.4 (10)
O1W—Ni1—N1—C4	93.7 (2)	C2—C1—C2'—N1	−67.1 (8)
O3—Ni1—N1—C2	175.2 (2)	C2—N1—C4—C5	−172.8 (3)
O1—Ni1—N1—C2	−4.6 (2)	C2'—N1—C4—C5	153.3 (7)
O3W—Ni1—N1—C2	85.7 (2)	Ni1—N1—C4—C5	0.0 (4)
O1W—Ni1—N1—C2	−93.3 (2)	N1—C4—C5—C6	179.8 (3)
O3—Ni1—N1—C2'	−154.0 (6)	N1—C4—C5—C10	−1.1 (4)
O1—Ni1—N1—C2'	26.2 (6)	C10—C5—C6—C7	0.9 (4)
O3W—Ni1—N1—C2'	116.5 (6)	C4—C5—C6—C7	−179.9 (2)
O1W—Ni1—N1—C2'	−62.5 (6)	C5—C6—C7—C8	−0.1 (4)
Ni1—O1—C1—O2	−172.5 (2)	C5—C6—C7—C11	−177.7 (2)
Ni1—O1—C1—C2	14.0 (3)	C6—C7—C8—C9	−0.6 (4)
Ni1—O1—C1—C2'	−17.7 (7)	C11—C7—C8—C9	176.9 (2)
C4—N1—C2—C3	−56.1 (6)	C7—C8—C9—C10	0.4 (4)
C2'—N1—C2—C3	46.6 (8)	Ni1—O3—C10—C5	4.8 (3)
Ni1—N1—C2—C3	130.3 (4)	Ni1—O3—C10—C9	−176.50 (17)
C4—N1—C2—C1	−174.9 (3)	C6—C5—C10—O3	177.6 (2)
C2'—N1—C2—C1	−72.2 (6)	C4—C5—C10—O3	−1.5 (4)
Ni1—N1—C2—C1	11.5 (4)	C6—C5—C10—C9	−1.1 (3)
O2—C1—C2—N1	169.1 (3)	C4—C5—C10—C9	179.8 (2)
O1—C1—C2—N1	−16.9 (4)	C8—C9—C10—O3	−178.3 (2)
C2'—C1—C2—N1	72.4 (6)	C8—C9—C10—C5	0.5 (4)
O2—C1—C2—C3	50.2 (5)	C6—C7—C11—O4	−179.7 (3)
O1—C1—C2—C3	−135.9 (4)	C8—C7—C11—O4	2.8 (4)
C2'—C1—C2—C3	−46.5 (8)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H1w1···O1^{i}	0.85 (1)	1.95 (1)	2.784 (2)	170 (3)
O1w—H1w2···O4^{ii}	0.84 (1)	1.97 (2)	2.786 (3)	162 (4)
O2w—H2w1···O3^{iii}	0.85 (1)	1.93 (1)	2.769 (2)	173 (4)
O2w—H2w2···O2^{i}	0.85 (1)	2.19 (2)	2.937 (3)	147 (3)
O3w—H3w1···O2^{iv}	0.84 (1)	1.95 (1)	2.753 (3)	161 (3)
O3w—H3w2···O4w^{v}	0.85 (1)	1.85 (1)	2.689 (3)	171 (4)
O4w—H4w1···O2	0.84 (1)	1.92 (1)	2.741 (3)	166 (3)
O4w—H4w2···O3^{vi}	0.84 (1)	2.11 (2)	2.929 (3)	165 (4)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+2, −*z*; (iii) −*x*+1, −*y*+2, −*z*+1; (iv) −*x*+2, −*y*+1, −*z*+1; (v) *x*, *y*+1, *z*; (vi) *x*+1, *y*−1, *z*.

Fig. 1