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Bis[2-(1*H*-benzimidazol-2-yl)acetato-κ^2N^3,O]bis(ethanol-κO)nickel(II)

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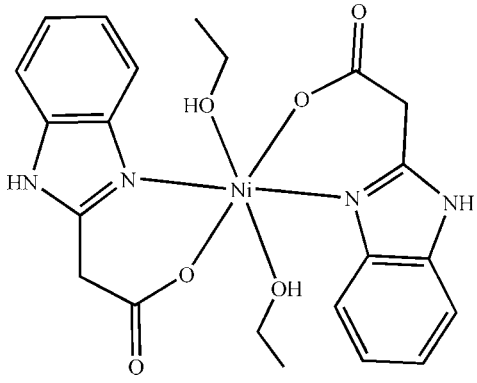
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.049; wR factor = 0.107; data-to-parameter ratio = 14.7.

In the title compound, $[Ni(C_9H_7N_2O_2)_2(C_2H_5OH)_2]$, the Ni^{II} ion is situated on an inversion center and is coordinated by two N and two O atoms from two 2-(1*H*-benzimidazol-2-yl)acetate (*L*) ligands and by two O atoms from two ethanol ligands in a distorted octahedral geometry. In the *L* ligand, the acetate group deviates significantly from the benzimidazole plane, the C—C—C—O(coordinating) torsion angle being 34.2 (5)°. In the crystal, O—H···O and N—H···O hydrogen bonds link the molecules into a two-dimensional supramolecular network parallel to the *bc* plane.

Related literature

For related structures, see: Chen *et al.* (2010); Gao *et al.* (2011); Guo *et al.* (2007); Peng *et al.* (2010).



Experimental

Crystal data

$[Ni(C_9H_7N_2O_2)_2(C_2H_6O)_2]$ M_r = 501.18
Monoclinic, $P2_1/c$
a = 10.441 (5) Å
b = 9.639 (4) Å
c = 11.480 (5) Å
β = 98.956 (6)°
V = 1141.3 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.90 mm^{-1}
T = 298 K
0.28 × 0.26 × 0.23 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.788, T_{max} = 0.821
6022 measured reflections
2231 independent reflections
1411 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.107
S = 1.04
2231 reflections
152 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O2^{i}	0.85	1.96	2.672 (3)	141
N2—H2A···O2^{ii}	0.86	1.93	2.788 (4)	173

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5355).

References

Bruker (2004). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Burnett, M. N. & Johnson, C. K. (1996). *ORTEPIII*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
Chen, W., Yang, B. Q., Ma, S. S., Shao, X. X. & Jiang, S. (2010). *Chin. J. Struct. Chem.* **29**, 1241–1249.
Gao, J., Wang, J. & Dai, C. (2011). *Acta Cryst.* E**67**, m75.
Guo, Z. G., Li, X. J., Gao, S. Y. & Li, Y. F. (2007). *J. Mol. Struct.* **846**, 123–127.
Peng, G., Qiu, Y. C., Liu, Z. H., Liu, B. & Deng, H. (2010). *Cryst. Growth Des.* **10**, 114–121.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supplementary materials

Acta Cryst. (2012). E**68**, m1461 [doi:10.1107/S160053681204514X]

Bis[2-(1*H*-benzimidazol-2-yl)acetato-κ^2N^3,O]bis(ethanol-κO)nickel(II)

Jun Wang and Jian-Hua Nie

Comment

Multidentate ligands containing N donors and carboxylic groups are often employed to construct new metal coordination polymers with different structures (Chen *et al.*, 2010; Gao *et al.*, 2011; Guo *et al.*, 2007; Peng *et al.*, 2010). The main reason is that they have various coordination modes and can form high-dimensional polymers through hydrogen-bonding interactions in the process of self-assembly. In this work, we chose 2-(1*H*-benzimidazol-2-yl)acetic acid (H*L*), which contains two N atoms of an imidazole group and one carboxylate group, as the building block to prepare new metal coordination polymers. To date, only three mononuclear complexes based on the H*L* ligand have been reported (Chen *et al.*,2010). In this paper, we report the synthesis and structure of the title compound, (I), obtained by the solvothermal reaction of $NiCl_2$ and H*L* ligand.

In (I) (Fig. 1), the Ni(II) ion is coordinated by two N and two O atoms from two bidentate chelating *L* ligands and two O atoms from two ethanol molecules in a distorted octahedral geometry. The Ni—N bond length is equal to 2.055 (3) Å, and the Ni—O distances vary from 2.037 (3) to 2.107 (2) Å. In the crystal, intermolecular O—H···O and N–H···O hydrogen bonds (Table1) involving the carboxylate O atoms, the imidazole N atoms and the coordinated ethanol O atoms link the molecules into a two-dimensional supramolecular network parallel to the *bc* plane (Fig. 2).

Experimental

A mixture of $NiCl_2$ (0.40 mmol), H*L* (0.40 mmol) and 8 ml C_2H_5OH was sealed into a 15 ml Teflon-lined stainless steel autoclave and then heated at 373 K for 72 h under autogenous pressure. After cooling to room temperature at a rate of 2 K /h, green block crystals of the title compound suitable for X-ray diffraction were obtained (yield: 35%).

Refinement

C– and N-bound H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.97 Å, N —H = 0.86 Å and with U_{iso}(H) = 1.2(1.5 for methyl)U_{eq}(C), U_{iso}(H) = 1.2U_{eq}(N). Hydroxy H atoms were located in a difference Fourier map and refined as riding, with O—H = 0.85 Å and U_{iso}(H)= 1.2U_{eq}(O).

Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

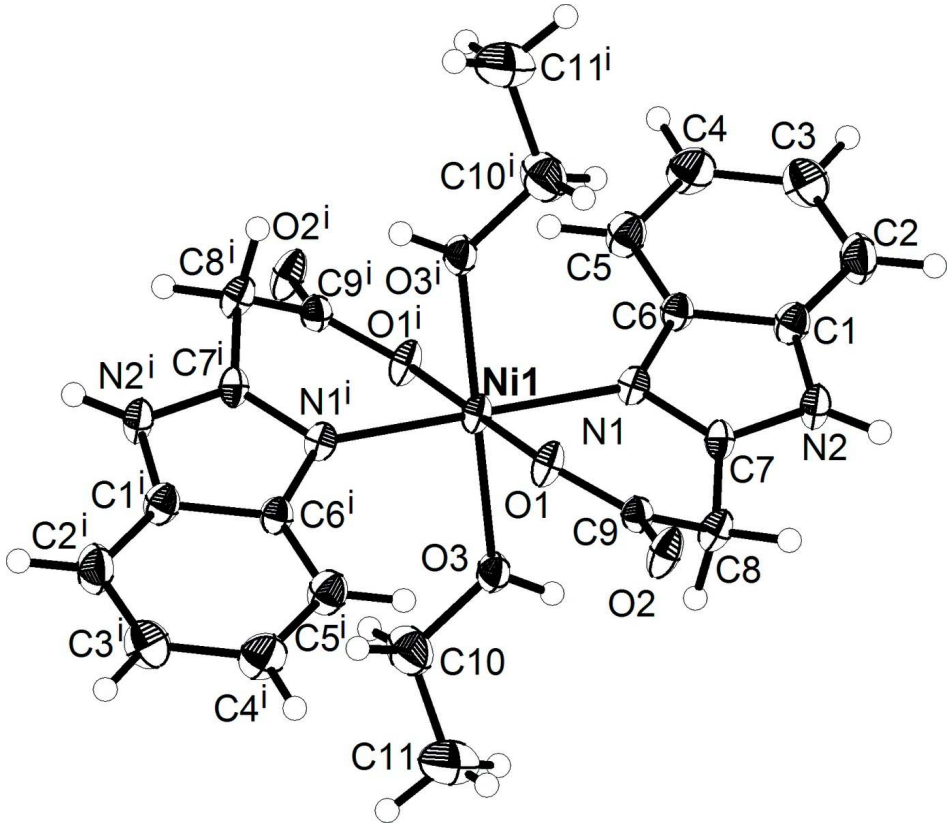

Figure 1

The molecular structure of (I) with displacement ellipsoids drawn at the 30% probability level [symmetry code\: (i) 1 - *x*, -*y*, -*z*].

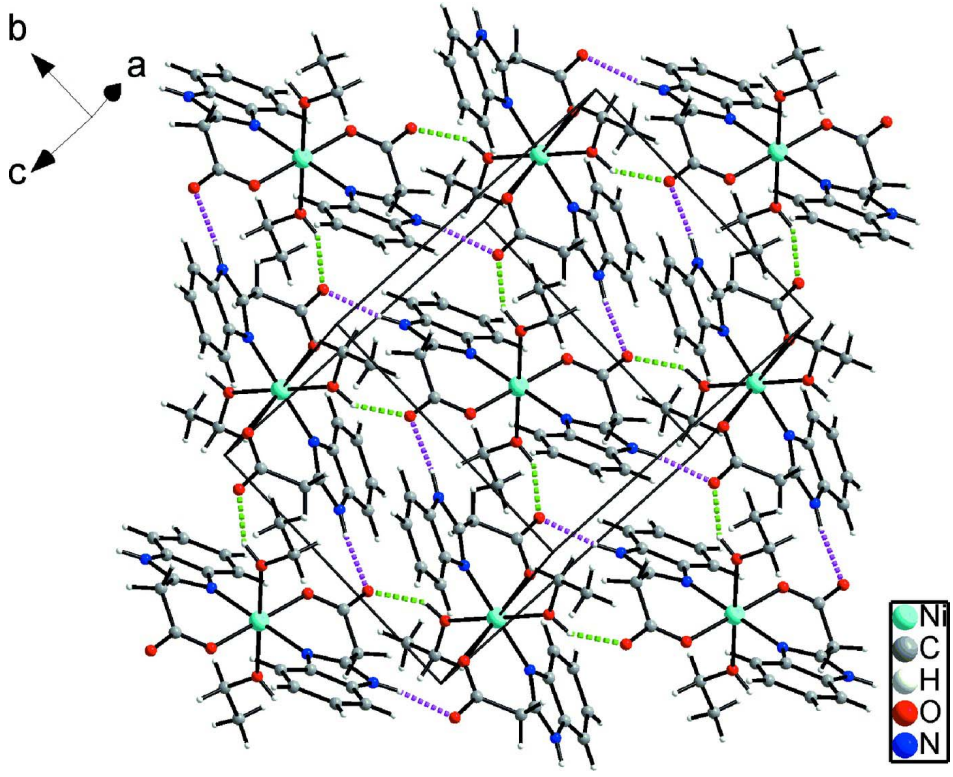

Figure 2

A portion of the crystal packing, showing the two-dimensional supramolecular network. Hydrogen bonds are shown as dashed lines.

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Crystal data

$[Ni(C_9H_7N_2O_2)_2(C_2H_6O)_2]$
M_r = 501.18
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 10.441 (5) Å
b = 9.639 (4) Å
c = 11.480 (5) Å
β = 98.956 (6)°
V = 1141.3 (9) Å^3
Z = 2
$F(000)$ = 524
D_x = 1.458 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1078 reflections
θ = 2.8–21.1°
μ = 0.90 mm^{-1}
T = 298 K
Block, green
0.28 × 0.26 × 0.23 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.788, T_{max} = 0.821
6022 measured reflections
2231 independent reflections
1411 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 26.0°, θ_{min} = 2.8°
h = −8→12
k = −11→11
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.107$
$S = 1.04$
2231 reflections
152 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
$w = 1/[\sigma^2(F_o^2) + (0.0364P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.45$ 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	0.5000	0.0000	0.0000	0.0295 (2)
C7	0.5632 (4)	0.2871 (4)	−0.0656 (3)	0.0303 (9)
C1	0.7327 (4)	0.3710 (4)	0.0516 (3)	0.0372 (10)
C6	0.7025 (4)	0.2385 (4)	0.0887 (3)	0.0310 (9)
C8	0.4525 (4)	0.2834 (4)	−0.1641 (3)	0.0357 (10)
H8A	0.4655	0.3559	−0.2197	0.043*
H8B	0.3741	0.3059	−0.1325	0.043*
C5	0.7763 (4)	0.1803 (4)	0.1874 (4)	0.0451 (11)
H5	0.7568	0.0929	0.2141	0.054*
C4	0.8787 (4)	0.2548 (5)	0.2444 (4)	0.0564 (13)
H4	0.9294	0.2178	0.3109	0.068*
C2	0.8367 (4)	0.4466 (4)	0.1082 (4)	0.0538 (12)
H2	0.8568	0.5341	0.0821	0.065*
C3	0.9081 (4)	0.3863 (4)	0.2039 (4)	0.0574 (13)
H3	0.9789	0.4340	0.2440	0.069*
C9	0.4305 (4)	0.1481 (4)	−0.2311 (3)	0.0302 (9)
O2	0.3884 (3)	0.1537 (2)	−0.3388 (2)	0.0435 (7)
O1	0.4545 (2)	0.0357 (2)	−0.1765 (2)	0.0357 (7)
N1	0.5959 (3)	0.1869 (3)	0.0125 (3)	0.0300 (8)
N2	0.6410 (3)	0.3986 (3)	−0.0456 (3)	0.0382 (8)
H2A	0.6347	0.4739	−0.0864	0.046*
O3	0.3382 (2)	0.1147 (2)	0.0343 (2)	0.0367 (7)
H3A	0.3398	0.2025	0.0416	0.044*
C10	0.2225 (5)	0.0637 (5)	0.0670 (5)	0.0627 (14)
H10A	0.2386	0.0401	0.1502	0.075*
H10B	0.1984	−0.0209	0.0233	0.075*

C11	0.1146 (5)	0.1594 (6)	0.0467 (6)	0.112 (2)
H11A	0.1364	0.2427	0.0913	0.168*
H11B	0.0397	0.1175	0.0710	0.168*
H11C	0.0962	0.1817	−0.0358	0.168*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0404 (5)	0.0212 (4)	0.0268 (4)	−0.0017 (3)	0.0044 (3)	0.0004 (3)
C7	0.039 (3)	0.022 (2)	0.031 (2)	−0.0052 (18)	0.0072 (18)	−0.0016 (17)
C1	0.045 (3)	0.029 (2)	0.037 (2)	−0.002 (2)	0.003 (2)	−0.0036 (18)
C6	0.035 (3)	0.027 (2)	0.031 (2)	−0.0018 (18)	0.0041 (19)	−0.0012 (17)
C8	0.050 (3)	0.024 (2)	0.031 (2)	0.0009 (19)	0.000 (2)	0.0009 (17)
C5	0.052 (3)	0.037 (2)	0.044 (3)	−0.003 (2)	−0.002 (2)	−0.002 (2)
C4	0.057 (4)	0.054 (3)	0.051 (3)	−0.001 (3)	−0.013 (2)	0.000 (2)
C2	0.059 (3)	0.038 (3)	0.060 (3)	−0.015 (2)	−0.002 (3)	0.004 (2)
C3	0.053 (3)	0.049 (3)	0.065 (3)	−0.014 (3)	−0.007 (3)	−0.015 (3)
C9	0.032 (2)	0.027 (2)	0.032 (2)	−0.0036 (18)	0.0043 (18)	−0.0002 (18)
O2	0.071 (2)	0.0274 (15)	0.0280 (16)	−0.0006 (14)	−0.0061 (14)	0.0026 (12)
O1	0.0565 (19)	0.0214 (14)	0.0283 (15)	0.0004 (12)	0.0041 (12)	0.0010 (11)
N1	0.038 (2)	0.0250 (17)	0.0270 (18)	−0.0005 (15)	0.0042 (15)	0.0012 (14)
N2	0.051 (2)	0.0258 (18)	0.037 (2)	−0.0079 (16)	0.0018 (17)	0.0063 (15)
O3	0.0414 (18)	0.0256 (14)	0.0448 (17)	−0.0020 (13)	0.0118 (13)	−0.0006 (12)
C10	0.058 (4)	0.051 (3)	0.083 (4)	−0.007 (3)	0.025 (3)	−0.014 (3)
C11	0.054 (4)	0.089 (5)	0.195 (8)	0.013 (4)	0.025 (4)	0.012 (5)

Geometric parameters (Å, º)

Ni1—O1^{i}	2.037 (3)	C5—H5	0.9300
Ni1—O1	2.037 (3)	C4—C3	1.400 (6)
Ni1—N1^{i}	2.055 (3)	C4—H4	0.9300
Ni1—N1	2.055 (3)	C2—C3	1.358 (6)
Ni1—O3^{i}	2.107 (2)	C2—H2	0.9300
Ni1—O3	2.107 (2)	C3—H3	0.9300
C7—N1	1.325 (4)	C9—O2	1.247 (4)
C7—N2	1.346 (4)	C9—O1	1.257 (4)
C7—C8	1.487 (5)	N2—H2A	0.8600
C1—N2	1.379 (5)	O3—C10	1.409 (5)
C1—C2	1.384 (5)	O3—H3A	0.8500
C1—C6	1.398 (5)	C10—C11	1.447 (6)
C6—C5	1.386 (5)	C10—H10A	0.9700
C6—N1	1.395 (5)	C10—H10B	0.9700
C8—C9	1.514 (5)	C11—H11A	0.9600
C8—H8A	0.9700	C11—H11B	0.9600
C8—H8B	0.9700	C11—H11C	0.9600
C5—C4	1.367 (5)		
O1^{i}—Ni1—O1	180.0	C5—C4—H4	119.6
O1^{i}—Ni1—N1^{i}	87.54 (10)	C3—C4—H4	119.6
O1—Ni1—N1^{i}	92.46 (10)	C3—C2—C1	116.5 (4)

O1^{i}—Ni1—N1	92.46 (10)	C3—C2—H2	121.7
O1—Ni1—N1	87.54 (10)	C1—C2—H2	121.7
N1^{i}—Ni1—N1	180.0	C2—C3—C4	122.3 (4)
O1^{i}—Ni1—O3^{i}	91.58 (10)	C2—C3—H3	118.8
O1—Ni1—O3^{i}	88.42 (10)	C4—C3—H3	118.8
N1^{i}—Ni1—O3^{i}	85.58 (11)	O2—C9—O1	123.0 (3)
N1—Ni1—O3^{i}	94.42 (11)	O2—C9—C8	117.9 (3)
O1^{i}—Ni1—O3	88.42 (10)	O1—C9—C8	119.1 (3)
O1—Ni1—O3	91.58 (10)	C9—O1—Ni1	129.7 (2)
N1^{i}—Ni1—O3	94.42 (11)	C7—N1—C6	105.1 (3)
N1—Ni1—O3	85.58 (11)	C7—N1—Ni1	121.3 (2)
O3^{i}—Ni1—O3	180.0	C6—N1—Ni1	133.5 (2)
N1—C7—N2	112.5 (3)	C7—N2—C1	107.9 (3)
N1—C7—C8	125.8 (3)	C7—N2—H2A	126.0
N2—C7—C8	121.7 (3)	C1—N2—H2A	126.0
N2—C1—C2	132.4 (4)	C10—O3—Ni1	127.8 (2)
N2—C1—C6	105.2 (3)	C10—O3—H3A	109.0
C2—C1—C6	122.4 (4)	Ni1—O3—H3A	122.5
C5—C6—N1	131.0 (3)	O3—C10—C11	114.4 (4)
C5—C6—C1	119.7 (4)	O3—C10—H10A	108.7
N1—C6—C1	109.3 (3)	C11—C10—H10A	108.7
C7—C8—C9	116.4 (3)	O3—C10—H10B	108.7
C7—C8—H8A	108.2	C11—C10—H10B	108.7
C9—C8—H8A	108.2	H10A—C10—H10B	107.6
C7—C8—H8B	108.2	C10—C11—H11A	109.5
C9—C8—H8B	108.2	C10—C11—H11B	109.5
H8A—C8—H8B	107.3	H11A—C11—H11B	109.5
C4—C5—C6	118.2 (4)	C10—C11—H11C	109.5
C4—C5—H5	120.9	H11A—C11—H11C	109.5
C6—C5—H5	120.9	H11B—C11—H11C	109.5
C5—C4—C3	120.8 (4)		

N2—C1—C6—C5	−178.9 (3)	N2—C7—N1—Ni1	−177.1 (2)
C2—C1—C6—C5	1.7 (6)	C8—C7—N1—Ni1	4.1 (5)
N2—C1—C6—N1	1.4 (4)	C5—C6—N1—C7	179.3 (4)
C2—C1—C6—N1	−178.0 (4)	C1—C6—N1—C7	−1.1 (4)
N1—C7—C8—C9	−41.6 (5)	C5—C6—N1—Ni1	−3.7 (6)
N2—C7—C8—C9	139.7 (3)	C1—C6—N1—Ni1	175.9 (2)
N1—C6—C5—C4	178.5 (4)	O1^{i}—Ni1—N1—C7	−154.3 (3)
C1—C6—C5—C4	−1.1 (6)	O1—Ni1—N1—C7	25.7 (3)
C6—C5—C4—C3	−0.1 (7)	O3^{i}—Ni1—N1—C7	114.0 (3)
N2—C1—C2—C3	179.8 (4)	O3—Ni1—N1—C7	−66.0 (3)
C6—C1—C2—C3	−1.0 (7)	O1^{i}—Ni1—N1—C6	29.2 (3)
C1—C2—C3—C4	−0.2 (7)	O1—Ni1—N1—C6	−150.8 (3)
C5—C4—C3—C2	0.8 (7)	O3^{i}—Ni1—N1—C6	−62.6 (3)
C7—C8—C9—O2	−146.1 (4)	O3—Ni1—N1—C6	117.4 (3)
C7—C8—C9—O1	34.2 (5)	N1—C7—N2—C1	0.5 (4)
O2—C9—O1—Ni1	−171.0 (3)	C8—C7—N2—C1	179.4 (3)
C8—C9—O1—Ni1	8.7 (5)	C2—C1—N2—C7	178.1 (4)

N1^{i}—Ni1—O1—C9	145.8 (3)	C6—C1—N2—C7	−1.2 (4)
N1—Ni1—O1—C9	−34.2 (3)	O1^{i}—Ni1—O3—C10	−73.1 (3)
O3^{i}—Ni1—O1—C9	−128.7 (3)	O1—Ni1—O3—C10	106.9 (3)
O3—Ni1—O1—C9	51.3 (3)	N1^{i}—Ni1—O3—C10	14.3 (3)
N2—C7—N1—C6	0.4 (4)	N1—Ni1—O3—C10	−165.7 (3)
C8—C7—N1—C6	−178.4 (4)	Ni1—O3—C10—C11	−160.5 (4)

Symmetry code: (i) −*x*+1, −*y*, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···O2^{ii}	0.85	1.96	2.672 (3)	141
N2—H2*A*···O2^{iii}	0.86	1.93	2.788 (4)	173

Symmetry codes: (ii) *x*, −*y*+1/2, *z*+1/2; (iii) −*x*+1, *y*+1/2, −*z*−1/2.