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Bis(2,2′,2″-nitrilotriacetamide-κ^3O,N,O')-nickel(II) dinitrate tetrahydrate

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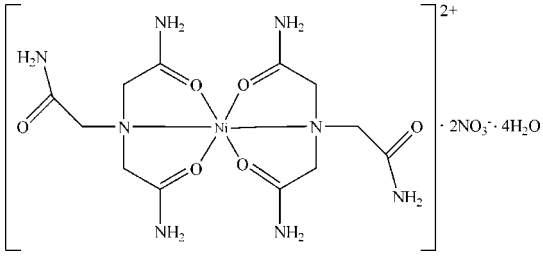
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.088; data-to-parameter ratio = 12.4.

In the title compound, $[Ni(C_6H_{12}N_4O_3)_2](NO_3)_2\cdot4H_2O$, the Ni^{II} cation is located on an inversion center and is N,O,O'-chelated by two nitrilotris(acetamide) molecules in a distorted octahedral geometry. The complex cations, nitrate anions and lattice water molecules are connected by O—H···O and N—H···O hydrogen bonds, forming a three-dimensional supramolecular structure.

Related literature

For related metal complexes, see: Niraj *et al.* (2012); Biswajit *et al.* (2009); Ben Amor *et al.* (1998). For the synthesis of the ligand, see: Donald & George (1974).



Experimental

Crystal data

$[Ni(C_6H_{12}N_4O_3)_2](NO_3)_2\cdot4H_2O$
M_r = 631.17
Triclinic, $P\overline{1}$
a = 8.557 (7) Å
b = 9.212 (8) Å
c = 9.367 (8) Å
α = 91.180 (14)°
β = 96.215 (14)°
γ = 111.136 (14)°
V = 683.2 (10) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.80 mm^{-1}
T = 296 K
0.42 × 0.38 × 0.33 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.731, T_{max} = 0.779
3732 measured reflections
2352 independent reflections
2219 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.088
S = 1.05
2352 reflections
190 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O8^{i}	0.86	2.14	2.988 (3)	169
N2—H2B···O6^{ii}	0.86	2.19	3.027 (4)	165
N3—H3A···O4^{iii}	0.86	2.28	3.056 (4)	150
N3—H3B···O3^{ii}	0.86	1.99	2.848 (3)	173
N4—H4A···O7^{iv}	0.86	2.22	3.002 (3)	152
N4—H4B···O7	0.86	2.32	3.068 (4)	145
O7—H7A···O4	0.87 (2)	2.08 (2)	2.913 (4)	162 (3)
O7—H7B···O8^{v}	0.87 (2)	1.98 (2)	2.843 (3)	174 (4)
O8—H8A···O1^{iii}	0.86 (2)	2.18 (2)	3.018 (3)	165 (3)
O8—H8B···O4	0.86 (2)	2.19 (2)	2.999 (4)	157 (3)
O8—H8B···O6	0.86 (2)	2.40 (3)	3.107 (4)	141 (3)

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* ; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5668).

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Xiao-Hui Deng, Qi-Jun Nie and Feng-Juan Zhu

S1. Comment

Coordination chemistry of nitrilotriacetic acid with metal ions is explored extensively owing to their flexible coordinating nature, but nitrilotriacetamide (H_3NTA) is hardly studied (Niraj *et al.*, 2012; Biswajit *et al.*, 2009; Ben Amor *et al.*, 1998). This is the first report of a bis(H_3NTA)–nickel(II) structure in which only H_3NTA acts as a tridentate ligand.

Complex I consists of a Ni(H_3NTA)$_2$ cation, two nitrate anions and four solvent water molecules (Scheme). Ni(II) has an octahedral coordination environment which is centrosymmetric as Ni(II) occupies an inversion center. The Ni atom is coordinated in a planar geometry by the nitrilotriacetamide N and O atoms. Two *trans* axial sites of this coordination environment is occupied by O2 and its symmetry related O2′ oxygen atoms from ligands(Fig. 1). In the equatorial plane the Ni—N1 distance is 2.131 (2) Å and the Ni—O1 distance is 2.098 (2) Å. The axial Ni—O2 bond is appreciably shortened which is 2.036 (2) Å. A few more selected bond distances and bond angles are presented in Table 1. The molecules are stacked along the *a* axis and display N—H···O and O—H···O hydrogen-bonds interaction (Fig. 2).

S2. Experimental

The synthesis of nitrilotriacetamide was carried out according to US patent 3799981 (Donald & George, 1974). The title compound was synthesized by adding solid Ni(NO_3)$_2$.6H_2O (291 mg, 1 mmol) to a solution of ligands (376 mg, 2 mmol) in ethanol/water (2:1, 20 ml), then the mixture was stirred for 2 h at room temperature. The solution was filtered and the filtrate was allowed to stand in air for 1 d, and blue crystals were formed at the bottom of the vessel on slow evaporation of the solvent at room temperature.Yield: 73%.

S3. Refinement

Water H atoms were located in a difference Fourier map and the positional parameters were refined, U_{iso}(H) = 1.5U_{eq}(O). Other H atoms were included in calculated positions with C—H = 0.93 or 0.97 and N—H = 0.86 Å, and refined using a riding-model with U_{iso}(H) = 1.2U_{eq}(C,N).

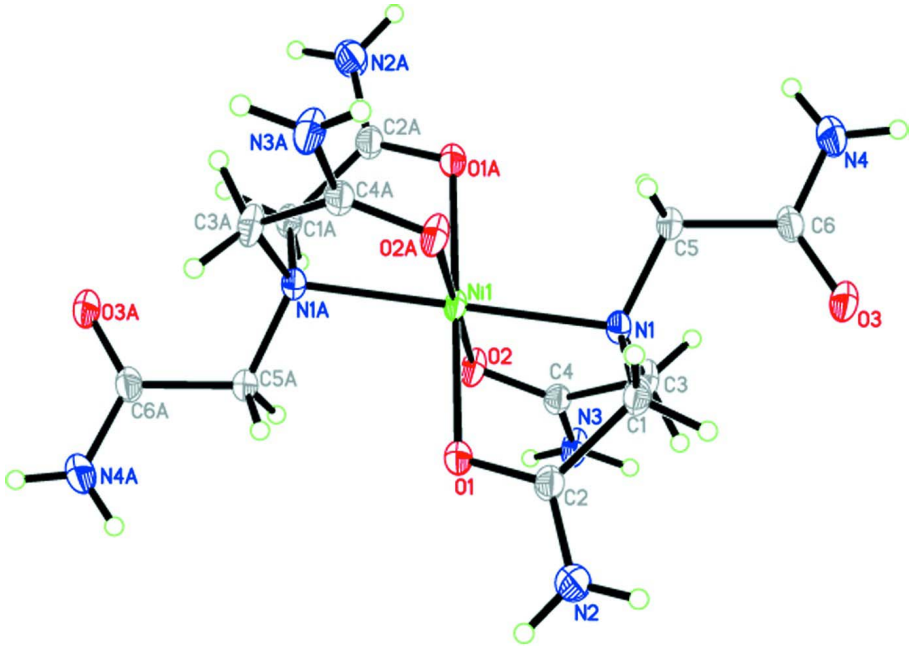

Figure 1

The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

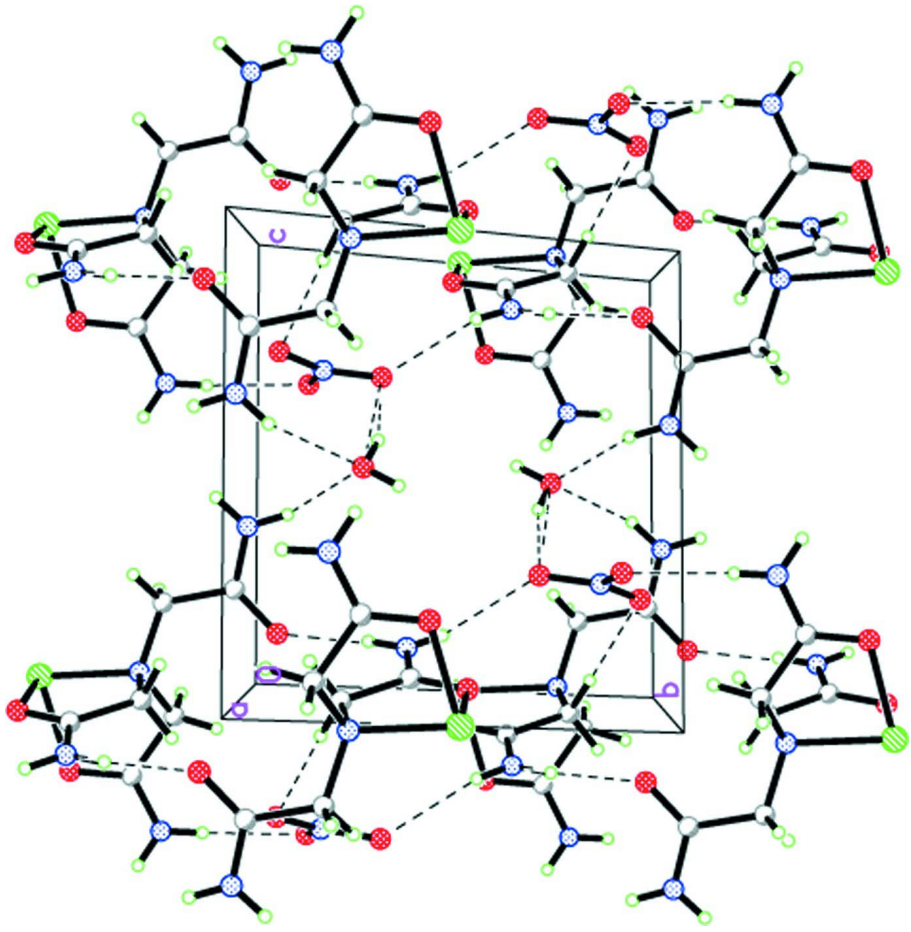

Figure 2

The packed diagram for the title compound, viewed down the *a* axis with hydrogen bonds drawn as dashed lines.

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Triclinic, $P\overline{1}$
Hall symbol: -P 1
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$c = 9.367$ (8) Å
$\alpha = 91.180$ (14)°
$\beta = 96.215$ (14)°
$\gamma = 111.136$ (14)°
$V = 683.2$ (10) Å^3
$Z = 1$
$F(000) = 330$
$D_x = 1.534$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2322 reflections
$\theta = 2.4$–28.2°
$\mu = 0.80$ mm^{-1}
$T = 296$ K
Block, blue
0.42 × 0.38 × 0.33 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.731$, $T_{max} = 0.779$
3732 measured reflections
2352 independent reflections

2219 reflections with $I > 2\sigma(I)$
$R_{int} = 0.014$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$
$h = -10 \rightarrow 10$
$k = -10 \rightarrow 10$
$l = -11 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.088$
$S = 1.05$
2352 reflections
190 parameters
6 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0494P)^2 + 0.3085P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Special details

Experimental. Selected IR data (cm^{-1}): 3315 (*s*), 3192 (*s*), 2935(w), 2783(w), 1666(*s*), 1596(*s*), 1276(*m*), 1134(*m*), 997(*m*), 867(*m*), 729(w), 561(*s*).

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	1.0000	0.5000	1.0000	0.02392 (14)
O1	1.0488 (2)	0.43473 (17)	1.20851 (16)	0.0346 (4)
O3	0.7111 (2)	−0.06864 (18)	0.86966 (18)	0.0445 (4)
O2	0.78448 (19)	0.51673 (16)	1.05845 (18)	0.0341 (4)
O4	0.3921 (3)	0.3138 (2)	0.7047 (3)	0.0796 (8)
O5	0.3643 (3)	0.0742 (3)	0.7446 (3)	0.0766 (7)
O6	0.1436 (3)	0.1309 (3)	0.6829 (3)	0.0760 (7)
O8	0.1390 (3)	0.4509 (2)	0.58844 (19)	0.0503 (5)
H8A	0.070 (4)	0.467 (4)	0.640 (3)	0.075*
H8B	0.188 (4)	0.396 (4)	0.635 (3)	0.075*
O7	0.6156 (3)	0.2788 (2)	0.5043 (2)	0.0618 (6)
H7A	0.563 (4)	0.311 (4)	0.564 (4)	0.093*
H7B	0.685 (4)	0.361 (3)	0.470 (4)	0.093*
N4	0.6721 (3)	−0.0015 (2)	0.6398 (2)	0.0488 (6)
H4A	0.6150	−0.0964	0.6083	0.059*
H4B	0.6905	0.0722	0.5816	0.059*
N1	0.8516 (2)	0.25706 (19)	0.97289 (18)	0.0255 (4)
N3	0.5292 (2)	0.3768 (2)	1.1244 (2)	0.0383 (5)
H3A	0.5150	0.4598	1.1533	0.046*

H3B	0.4526	0.2868	1.1308	0.046*
N2	1.0204 (3)	0.2211 (2)	1.3335 (2)	0.0504 (6)
H2A	1.0547	0.2765	1.4138	0.060*
H2B	0.9931	0.1216	1.3325	0.060*
N5	0.3008 (3)	0.1727 (3)	0.7132 (3)	0.0495 (6)
C4	0.6690 (3)	0.3874 (2)	1.0699 (2)	0.0278 (4)
C1	0.9486 (3)	0.1859 (2)	1.0730 (2)	0.0301 (5)
H1A	1.0441	0.1794	1.0299	0.036*
H1B	0.8767	0.0813	1.0920	0.036*
C6	0.7323 (3)	0.0313 (2)	0.7789 (2)	0.0313 (5)
C2	1.0099 (3)	0.2884 (2)	1.2128 (2)	0.0316 (5)
C5	0.8390 (3)	0.2040 (2)	0.8193 (2)	0.0322 (5)
H5A	0.9522	0.2242	0.7956	0.039*
H5B	0.7918	0.2669	0.7599	0.039*
C3	0.6822 (3)	0.2338 (2)	1.0189 (3)	0.0346 (5)
H3C	0.6623	0.1635	1.0963	0.041*
H3D	0.5953	0.1855	0.9388	0.041*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0223 (2)	0.0156 (2)	0.0283 (2)	0.00044 (14)	0.00210 (14)	0.00082 (14)
O1	0.0430 (9)	0.0214 (8)	0.0311 (8)	0.0035 (7)	−0.0013 (7)	0.0001 (6)
O3	0.0518 (11)	0.0231 (8)	0.0437 (9)	−0.0027 (7)	0.0006 (8)	0.0012 (7)
O2	0.0284 (8)	0.0193 (7)	0.0515 (9)	0.0033 (6)	0.0110 (7)	0.0018 (6)
O4	0.0941 (18)	0.0344 (11)	0.1007 (18)	0.0035 (11)	0.0446 (15)	−0.0048 (11)
O5	0.0583 (14)	0.0618 (14)	0.109 (2)	0.0227 (12)	0.0036 (13)	0.0220 (13)
O6	0.0538 (13)	0.0572 (13)	0.123 (2)	0.0250 (11)	0.0171 (13)	0.0198 (13)
O8	0.0604 (13)	0.0489 (11)	0.0404 (10)	0.0185 (10)	0.0068 (9)	0.0036 (8)
O7	0.0663 (14)	0.0445 (11)	0.0573 (13)	−0.0015 (10)	0.0122 (10)	−0.0014 (9)
N4	0.0606 (14)	0.0304 (11)	0.0401 (11)	0.0019 (10)	−0.0052 (10)	−0.0068 (9)
N1	0.0240 (9)	0.0187 (8)	0.0296 (9)	0.0033 (7)	0.0013 (7)	−0.0007 (7)
N3	0.0323 (10)	0.0231 (9)	0.0577 (13)	0.0052 (8)	0.0156 (9)	0.0004 (9)
N2	0.0761 (16)	0.0300 (11)	0.0355 (11)	0.0115 (11)	−0.0064 (10)	0.0045 (9)
N5	0.0567 (15)	0.0376 (12)	0.0546 (13)	0.0139 (11)	0.0196 (11)	0.0053 (10)
C4	0.0258 (10)	0.0242 (11)	0.0303 (11)	0.0062 (9)	0.0010 (8)	0.0019 (8)
C1	0.0325 (11)	0.0195 (10)	0.0342 (11)	0.0060 (9)	−0.0007 (9)	0.0019 (8)
C6	0.0305 (11)	0.0234 (11)	0.0358 (11)	0.0050 (9)	0.0040 (9)	−0.0054 (9)
C2	0.0307 (11)	0.0252 (11)	0.0332 (11)	0.0050 (9)	−0.0017 (9)	0.0021 (9)
C5	0.0372 (12)	0.0216 (10)	0.0292 (11)	0.0011 (9)	0.0024 (9)	−0.0001 (8)
C3	0.0247 (11)	0.0211 (10)	0.0529 (14)	0.0017 (9)	0.0079 (10)	−0.0008 (9)

Geometric parameters (Å, º)

Ni1—O2	2.036 (2)	N1—C5	1.490 (3)
Ni1—O2^{i}	2.036 (2)	N1—C3	1.499 (3)
Ni1—O1^{i}	2.098 (2)	N1—C1	1.499 (3)
Ni1—O1	2.098 (2)	N3—C4	1.323 (3)

Ni1—N1	2.131 (2)	N3—H3A	0.8600
Ni1—N1^{i}	2.131 (2)	N3—H3B	0.8600
O1—C2	1.270 (3)	N2—C2	1.311 (3)
O3—C6	1.244 (3)	N2—H2A	0.8600
O2—C4	1.259 (3)	N2—H2B	0.8600
O4—N5	1.262 (3)	C4—C3	1.530 (3)
O5—N5	1.239 (3)	C1—C2	1.525 (3)
O6—N5	1.256 (3)	C1—H1A	0.9700
O8—H8A	0.856 (17)	C1—H1B	0.9700
O8—H8B	0.859 (17)	C6—C5	1.537 (3)
O7—H7A	0.868 (18)	C5—H5A	0.9700
O7—H7B	0.866 (18)	C5—H5B	0.9700
N4—C6	1.335 (3)	C3—H3C	0.9700
N4—H4A	0.8600	C3—H3D	0.9700
N4—H4B	0.8600		

O2—Ni1—O2^{i}	180.0	C2—N2—H2B	120.0
O2—Ni1—O1^{i}	92.01 (7)	H2A—N2—H2B	120.0
O2^{i}—Ni1—O1^{i}	87.99 (7)	O5—N5—O6	119.8 (2)
O2—Ni1—O1	87.99 (7)	O5—N5—O4	121.1 (3)
O2^{i}—Ni1—O1	92.01 (7)	O6—N5—O4	119.1 (3)
O1^{i}—Ni1—O1	180.000 (1)	O2—C4—N3	122.14 (19)
O2—Ni1—N1	83.50 (8)	O2—C4—C3	121.45 (19)
O2^{i}—Ni1—N1	96.50 (7)	N3—C4—C3	116.40 (18)
O1^{i}—Ni1—N1	99.63 (7)	N1—C1—C2	108.21 (17)
O1—Ni1—N1	80.37 (7)	N1—C1—H1A	110.1
O2—Ni1—N1^{i}	96.50 (7)	C2—C1—H1A	110.1
O2^{i}—Ni1—N1^{i}	83.50 (8)	N1—C1—H1B	110.1
O1^{i}—Ni1—N1^{i}	80.37 (7)	C2—C1—H1B	110.1
O1—Ni1—N1^{i}	99.63 (7)	H1A—C1—H1B	108.4
N1—Ni1—N1^{i}	180.0	O3—C6—N4	123.8 (2)
C2—O1—Ni1	112.16 (13)	O3—C6—C5	121.5 (2)
C4—O2—Ni1	114.27 (14)	N4—C6—C5	114.6 (2)
H8A—O8—H8B	109 (2)	O1—C2—N2	122.5 (2)
H7A—O7—H7B	107 (2)	O1—C2—C1	119.24 (18)
C6—N4—H4A	120.0	N2—C2—C1	118.3 (2)
C6—N4—H4B	120.0	N1—C5—C6	115.90 (17)
H4A—N4—H4B	120.0	N1—C5—H5A	108.3
C5—N1—C3	112.27 (17)	C6—C5—H5A	108.3
C5—N1—C1	112.83 (17)	N1—C5—H5B	108.3
C3—N1—C1	111.36 (17)	C6—C5—H5B	108.3
C5—N1—Ni1	108.65 (12)	H5A—C5—H5B	107.4
C3—N1—Ni1	107.87 (12)	N1—C3—C4	112.21 (16)
C1—N1—Ni1	103.32 (13)	N1—C3—H3C	109.2
C4—N3—H3A	120.0	C4—C3—H3C	109.2
C4—N3—H3B	120.0	N1—C3—H3D	109.2
H3A—N3—H3B	120.0	C4—C3—H3D	109.2
C2—N2—H2A	120.0	H3C—C3—H3D	107.9

O2—Ni1—O1—C2	100.65 (16)	O1^{i}—Ni1—N1—C1	147.65 (13)
O2^{i}—Ni1—O1—C2	−79.35 (16)	O1—Ni1—N1—C1	−32.35 (13)
O1^{i}—Ni1—O1—C2	177 (100)	N1^{i}—Ni1—N1—C1	−136 (100)
N1—Ni1—O1—C2	16.91 (15)	Ni1—O2—C4—N3	171.21 (17)
N1^{i}—Ni1—O1—C2	−163.09 (15)	Ni1—O2—C4—C3	−9.8 (3)
O2^{i}—Ni1—O2—C4	178 (100)	C5—N1—C1—C2	159.20 (17)
O1^{i}—Ni1—O2—C4	106.73 (15)	C3—N1—C1—C2	−73.5 (2)
O1—Ni1—O2—C4	−73.27 (15)	Ni1—N1—C1—C2	42.05 (18)
N1—Ni1—O2—C4	7.27 (15)	Ni1—O1—C2—N2	−175.82 (19)
N1^{i}—Ni1—O2—C4	−172.73 (15)	Ni1—O1—C2—C1	4.2 (3)
O2—Ni1—N1—C5	118.55 (14)	N1—C1—C2—O1	−33.3 (3)
O2^{i}—Ni1—N1—C5	−61.45 (14)	N1—C1—C2—N2	146.7 (2)
O1^{i}—Ni1—N1—C5	27.60 (14)	C3—N1—C5—C6	−59.4 (2)
O1—Ni1—N1—C5	−152.40 (14)	C1—N1—C5—C6	67.4 (2)
N1^{i}—Ni1—N1—C5	103 (100)	Ni1—N1—C5—C6	−178.62 (15)
O2—Ni1—N1—C3	−3.40 (13)	O3—C6—C5—N1	−25.7 (3)
O2^{i}—Ni1—N1—C3	176.60 (13)	N4—C6—C5—N1	157.0 (2)
O1^{i}—Ni1—N1—C3	−94.34 (14)	C5—N1—C3—C4	−119.78 (19)
O1—Ni1—N1—C3	85.66 (14)	C1—N1—C3—C4	112.6 (2)
N1^{i}—Ni1—N1—C3	−18 (100)	Ni1—N1—C3—C4	−0.1 (2)
O2—Ni1—N1—C1	−121.40 (14)	O2—C4—C3—N1	6.6 (3)
O2^{i}—Ni1—N1—C1	58.60 (14)	N3—C4—C3—N1	−174.31 (19)

Symmetry code: (i) −*x*+2, −*y*+1, −*z*+2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O8^{ii}	0.86	2.14	2.988 (3)	169
N2—H2*B*···O6^{iii}	0.86	2.19	3.027 (4)	165
N3—H3*A*···O4^{iv}	0.86	2.28	3.056 (4)	150
N3—H3*B*···O3^{iii}	0.86	1.99	2.848 (3)	173
N4—H4*A*···O7^{v}	0.86	2.22	3.002 (3)	152
N4—H4*B*···O7	0.86	2.32	3.068 (4)	145
O7—H7*A*···O4	0.87 (2)	2.08 (2)	2.913 (4)	162 (3)
O7—H7*B*···O8^{vi}	0.87 (2)	1.98 (2)	2.843 (3)	174 (4)
O8—H8*A*···O1^{iv}	0.86 (2)	2.18 (2)	3.018 (3)	165 (3)
O8—H8*B*···O4	0.86 (2)	2.19 (2)	2.999 (4)	157 (3)
O8—H8*B*···O6	0.86 (2)	2.40 (3)	3.107 (4)	141 (3)

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