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Bis{*N*-[2-(2-hydroxy-3-methoxybenzylamino)ethyl]-*N*′-(2-hydroxy-3-methoxybenzyl)ethane-1,2-diamine}nickel(II) dinitrate 1.25-hydrate

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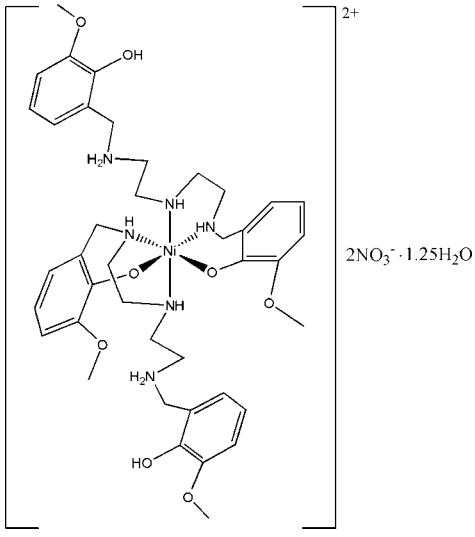
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.009 Å; disorder in solvent or counterion; R factor = 0.064; wR factor = 0.154; data-to-parameter ratio = 13.4.

In the title compound, $[Ni(C_{20}H_{29}N_3O_4)_2](NO_3)_2\cdot1.25H_2O$, the asymmetric unit consists of one cation, two nitrate anions, one complete water molecule and a half-occupancy water molecule lying on a twofold rotation axis. The Ni atom is situated in a distorted octahedral geometry. The molecules are linked into a three-dimensional network by O—H···O, N—H···O and C—H···O hydrogen bonds. Two nitrate O atoms are disordered over two sites in the ratio 0.64:0.36.

Related literature

For related literature, see: Xia *et al.* (2007).



Experimental

Crystal data

$[Ni(C_{20}H_{29}N_3O_4)_2](NO_3)_2\cdot1.25H_2O$
M_r = 3824.70
Monoclinic, $C2/c$
a = 43.710 (3) Å
b = 9.5091 (16) Å
c = 28.476 (3) Å
β = 130.370 (3)°
V = 9017.5 (18) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.51 mm^{-1}
T = 298 (2) K
0.40 × 0.16 × 0.13 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.823, T_{max} = 0.937
22092 measured reflections
7920 independent reflections
3683 reflections with $I > 2\sigma(I)$
R_{int} = 0.074

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.154
S = 1.00
7920 reflections
593 parameters
116 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.39 e Å^{-3}
$\Delta\rho_{min}$ = −1.20 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	2.025 (3)	Ni1—N1	2.110 (4)
Ni1—O5	2.041 (3)	Ni1—N2	2.184 (4)
Ni1—N4	2.102 (4)	Ni1—N5	2.212 (4)
O1—Ni1—O5	84.85 (12)	N4—Ni1—N2	92.02 (17)
O1—Ni1—N4	171.59 (16)	N1—Ni1—N2	81.37 (16)
O5—Ni1—N4	89.52 (15)	O1—Ni1—N5	91.79 (14)
O1—Ni1—N1	89.02 (14)	O5—Ni1—N5	91.33 (14)
O5—Ni1—N1	172.66 (15)	N4—Ni1—N5	82.08 (16)
N4—Ni1—N1	97.00 (16)	N1—Ni1—N5	92.89 (16)
O1—Ni1—N2	94.69 (14)	N2—Ni1—N5	171.25 (15)
O5—Ni1—N2	95.09 (14)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O9^{i}	0.91	2.38	3.122 (6)	139
N1—H1···O10^{i}	0.91	2.31	3.163 (6)	156
N2—H2···O13′^{ii}	0.91	2.14	2.976 (11)	152
N4—H4···O12^{ii}	0.91	2.21	3.021 (8)	148
O15—H42···O10^{iii}	0.85	2.32	3.013 (6)	138
O15—H42···O11^{iii}	0.85	2.14	2.965 (6)	163
C9—H9*B*···O14′^{iv}	0.97	2.48	3.420 (10)	163
C17—H17*A*···O12^{ii}	0.97	2.59	3.445 (9)	147
C34—H34···O11^{v}	0.93	2.59	3.419 (8)	149
O16—H43···O13′^{iv}	0.85	1.66	2.464 (17)	156
O3—H3···O15	0.82	1.98	2.653 (5)	139
O3—H3···O4	0.82	2.21	2.659 (5)	115
N3—H3*A*···O5	0.90	1.73	2.617 (5)	168
N3—H3*B*···O2	0.90	2.53	3.211 (5)	133
N3—H3*B*···O3	0.90	2.23	2.838 (5)	124
N5—H5···O9	0.91	2.24	3.123 (6)	165
N6—H6*A*···O5	0.90	2.49	2.936 (5)	111
N6—H6*A*···O6	0.90	2.10	2.961 (6)	161
N6—H6*B*···O1	0.90	1.72	2.612 (5)	169
O7—H7···O8	0.82	2.20	2.633 (6)	113
O7—H7···O15	0.82	2.13	2.872 (6)	151
O15—H41···O12	0.85	2.21	3.037 (8)	166
C1—H1*B*···O9	0.97	2.49	3.438 (7)	165
C29—H29*A*···O2	0.97	2.50	3.382 (6)	151

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D—H···A	D—H	H···A	D···A	D—H···A
C29—H29A···O7	0.97	2.39	2.757 (7)	102
C40—H40B···O9	0.97	2.56	3.369 (7)	141
C40—H40B···O11	0.97	2.53	3.456 (7)	160
C39—H39B···O5	0.97	2.55	3.087 (6)	115

Symmetry codes: (i) $-x+\frac{3}{2}, -y+\frac{3}{2}, -z+2$; (ii) $x, -y+1, z+\frac{1}{2}$; (iii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x+1, -y+1, -z+1$; (v) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: AT2393).

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supplementary materials

Acta Cryst. (2007). E**63**, m2512-m2513 [**doi:10.1107/S160053680704353X**]

Bis{*N*-[2-(2-hydroxy-3-methoxybenzylamino)ethyl]-*N*'-(2-hydroxy-3-methoxybenzyl)ethane-1,2-diamine}nickel(II) dinitrate 1.25-hydrate

H.-T. Xia, Y.-F. Liu, D.-Q. Wang and S.-P. Yang

Comment

We have recently reported crystal structure of nickel complex with diamine derivatives (Xia *et al.*, 2007). We have now continued our studied in this area with the title complex, (I).

In (I), the asymmetric unit consists of one cation, two anions, one water molecules and one OH group. The Ni atom is six coordinated by four nitrogen and two oxygen atoms (Fig. 1). The equatorial plane are formed by N1, N4, O1 and O5 atoms, the axial positions are occupied by atoms O2 and N5. The Ni atom is shifted by 0.0217 (16)Å from the equatorial plane toward the axial N2 atom, and the coordinating N1, N4, O1and O5 atoms show the distortions with deviations of 0.0820 (14) Å, −0.0824 (13) Å, 0.0947 (16)Å and −0.944 (16)Å from the least-square N_2O_2 plane. The dihedral angles between equatorial plane and aryl rings are 20.03 (18)° for the ring (C2–C7), 71.03 (11)° for the ring (C10–C15), 24.12 (18)° for the ring (C22–C27) and 83.08 (10)° for the ring (C30–C35).

The molecules of the title complex (I) are linked into a three-dimensional network by O—H···O, N—H···O and C—H···O hydrogen bonds (Table 2).

Experimental

N-[2-(2-hydroxy-3-methoxybenzylamino)ethyl]-*N*′-[2-hydroxy-3-methoxybenzyl] ethane-1,2diamine (1 mmol) was dissolved in 10 ml e thanol, and 10 ml aqueous solution of nickel(II) nitrate (1 mmol) was added. The reaction mixture was stirred 2 h and filtered. The blue crystals of (I) suitable for X-ray diffraction was obtained by evaporation of an solution.

Refinement

All H atoms were located in difference Fourier maps. The O13, O14, O13' and O14' bond to N8 of the nitrate were to be disordered over two sites. The coordinates of these two sites were refined with the occupancies tied to sum to unity. The site occupancies for O13, O14 and O13', O14' refined to 0.360 and 0.640, and at the same time O16 with attached H atoms was, found to be disordered in occupancies which were refined to half unity. H atoms bonded to C, N and O atoms were treated as riding atoms, with C—H distances of 0.93 Å (aryl), 0.96 Å (methyl), 0.97 Å(methylene), O—H distance of 0.85 Å and N—H distance of 0.91 Å (amine), and with U_{iso}(H) = 1.2U_{eq}(C,*N*) (aryl, methylene, amine) and 1.5U_{eq}(C,*O*) (methyl and water).

Figures

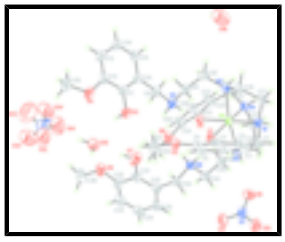

Fig. 1. The structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are at the 30% probability level.

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Crystal data

$[Ni(C_{20}H_{29}N_3O_4)_2](NO_3)_2\cdot 1.25H_2O$	$F_{000} = 4052$
$M_r = 3824.70$	$D_x = 1.409$ Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 2390 reflections
a = 43.710 (3) Å	θ = 2.6–18.2º
b = 9.5091 (16) Å	μ = 0.51 mm^{-1}
c = 28.476 (3) Å	*T* = 298 (2) K
β = 130.370 (3)º	Block, blue
V = 9017.5 (18) Å^3	0.40 × 0.16 × 0.13 mm
Z = 8	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	7920 independent reflections
Radiation source: fine-focus sealed tube	3683 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.074$
T = 298(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.4$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −51→51
$T_{min} = 0.823$, $T_{max} = 0.937$	*k* = −11→11
22092 measured reflections	*l* = −33→31

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.064$	H-atom parameters constrained
$wR(F^2) = 0.154$	$w = 1/[\sigma^2(F_o^2) + (0.0509P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.016$
7920 reflections	$\Delta\rho_{max} = 1.39$ e Å^{-3}
593 parameters	$\Delta\rho_{min} = -1.20$ e Å^{-3}
116 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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}	Occ. (<1)
Ni1	0.641419 (19)	0.66303 (7)	0.83507 (3)	0.0421 (2)	
N1	0.67961 (12)	0.5637 (5)	0.92197 (18)	0.0470 (11)	
H1	0.6824	0.6245	0.9492	0.056*	
N2	0.60570 (12)	0.4742 (4)	0.81236 (18)	0.0453 (11)	
H2	0.5900	0.4979	0.8217	0.054*	
N3	0.59205 (12)	0.5073 (4)	0.68534 (18)	0.0503 (12)	
H3A	0.6004	0.5837	0.7095	0.060*	
H3B	0.6092	0.4943	0.6783	0.060*	
N4	0.60783 (12)	0.7801 (5)	0.85042 (19)	0.0495 (12)	
H4	0.6088	0.7336	0.8793	0.059*	
N5	0.67810 (11)	0.8570 (4)	0.87038 (17)	0.0446 (11)	
H5	0.7044	0.8311	0.8952	0.053*	
N6	0.67847 (11)	0.7963 (4)	0.76456 (18)	0.0457 (11)	
H6A	0.6527	0.8062	0.7299	0.055*	
H6B	0.6795	0.7251	0.7864	0.055*	
N7	0.79795 (17)	0.8175 (6)	0.9440 (3)	0.0647 (14)	
N8	0.5515 (3)	0.4732 (12)	0.3733 (4)	0.166 (3)	
O1	0.67406 (9)	0.5765 (4)	0.81493 (14)	0.0434 (9)	
O2	0.68190 (10)	0.4173 (4)	0.74696 (16)	0.0532 (10)	
O3	0.59061 (11)	0.4258 (4)	0.58805 (17)	0.0726 (12)	
H3	0.6000	0.3898	0.5736	0.109*	
O4	0.56196 (12)	0.2248 (5)	0.50398 (18)	0.0799 (13)	
O5	0.60564 (9)	0.7372 (3)	0.74682 (14)	0.0394 (8)	
O6	0.59622 (13)	0.8973 (4)	0.66216 (17)	0.0809 (9)	
O7	0.64853 (14)	0.6522 (5)	0.62992 (19)	0.1009 (16)	

H7	0.6368	0.6205	0.5953	0.151*	
O8	0.62619 (13)	0.7786 (4)	0.52971 (19)	0.0809 (9)	
O9	0.77001 (13)	0.8176 (6)	0.9444 (2)	0.0993 (17)	
O10	0.83138 (14)	0.7824 (5)	0.9913 (2)	0.0956 (16)	
O11	0.79332 (12)	0.8545 (5)	0.8982 (2)	0.0886 (15)	
O12	0.5796 (2)	0.4142 (10)	0.3996 (3)	0.198 (3)	
O13	0.5197 (4)	0.418 (3)	0.3255 (11)	0.239 (8)	0.360 (10)
O14	0.5441 (6)	0.554 (3)	0.3961 (9)	0.215 (6)	0.360 (10)
O13'	0.5460 (3)	0.5510 (16)	0.3304 (6)	0.224 (5)	0.640 (10)
O14'	0.5220 (3)	0.4543 (18)	0.3637 (6)	0.195 (4)	0.640 (10)
O15	0.62322 (12)	0.4501 (5)	0.53586 (19)	0.0917 (15)	
H41	0.6075	0.4356	0.4972	0.138*	
H42	0.6448	0.4093	0.5489	0.138*	
O16	0.5000	0.2747 (19)	0.7500	0.166 (7)	0.50
H43	0.4795	0.3158	0.7182	0.250*	0.50
C1	0.72074 (15)	0.5365 (6)	0.9449 (2)	0.0542 (15)	
H1A	0.7367	0.4966	0.9860	0.065*	
H1B	0.7328	0.6256	0.9483	0.065*	
C2	0.72261 (14)	0.4396 (6)	0.9053 (2)	0.0449 (14)	
C3	0.70035 (14)	0.4694 (5)	0.8429 (2)	0.0408 (13)	
C4	0.70488 (15)	0.3824 (5)	0.8079 (3)	0.0425 (14)	
C5	0.73178 (16)	0.2706 (6)	0.8355 (3)	0.0525 (15)	
H5A	0.7351	0.2143	0.8124	0.063*	
C6	0.75355 (17)	0.2434 (6)	0.8974 (3)	0.0651 (17)	
H6	0.7713	0.1679	0.9158	0.078*	
C7	0.74916 (15)	0.3271 (6)	0.9317 (3)	0.0580 (16)	
H7A	0.7642	0.3084	0.9735	0.070*	
C8	0.68558 (16)	0.3331 (6)	0.7093 (2)	0.0658 (17)	
H8A	0.7133	0.3268	0.7281	0.099*	
H8B	0.6706	0.3754	0.6693	0.099*	
H8C	0.6753	0.2406	0.7052	0.099*	
C9	0.55143 (15)	0.5370 (6)	0.6253 (2)	0.0548 (15)	
H9A	0.5530	0.6196	0.6070	0.066*	
H9B	0.5333	0.5586	0.6330	0.066*	
C10	0.53406 (16)	0.4178 (6)	0.5800 (2)	0.0466 (14)	
C11	0.55433 (15)	0.3678 (6)	0.5615 (2)	0.0492 (15)	
C12	0.53789 (18)	0.2648 (6)	0.5165 (2)	0.0553 (16)	
C13	0.50100 (19)	0.2091 (6)	0.4911 (3)	0.0640 (17)	
H13	0.4899	0.1379	0.4618	0.077*	
C14	0.48067 (18)	0.2600 (7)	0.5094 (3)	0.0665 (18)	
H14	0.4554	0.2244	0.4913	0.080*	
C15	0.49687 (17)	0.3610 (7)	0.5532 (3)	0.0558 (16)	
H15	0.4828	0.3924	0.5655	0.067*	
C16	0.5453 (2)	0.1424 (7)	0.4510 (3)	0.095 (2)	
H16A	0.5380	0.0517	0.4559	0.143*	
H16B	0.5647	0.1312	0.4457	0.143*	
H16C	0.5219	0.1882	0.4155	0.143*	
C17	0.65999 (16)	0.4377 (6)	0.9215 (2)	0.0588 (16)	
H17A	0.6439	0.4638	0.9326	0.071*	

H17B	0.6803	0.3717	0.9522	0.071*
C18	0.63343 (16)	0.3673 (6)	0.8591 (2)	0.0545 (15)
H18A	0.6497	0.3279	0.8503	0.065*
H18B	0.6183	0.2918	0.8586	0.065*
C19	0.57708 (16)	0.4114 (6)	0.7500 (2)	0.0612 (16)
H19A	0.5544	0.4744	0.7238	0.073*
H19B	0.5671	0.3237	0.7529	0.073*
C20	0.59466 (17)	0.3830 (6)	0.7197 (2)	0.0562 (16)
H20A	0.6226	0.3562	0.7510	0.067*
H20B	0.5805	0.3047	0.6914	0.067*
C21	0.56470 (15)	0.7916 (6)	0.7938 (2)	0.0550 (16)
H21A	0.5499	0.8349	0.8046	0.066*
H21B	0.5539	0.6979	0.7784	0.066*
C22	0.55834 (14)	0.8767 (5)	0.7434 (2)	0.0420 (14)
C23	0.57919 (14)	0.8421 (6)	0.7233 (2)	0.0376 (12)
C24	0.57242 (15)	0.9306 (6)	0.6775 (2)	0.0412 (13)
C25	0.54597 (14)	1.0401 (6)	0.6519 (2)	0.0483 (14)
H25	0.5420	1.0943	0.6212	0.058*
C26	0.52528 (15)	1.0701 (6)	0.6717 (3)	0.0543 (16)
H26	0.5069	1.1437	0.6541	0.065*
C27	0.53190 (15)	0.9910 (6)	0.7175 (3)	0.0563 (16)
H27	0.5185	1.0136	0.7319	0.068*
C28	0.5962 (2)	0.9959 (8)	0.6247 (3)	0.0952 (16)
H28A	0.5704	0.9957	0.5840	0.143*
H28B	0.6165	0.9706	0.6224	0.143*
H28C	0.6017	1.0881	0.6422	0.143*
C29	0.70348 (15)	0.7592 (6)	0.7475 (2)	0.0519 (15)
H29A	0.7009	0.6591	0.7391	0.062*
H29B	0.7314	0.7781	0.7826	0.062*
C30	0.69241 (16)	0.8374 (6)	0.6927 (3)	0.0483 (14)
C31	0.66558 (19)	0.7776 (7)	0.6360 (3)	0.0632 (17)
C32	0.6551 (2)	0.8495 (8)	0.5839 (3)	0.0768 (19)
C33	0.6706 (2)	0.9770 (8)	0.5890 (4)	0.080 (2)
H33	0.6627	1.0250	0.5542	0.095*
C34	0.6981 (2)	1.0331 (7)	0.6462 (4)	0.081 (2)
H34	0.7097	1.1194	0.6505	0.097*
C35	0.70907 (18)	0.9656 (7)	0.6977 (3)	0.0659 (17)
H35	0.7279	1.0065	0.7363	0.079*
C36	0.6178 (2)	0.8226 (8)	0.4753 (3)	0.0952 (16)
H36A	0.6071	0.9164	0.4654	0.143*
H36B	0.5984	0.7603	0.4423	0.143*
H36C	0.6420	0.8212	0.4811	0.143*
C37	0.62605 (16)	0.9192 (6)	0.8758 (3)	0.0600 (16)
H37A	0.6216	0.9490	0.9035	0.072*
H37B	0.6133	0.9870	0.8425	0.072*
C38	0.67043 (16)	0.9163 (6)	0.9101 (2)	0.0590 (16)
H38A	0.6812	1.0109	0.9226	0.071*
H38B	0.6839	0.8594	0.9470	0.071*
C39	0.67105 (15)	0.9631 (6)	0.8263 (2)	0.0516 (15)

H39A	0.6805	1.0538	0.8467	0.062*
H39B	0.6424	0.9708	0.7922	0.062*
C40	0.69177 (15)	0.9282 (6)	0.8014 (2)	0.0524 (15)
H40A	0.6877	1.0058	0.7758	0.063*
H40B	0.7204	0.9212	0.8358	0.063*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0469 (4)	0.0429 (4)	0.0366 (4)	0.0007 (4)	0.0271 (3)	−0.0002 (3)
N1	0.055 (3)	0.047 (3)	0.041 (3)	−0.001 (2)	0.032 (2)	−0.003 (2)
N2	0.048 (3)	0.052 (3)	0.038 (3)	−0.002 (2)	0.029 (2)	0.003 (2)
N3	0.056 (3)	0.045 (3)	0.045 (3)	−0.004 (2)	0.031 (3)	−0.008 (2)
N4	0.058 (3)	0.056 (3)	0.043 (3)	−0.002 (3)	0.036 (3)	−0.002 (2)
N5	0.042 (2)	0.046 (3)	0.038 (3)	0.003 (2)	0.022 (2)	0.001 (2)
N6	0.044 (3)	0.046 (3)	0.046 (3)	0.003 (2)	0.029 (2)	0.010 (2)
N7	0.065 (4)	0.077 (4)	0.052 (4)	−0.001 (3)	0.038 (3)	−0.012 (3)
N8	0.142 (7)	0.275 (10)	0.158 (8)	−0.020 (7)	0.132 (7)	−0.078 (6)
O1	0.048 (2)	0.041 (2)	0.042 (2)	0.0081 (18)	0.0299 (19)	0.0072 (18)
O2	0.068 (2)	0.046 (2)	0.054 (3)	0.011 (2)	0.044 (2)	0.001 (2)
O3	0.060 (3)	0.090 (3)	0.068 (3)	−0.019 (2)	0.041 (2)	−0.033 (2)
O4	0.076 (3)	0.094 (4)	0.064 (3)	−0.022 (3)	0.043 (3)	−0.038 (3)
O5	0.045 (2)	0.034 (2)	0.042 (2)	0.0036 (18)	0.0297 (18)	0.0019 (17)
O6	0.109 (2)	0.073 (2)	0.056 (2)	0.0023 (19)	0.051 (2)	0.0137 (17)
O7	0.134 (4)	0.068 (3)	0.064 (3)	−0.039 (3)	0.048 (3)	−0.003 (2)
O8	0.109 (2)	0.073 (2)	0.056 (2)	0.0023 (19)	0.051 (2)	0.0137 (17)
O9	0.064 (3)	0.153 (5)	0.088 (4)	−0.009 (3)	0.053 (3)	0.002 (3)
O10	0.071 (3)	0.147 (5)	0.059 (3)	0.016 (3)	0.037 (3)	0.007 (3)
O11	0.090 (3)	0.126 (4)	0.061 (3)	0.010 (3)	0.054 (3)	0.006 (3)
O12	0.130 (6)	0.308 (9)	0.181 (6)	−0.021 (5)	0.111 (6)	−0.106 (6)
O13	0.168 (9)	0.305 (12)	0.206 (11)	−0.010 (9)	0.104 (9)	−0.091 (10)
O14	0.173 (9)	0.318 (12)	0.193 (10)	−0.016 (9)	0.136 (8)	−0.096 (9)
O13'	0.172 (7)	0.352 (11)	0.211 (9)	−0.043 (7)	0.151 (7)	−0.054 (8)
O14'	0.143 (7)	0.308 (11)	0.206 (9)	−0.025 (7)	0.145 (7)	−0.055 (8)
O15	0.089 (3)	0.114 (4)	0.093 (3)	−0.015 (3)	0.068 (3)	−0.026 (3)
O16	0.201 (10)	0.167 (11)	0.208 (11)	0.000	0.166 (9)	0.000
C1	0.054 (4)	0.058 (4)	0.034 (3)	0.006 (3)	0.021 (3)	0.008 (3)
C2	0.038 (3)	0.042 (4)	0.045 (4)	0.005 (3)	0.022 (3)	0.010 (3)
C3	0.039 (3)	0.034 (3)	0.046 (4)	0.000 (3)	0.026 (3)	0.004 (3)
C4	0.048 (3)	0.033 (4)	0.044 (4)	−0.005 (3)	0.029 (3)	−0.001 (3)
C5	0.057 (4)	0.036 (4)	0.068 (4)	0.002 (3)	0.042 (4)	−0.002 (3)
C6	0.060 (4)	0.049 (4)	0.072 (5)	0.015 (3)	0.037 (4)	0.016 (4)
C7	0.049 (4)	0.058 (4)	0.054 (4)	0.011 (3)	0.028 (3)	0.018 (3)
C8	0.072 (4)	0.070 (5)	0.061 (4)	0.012 (4)	0.045 (4)	−0.005 (4)
C9	0.061 (4)	0.048 (4)	0.045 (4)	0.007 (3)	0.030 (3)	0.002 (3)
C10	0.049 (4)	0.039 (4)	0.041 (3)	0.005 (3)	0.025 (3)	0.007 (3)
C11	0.038 (3)	0.052 (4)	0.038 (3)	−0.005 (3)	0.016 (3)	−0.005 (3)
C12	0.055 (4)	0.057 (4)	0.039 (4)	−0.002 (3)	0.024 (3)	−0.003 (3)

C13	0.065 (4)	0.055 (4)	0.042 (4)	−0.008 (4)	0.022 (4)	−0.003 (3)
C14	0.054 (4)	0.062 (5)	0.055 (4)	−0.009 (4)	0.023 (4)	0.001 (4)
C15	0.050 (4)	0.066 (5)	0.047 (4)	0.015 (3)	0.030 (3)	0.014 (3)
C16	0.108 (5)	0.095 (6)	0.073 (5)	−0.014 (5)	0.055 (5)	−0.037 (4)
C17	0.061 (4)	0.074 (5)	0.047 (4)	0.006 (3)	0.037 (3)	0.013 (3)
C18	0.060 (4)	0.044 (4)	0.056 (4)	0.000 (3)	0.036 (3)	0.008 (3)
C19	0.065 (4)	0.062 (4)	0.056 (4)	−0.015 (3)	0.039 (4)	−0.003 (3)
C20	0.072 (4)	0.040 (4)	0.047 (4)	−0.002 (3)	0.034 (3)	−0.001 (3)
C21	0.051 (4)	0.064 (4)	0.061 (4)	0.006 (3)	0.041 (4)	0.001 (3)
C22	0.043 (3)	0.040 (4)	0.044 (3)	0.005 (3)	0.029 (3)	−0.002 (3)
C23	0.040 (3)	0.034 (3)	0.039 (3)	−0.006 (3)	0.026 (3)	−0.009 (3)
C24	0.045 (3)	0.037 (4)	0.043 (3)	−0.008 (3)	0.029 (3)	−0.009 (3)
C25	0.046 (3)	0.040 (4)	0.049 (4)	0.004 (3)	0.027 (3)	0.006 (3)
C26	0.042 (3)	0.047 (4)	0.062 (4)	0.003 (3)	0.028 (3)	−0.006 (3)
C27	0.046 (4)	0.066 (5)	0.065 (4)	0.005 (3)	0.040 (3)	−0.006 (4)
C28	0.119 (4)	0.103 (4)	0.073 (3)	0.023 (3)	0.066 (3)	0.018 (3)
C29	0.054 (3)	0.051 (4)	0.063 (4)	0.003 (3)	0.043 (3)	0.002 (3)
C30	0.053 (3)	0.042 (4)	0.067 (4)	0.003 (3)	0.046 (3)	0.003 (3)
C31	0.077 (5)	0.053 (5)	0.065 (5)	−0.007 (4)	0.049 (4)	0.001 (4)
C32	0.095 (5)	0.067 (5)	0.059 (5)	−0.016 (4)	0.046 (4)	−0.015 (4)
C33	0.122 (6)	0.056 (5)	0.095 (6)	0.014 (5)	0.086 (6)	0.015 (4)
C34	0.113 (6)	0.053 (5)	0.117 (7)	−0.010 (4)	0.093 (6)	0.003 (5)
C35	0.077 (4)	0.054 (5)	0.083 (5)	−0.008 (4)	0.059 (4)	−0.008 (4)
C36	0.119 (4)	0.103 (4)	0.073 (3)	0.023 (3)	0.066 (3)	0.018 (3)
C37	0.072 (4)	0.059 (4)	0.058 (4)	−0.001 (4)	0.046 (4)	−0.013 (3)
C38	0.074 (4)	0.050 (4)	0.052 (4)	−0.006 (3)	0.040 (4)	−0.013 (3)
C39	0.063 (4)	0.039 (4)	0.053 (4)	−0.006 (3)	0.037 (3)	−0.006 (3)
C40	0.060 (4)	0.043 (4)	0.051 (4)	−0.005 (3)	0.035 (3)	−0.002 (3)

Geometric parameters (Å, °)

Ni1—O1	2.025 (3)	C9—C10	1.503 (7)
Ni1—O5	2.041 (3)	C9—H9A	0.9700
Ni1—N4	2.102 (4)	C9—H9B	0.9700
Ni1—N1	2.110 (4)	C10—C11	1.376 (7)
Ni1—N2	2.184 (4)	C10—C15	1.382 (7)
Ni1—N5	2.212 (4)	C11—C12	1.386 (7)
N1—C17	1.468 (6)	C12—C13	1.375 (7)
N1—C1	1.485 (6)	C13—C14	1.376 (7)
N1—H1	0.9100	C13—H13	0.9300
N2—C18	1.478 (6)	C14—C15	1.356 (8)
N2—C19	1.483 (6)	C14—H14	0.9300
N2—H2	0.9100	C15—H15	0.9300
N3—C9	1.491 (6)	C16—H16A	0.9600
N3—C20	1.491 (6)	C16—H16B	0.9600
N3—H3A	0.9000	C16—H16C	0.9600
N3—H3B	0.9000	C17—C18	1.510 (7)
N4—C37	1.470 (7)	C17—H17A	0.9700
N4—C21	1.492 (6)	C17—H17B	0.9700

N4—H4	0.9100	C18—H18A	0.9700
N5—C39	1.480 (6)	C18—H18B	0.9700
N5—C38	1.485 (6)	C19—C20	1.504 (7)
N5—H5	0.9100	C19—H19A	0.9700
N6—C40	1.489 (6)	C19—H19B	0.9700
N6—C29	1.497 (5)	C20—H20A	0.9700
N6—H6A	0.9000	C20—H20B	0.9700
N6—H6B	0.9000	C21—C22	1.510 (7)
N7—O9	1.229 (11)	C21—H21A	0.9700
N7—O10	1.229 (5)	C21—H21B	0.9700
N7—O11	1.235 (6)	C22—C23	1.393 (6)
N8—O12	1.093 (10)	C22—C27	1.399 (7)
N8—O14'	1.148 (10)	C23—C24	1.412 (7)
N8—O14	1.178 (12)	C24—C25	1.364 (6)
N8—O13	1.266 (13)	C25—C26	1.370 (6)
N8—O13'	1.310 (12)	C25—H25	0.9300
O1—C3	1.344 (5)	C26—C27	1.364 (7)
O2—C4	1.369 (6)	C26—H26	0.9300
O2—C8	1.428 (6)	C27—H27	0.9300
O3—C11	1.355 (6)	C28—H28A	0.9600
O3—H3	0.8200	C28—H28B	0.9600
O4—C12	1.367 (6)	C28—H28C	0.9600
O4—C16	1.413 (6)	C29—C30	1.499 (7)
O5—C23	1.333 (5)	C29—H29A	0.9700
O6—C24	1.402 (6)	C29—H29B	0.9700
O6—C28	1.421 (7)	C30—C31	1.361 (7)
O7—C31	1.357 (7)	C30—C35	1.379 (7)
O7—H7	0.8200	C31—C32	1.414 (8)
O8—C32	1.381 (7)	C32—C33	1.350 (8)
O8—C36	1.403 (6)	C33—C34	1.359 (8)
O15—H41	0.8501	C33—H33	0.9300
O15—H42	0.8501	C34—C35	1.372 (8)
O16—H43	0.8500	C34—H34	0.9300
C1—C2	1.500 (7)	C35—H35	0.9300
C1—H1A	0.9700	C36—H36A	0.9600
C1—H1B	0.9700	C36—H36B	0.9600
C2—C7	1.388 (7)	C36—H36C	0.9600
C2—C3	1.393 (6)	C37—C38	1.504 (7)
C3—C4	1.405 (6)	C37—H37A	0.9700
C4—C5	1.390 (7)	C37—H37B	0.9700
C5—C6	1.379 (7)	C38—H38A	0.9700
C5—H5A	0.9300	C38—H38B	0.9700
C6—C7	1.367 (7)	C39—C40	1.506 (6)
C6—H6	0.9300	C39—H39A	0.9700
C7—H7A	0.9300	C39—H39B	0.9700
C8—H8A	0.9600	C40—H40A	0.9700
C8—H8B	0.9600	C40—H40B	0.9700
C8—H8C	0.9600		
O1—Ni1—O5	84.85 (12)	C15—C14—C13	121.2 (6)

O1—Ni1—N4	171.59 (16)	C15—C14—H14	119.4
O5—Ni1—N4	89.52 (15)	C13—C14—H14	119.4
O1—Ni1—N1	89.02 (14)	C14—C15—C10	120.7 (6)
O5—Ni1—N1	172.66 (15)	C14—C15—H15	119.7
N4—Ni1—N1	97.00 (16)	C10—C15—H15	119.7
O1—Ni1—N2	94.69 (14)	O4—C16—H16A	109.5
O5—Ni1—N2	95.09 (14)	O4—C16—H16B	109.5
N4—Ni1—N2	92.02 (17)	H16A—C16—H16B	109.5
N1—Ni1—N2	81.37 (16)	O4—C16—H16C	109.5
O1—Ni1—N5	91.79 (14)	H16A—C16—H16C	109.5
O5—Ni1—N5	91.33 (14)	H16B—C16—H16C	109.5
N4—Ni1—N5	82.08 (16)	N1—C17—C18	111.8 (4)
N1—Ni1—N5	92.89 (16)	N1—C17—H17A	109.3
N2—Ni1—N5	171.25 (15)	C18—C17—H17A	109.3
C17—N1—C1	113.3 (4)	N1—C17—H17B	109.3
C17—N1—Ni1	110.0 (3)	C18—C17—H17B	109.3
C1—N1—Ni1	114.0 (3)	H17A—C17—H17B	107.9
C17—N1—H1	106.3	N2—C18—C17	108.2 (5)
C1—N1—H1	106.3	N2—C18—H18A	110.1
Ni1—N1—H1	106.3	C17—C18—H18A	110.1
C18—N2—C19	111.4 (4)	N2—C18—H18B	110.1
C18—N2—Ni1	106.7 (3)	C17—C18—H18B	110.1
C19—N2—Ni1	124.9 (3)	H18A—C18—H18B	108.4
C18—N2—H2	103.9	N2—C19—C20	114.3 (4)
C19—N2—H2	103.9	N2—C19—H19A	108.7
Ni1—N2—H2	103.9	C20—C19—H19A	108.7
C9—N3—C20	115.5 (4)	N2—C19—H19B	108.7
C9—N3—H3A	108.4	C20—C19—H19B	108.7
C20—N3—H3A	108.4	H19A—C19—H19B	107.6
C9—N3—H3B	108.4	N3—C20—C19	112.5 (5)
C20—N3—H3B	108.4	N3—C20—H20A	109.1
H3A—N3—H3B	107.5	C19—C20—H20A	109.1
C37—N4—C21	111.6 (4)	N3—C20—H20B	109.1
C37—N4—Ni1	110.5 (3)	C19—C20—H20B	109.1
C21—N4—Ni1	112.2 (3)	H20A—C20—H20B	107.8
C37—N4—H4	107.4	N4—C21—C22	113.1 (4)
C21—N4—H4	107.4	N4—C21—H21A	109.0
Ni1—N4—H4	107.4	C22—C21—H21A	109.0
C39—N5—C38	111.3 (4)	N4—C21—H21B	109.0
C39—N5—Ni1	119.4 (3)	C22—C21—H21B	109.0
C38—N5—Ni1	102.0 (3)	H21A—C21—H21B	107.8
C39—N5—H5	107.9	C23—C22—C27	120.3 (5)
C38—N5—H5	107.9	C23—C22—C21	119.9 (5)
Ni1—N5—H5	107.9	C27—C22—C21	119.8 (5)
C40—N6—C29	113.1 (4)	O5—C23—C22	123.7 (5)
C40—N6—H6A	109.0	O5—C23—C24	120.4 (4)
C29—N6—H6A	109.0	C22—C23—C24	115.9 (5)
C40—N6—H6B	109.0	C25—C24—O6	123.3 (5)
C29—N6—H6B	109.0	C25—C24—C23	123.1 (5)

H6A—N6—H6B	107.8	O6—C24—C23	113.5 (5)
O9—N7—O10	118.3 (6)	C24—C25—C26	119.7 (5)
O9—N7—O11	121.7 (6)	C24—C25—H25	120.1
O10—N7—O11	120.0 (5)	C26—C25—H25	120.1
O12—N8—O14'	132.4 (14)	C27—C26—C25	119.4 (5)
O12—N8—O14	123.0 (13)	C27—C26—H26	120.3
O14'—N8—O14	64.3 (11)	C25—C26—H26	120.3
O12—N8—O13	119.4 (14)	C26—C27—C22	121.5 (5)
O14'—N8—O13	53.0 (13)	C26—C27—H27	119.2
O14—N8—O13	111.0 (12)	C22—C27—H27	119.2
O12—N8—O13'	112.0 (9)	O6—C28—H28A	109.5
O14'—N8—O13'	111.7 (11)	O6—C28—H28B	109.5
O14—N8—O13'	101 (2)	H28A—C28—H28B	109.5
O13—N8—O13'	79.6 (19)	O6—C28—H28C	109.5
C3—O1—Ni1	128.9 (3)	H28A—C28—H28C	109.5
C4—O2—C8	118.0 (4)	H28B—C28—H28C	109.5
C11—O3—H3	109.5	N6—C29—C30	114.2 (4)
C12—O4—C16	118.8 (5)	N6—C29—H29A	108.7
C23—O5—Ni1	126.9 (3)	C30—C29—H29A	108.7
C24—O6—C28	116.5 (5)	N6—C29—H29B	108.7
C31—O7—H7	109.8	C30—C29—H29B	108.7
C32—O8—C36	119.0 (5)	H29A—C29—H29B	107.6
H41—O15—H42	103.3	C31—C30—C35	118.9 (6)
N1—C1—C2	114.6 (4)	C31—C30—C29	118.5 (6)
N1—C1—H1A	108.6	C35—C30—C29	122.6 (6)
C2—C1—H1A	108.6	O7—C31—C30	120.0 (6)
N1—C1—H1B	108.6	O7—C31—C32	120.9 (6)
C2—C1—H1B	108.6	C30—C31—C32	119.2 (6)
H1A—C1—H1B	107.6	C33—C32—O8	126.2 (7)
C7—C2—C3	119.8 (5)	C33—C32—C31	121.6 (6)
C7—C2—C1	120.0 (5)	O8—C32—C31	112.1 (6)
C3—C2—C1	120.0 (5)	C32—C33—C34	118.3 (7)
O1—C3—C2	122.2 (5)	C32—C33—H33	120.9
O1—C3—C4	119.0 (5)	C34—C33—H33	120.9
C2—C3—C4	118.7 (5)	C33—C34—C35	121.5 (7)
O2—C4—C5	124.1 (5)	C33—C34—H34	119.2
O2—C4—C3	115.6 (5)	C35—C34—H34	119.2
C5—C4—C3	120.4 (5)	C34—C35—C30	120.5 (6)
C6—C5—C4	119.8 (5)	C34—C35—H35	119.7
C6—C5—H5A	120.1	C30—C35—H35	119.7
C4—C5—H5A	120.1	O8—C36—H36A	109.5
C7—C6—C5	120.2 (6)	O8—C36—H36B	109.5
C7—C6—H6	119.9	H36A—C36—H36B	109.5
C5—C6—H6	119.9	O8—C36—H36C	109.5
C6—C7—C2	121.1 (5)	H36A—C36—H36C	109.5
C6—C7—H7A	119.5	H36B—C36—H36C	109.5
C2—C7—H7A	119.5	N4—C37—C38	111.3 (5)
O2—C8—H8A	109.5	N4—C37—H37A	109.4
O2—C8—H8B	109.5	C38—C37—H37A	109.4

H8A—C8—H8B	109.5	N4—C37—H37B	109.4
O2—C8—H8C	109.5	C38—C37—H37B	109.4
H8A—C8—H8C	109.5	H37A—C37—H37B	108.0
H8B—C8—H8C	109.5	N5—C38—C37	110.1 (4)
N3—C9—C10	114.0 (4)	N5—C38—H38A	109.6
N3—C9—H9A	108.8	C37—C38—H38A	109.6
C10—C9—H9A	108.8	N5—C38—H38B	109.6
N3—C9—H9B	108.8	C37—C38—H38B	109.6
C10—C9—H9B	108.8	H38A—C38—H38B	108.1
H9A—C9—H9B	107.7	N5—C39—C40	113.0 (4)
C11—C10—C15	118.3 (5)	N5—C39—H39A	109.0
C11—C10—C9	119.8 (5)	C40—C39—H39A	109.0
C15—C10—C9	121.8 (5)	N5—C39—H39B	109.0
O3—C11—C10	117.2 (5)	C40—C39—H39B	109.0
O3—C11—C12	121.5 (5)	H39A—C39—H39B	107.8
C10—C11—C12	121.3 (5)	N6—C40—C39	115.9 (4)
O4—C12—C13	126.4 (6)	N6—C40—H40A	108.3
O4—C12—C11	114.3 (5)	C39—C40—H40A	108.3
C13—C12—C11	119.3 (6)	N6—C40—H40B	108.3
C12—C13—C14	119.3 (6)	C39—C40—H40B	108.3
C12—C13—H13	120.4	H40A—C40—H40B	107.4
C14—C13—H13	120.4		
O1—Ni1—N1—C17	−101.5 (3)	C16—O4—C12—C11	−167.4 (5)
N4—Ni1—N1—C17	84.4 (3)	O3—C11—C12—O4	2.4 (8)
N2—Ni1—N1—C17	−6.6 (3)	C10—C11—C12—O4	−179.0 (5)
N5—Ni1—N1—C17	166.8 (3)	O3—C11—C12—C13	179.8 (5)
O1—Ni1—N1—C1	27.1 (4)	C10—C11—C12—C13	−1.6 (8)
N4—Ni1—N1—C1	−147.0 (4)	O4—C12—C13—C14	179.1 (5)
N2—Ni1—N1—C1	122.0 (4)	C11—C12—C13—C14	2.0 (9)
N5—Ni1—N1—C1	−64.7 (4)	C12—C13—C14—C15	−1.9 (9)
O1—Ni1—N2—C18	67.5 (3)	C13—C14—C15—C10	1.3 (9)
O5—Ni1—N2—C18	152.8 (3)	C11—C10—C15—C14	−0.8 (8)
N4—Ni1—N2—C18	−117.5 (3)	C9—C10—C15—C14	175.5 (5)
N1—Ni1—N2—C18	−20.7 (3)	C1—N1—C17—C18	−95.6 (5)
O1—Ni1—N2—C19	−64.8 (4)	Ni1—N1—C17—C18	33.3 (5)
O5—Ni1—N2—C19	20.4 (4)	C19—N2—C18—C17	−177.0 (4)
N4—Ni1—N2—C19	110.1 (4)	Ni1—N2—C18—C17	43.6 (5)
N1—Ni1—N2—C19	−153.1 (4)	N1—C17—C18—N2	−52.6 (6)
O5—Ni1—N4—C37	−92.2 (3)	C18—N2—C19—C20	−77.6 (6)
N1—Ni1—N4—C37	91.1 (4)	Ni1—N2—C19—C20	53.0 (6)
N2—Ni1—N4—C37	172.7 (3)	C9—N3—C20—C19	−75.2 (5)
N5—Ni1—N4—C37	−0.8 (3)	N2—C19—C20—N3	−87.0 (6)
O5—Ni1—N4—C21	33.0 (3)	C37—N4—C21—C22	58.1 (6)
N1—Ni1—N4—C21	−143.6 (3)	Ni1—N4—C21—C22	−66.5 (5)
N2—Ni1—N4—C21	−62.0 (3)	N4—C21—C22—C23	53.5 (6)
N5—Ni1—N4—C21	124.5 (3)	N4—C21—C22—C27	−125.7 (5)
O1—Ni1—N5—C39	78.0 (3)	Ni1—O5—C23—C22	−30.3 (6)
O5—Ni1—N5—C39	−6.9 (3)	Ni1—O5—C23—C24	146.3 (4)
N4—Ni1—N5—C39	−96.2 (4)	C27—C22—C23—O5	178.1 (4)

N1—Ni1—N5—C39	167.1 (3)	C21—C22—C23—O5	−1.1 (7)
O1—Ni1—N5—C38	−158.9 (3)	C27—C22—C23—C24	1.4 (7)
O5—Ni1—N5—C38	116.2 (3)	C21—C22—C23—C24	−177.8 (4)
N4—Ni1—N5—C38	26.9 (3)	C28—O6—C24—C25	9.0 (7)
N1—Ni1—N5—C38	−69.8 (3)	C28—O6—C24—C23	−169.4 (5)
O5—Ni1—O1—C3	−159.8 (4)	O5—C23—C24—C25	−179.6 (4)
N1—Ni1—O1—C3	16.1 (4)	C22—C23—C24—C25	−2.8 (7)
N2—Ni1—O1—C3	−65.1 (4)	O5—C23—C24—O6	−1.1 (6)
N5—Ni1—O1—C3	109.0 (4)	C22—C23—C24—O6	175.7 (4)
O1—Ni1—O5—C23	−161.8 (4)	O6—C24—C25—C26	−176.7 (5)
N4—Ni1—O5—C23	12.0 (4)	C23—C24—C25—C26	1.6 (8)
N2—Ni1—O5—C23	104.0 (4)	C24—C25—C26—C27	1.0 (8)
N5—Ni1—O5—C23	−70.1 (4)	C25—C26—C27—C22	−2.2 (8)
C17—N1—C1—C2	64.7 (6)	C23—C22—C27—C26	1.0 (8)
Ni1—N1—C1—C2	−62.1 (5)	C21—C22—C27—C26	−179.8 (5)
N1—C1—C2—C7	−130.7 (5)	C40—N6—C29—C30	−81.1 (6)
N1—C1—C2—C3	55.0 (7)	N6—C29—C30—C31	−92.7 (6)
Ni1—O1—C3—C2	−29.2 (6)	N6—C29—C30—C35	88.9 (6)
Ni1—O1—C3—C4	149.2 (4)	C35—C30—C31—O7	−179.4 (5)
C7—C2—C3—O1	179.6 (4)	C29—C30—C31—O7	2.2 (8)
C1—C2—C3—O1	−6.1 (7)	C35—C30—C31—C32	−1.1 (9)
C7—C2—C3—C4	1.2 (7)	C29—C30—C31—C32	−179.5 (5)
C1—C2—C3—C4	175.5 (5)	C36—O8—C32—C33	15.4 (10)
C8—O2—C4—C5	0.5 (7)	C36—O8—C32—C31	−168.7 (5)
C8—O2—C4—C3	179.4 (4)	O7—C31—C32—C33	177.4 (6)
O1—C3—C4—O2	1.1 (7)	C30—C31—C32—C33	−1.0 (10)
C2—C3—C4—O2	179.6 (4)	O7—C31—C32—O8	1.3 (9)
O1—C3—C4—C5	−179.9 (4)	C30—C31—C32—O8	−177.1 (5)
C2—C3—C4—C5	−1.4 (7)	O8—C32—C33—C34	178.1 (6)
O2—C4—C5—C6	−179.8 (5)	C31—C32—C33—C34	2.5 (10)
C3—C4—C5—C6	1.3 (8)	C32—C33—C34—C35	−2.1 (10)
C4—C5—C6—C7	−0.9 (9)	C33—C34—C35—C30	0.1 (10)
C5—C6—C7—C2	0.7 (9)	C31—C30—C35—C34	1.5 (9)
C3—C2—C7—C6	−0.9 (8)	C29—C30—C35—C34	179.8 (5)
C1—C2—C7—C6	−175.2 (5)	C21—N4—C37—C38	−152.0 (4)
C20—N3—C9—C10	−58.8 (6)	Ni1—N4—C37—C38	−26.4 (5)
N3—C9—C10—C11	−58.7 (7)	C39—N5—C38—C37	79.4 (5)
N3—C9—C10—C15	125.1 (5)	Ni1—N5—C38—C37	−49.1 (5)
C15—C10—C11—O3	179.6 (5)	N4—C37—C38—N5	53.2 (6)
C9—C10—C11—O3	3.2 (7)	C38—N5—C39—C40	159.5 (4)
C15—C10—C11—C12	1.0 (8)	Ni1—N5—C39—C40	−82.1 (5)
C9—C10—C11—C12	−175.4 (5)	C29—N6—C40—C39	−173.2 (4)
C16—O4—C12—C13	15.4 (9)	N5—C39—C40—N6	63.0 (6)

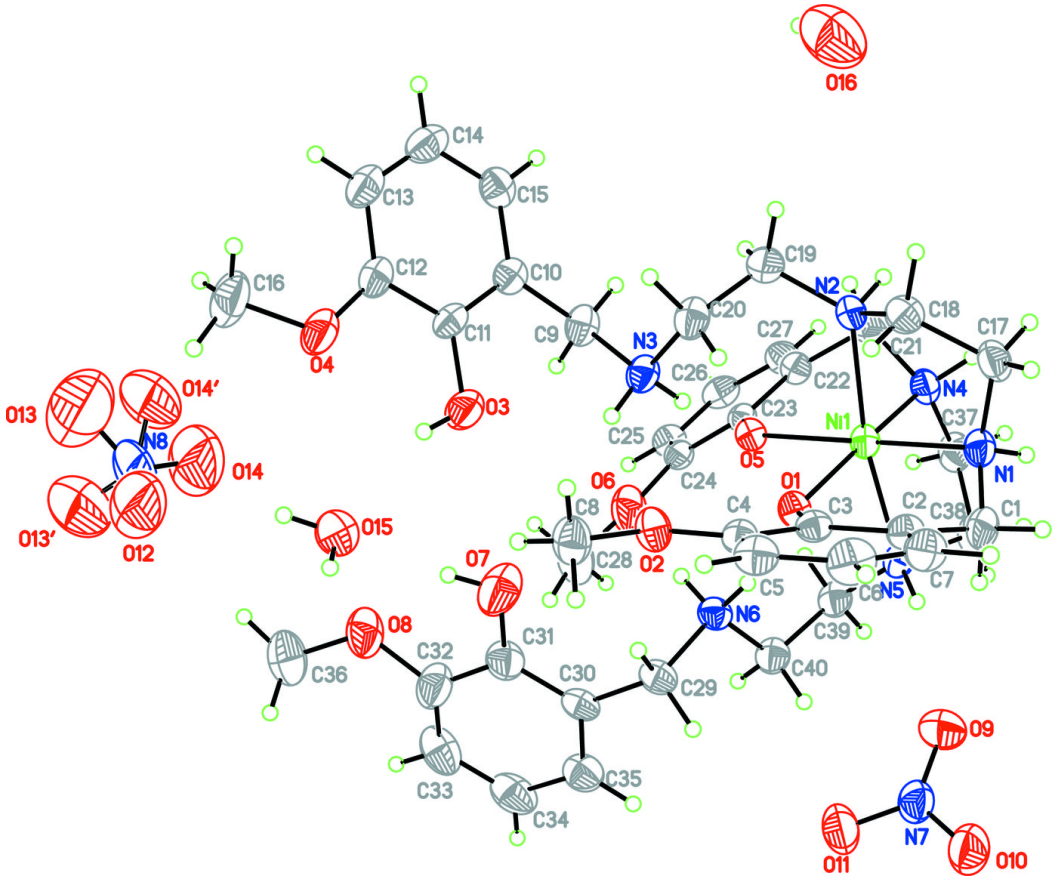
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O9^{i}	0.91	2.38	3.122 (6)	139
N1—H1···O10^{i}	0.91	2.31	3.163 (6)	156

N2—H2···O13^{ii}	0.91	2.14	2.976 (11)	152
N4—H4···O12^{ii}	0.91	2.21	3.021 (8)	148
O15—H42···O10^{iii}	0.85	2.32	3.013 (6)	138
O15—H42···O11^{iii}	0.85	2.14	2.965 (6)	163
C9—H9B···O14^{iv}	0.97	2.48	3.420 (10)	163
C17—H17A···O12^{ii}	0.97	2.59	3.445 (9)	147
C34—H34···O11^{v}	0.93	2.59	3.419 (8)	149
O16—H43···O13^{iv}	0.85	1.66	2.464 (17)	156
O3—H3···O15	0.82	1.98	2.653 (5)	139
O3—H3···O4	0.82	2.21	2.659 (5)	115
N3—H3A···O5	0.90	1.73	2.617 (5)	168
N3—H3B···O2	0.90	2.53	3.211 (5)	133
N3—H3B···O3	0.90	2.23	2.838 (5)	124
N5—H5···O9	0.91	2.24	3.123 (6)	165
N6—H6A···O5	0.90	2.49	2.936 (5)	111
N6—H6A···O6	0.90	2.10	2.961 (6)	161
N6—H6B···O1	0.90	1.72	2.612 (5)	169
O7—H7···O8	0.82	2.20	2.633 (6)	113
O7—H7···O15	0.82	2.13	2.872 (6)	151
O15—H41···O12	0.85	2.21	3.037 (8)	166
C1—H1B···O9	0.97	2.49	3.438 (7)	165
C29—H29A···O2	0.97	2.50	3.382 (6)	151
C29—H29A···O7	0.97	2.39	2.757 (7)	102
C40—H40B···O9	0.97	2.56	3.369 (7)	141
C40—H40B···O11	0.97	2.53	3.456 (7)	160
C39—H39B···O5	0.97	2.55	3.087 (6)	115

Symmetry codes: (i) −*x*+3/2, −*y*+3/2, −*z*+2; (ii) *x*, −*y*+1, *z*+1/2; (iii) −*x*+3/2, *y*−1/2, −*z*+3/2; (iv) −*x*+1, −*y*+1, −*z*+1; (v) −*x*+3/2, *y*+1/2, −*z*+3/2.

Fig. 1


O16
C14
C13
C15
C16
C12
C10
C11
C9
O4
O3
N3
C19
N2
C20
C27
C18
C17
C21
C26
C22
N4
C23
Ni1
C37
C25
O5
N1
C24
O6
O1
C8
C4
C3
C2
C38
C1
O15
O7
C28
O2
C5
C6
N5
C7
N6
C39
O8
C31
C32
C36
C30
C29
C40
C33
C35
C34
O9
N7
O11
O10
O13
O14′
N8
O14
O13′
O12