Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diaquabis{2-[2-(isopropylammonio)-ethyliminomethyl]-6-methoxyphenolato}-nickel(II) dinitrate dihydrate

Ying-Zhen Wang,[a] Lan-Lan Li,[b] Yong-Qing Su[c]* and Cong Li[c]

[a]Kunming Teachers College, Kunming 650031, People's Republic of China, [b]Faculty of Chemical Science and Engineering, Yunnan University, Kunming 650091, People's Republic of China, and [c]Faculty of Chemistry and Chemical Engineering, Yunnan Normal University, Kunming 650092, People's Republic of China
Correspondence e-mail: yongqing_su@163.com

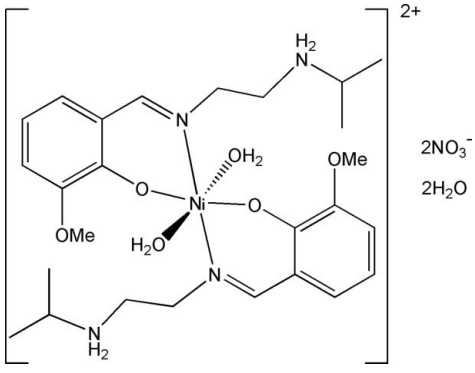
Received 25 October 2007; accepted 31 October 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.108; data-to-parameter ratio = 17.3.

The title compound, $[Ni(C_{13}H_{20}N_2O_2)_2(H_2O)_2](NO_3)_2\cdot 2H_2O$, consists of a mononuclear nickel(II) complex, two nitrate anions and two solvent water molecules. The Ni atom lies on an inversion centre and is chelated by the phenolic O and imine N atoms from two Schiff base ligands, and coordinated by the O atoms from two water molecules, giving a slightly distorted octahedral geometry. Within the crystal structure, the components form chains parallel to the a axis by intermolecular N—H···O, O—H···O and O—H···N hydrogen bonds.

Related literature

For related literature, see: Ali *et al.* (2004); Averseng *et al.* (1999); Di Bella *et al.* (1994); Fun *et al.* (2001); Gomes *et al.* (2000); Lacroix *et al.* (1996); Sarı *et al.* (2006); Su *et al.* (2006); Wang (2005); Wei (2005); Zhang *et al.* (2005).



Experimental

Crystal data

$[Ni(C_{13}H_{20}N_2O_2)_2(H_2O)_2](NO_3)_2\cdot 2H_2O$
M_r = 727.39
Orthorhombic, *Pbca*
a = 14.101 (4) Å
b = 10.369 (3) Å
c = 23.627 (6) Å
V = 3454.7 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.63 mm^{-1}
T = 298 (2) K
0.30 × 0.27 × 0.23 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.833, T_{max} = 0.868
27825 measured reflections
3967 independent reflections
3000 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.108
S = 1.02
3967 reflections
229 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1^{i}	0.90	1.78	2.631 (2)	158
N2—H2A···O2^{i}	0.90	2.46	3.086 (2)	127
N2—H2B···O7^{ii}	0.90	2.03	2.907 (3)	166
O3—H3A···O7^{iii}	0.85 (3)	1.965 (15)	2.765 (2)	157 (3)
O3—H3B···O5^{iii}	0.85 (3)	2.118 (18)	2.859 (3)	146 (2)
O7—H7D···O4	0.85 (3)	1.939 (12)	2.765 (3)	166 (3)
O7—H7D···N3	0.85 (3)	2.588 (18)	3.300 (3)	143 (3)
O7—H7D···O5	0.85 (3)	2.65 (2)	3.175 (3)	121 (2)
O7—H7E···O6^{iv}	0.84 (3)	2.041 (11)	2.875 (3)	172 (3)
O7—H7E···O4^{iv}	0.84 (3)	2.55 (2)	3.202 (3)	135 (3)
O7—H7E···N3^{iv}	0.84 (3)	2.641 (13)	3.449 (3)	162 (3)

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2060).

References

Ali, H. M., Khamis, N. A. & Yamin, B. M. (2004). *Acta Cryst.* E**60**, m1708–m1709.
Averseng, F., Lacroix, P. G., Malfant, I., Lenoble, G., Cassoux, P., Nakatani, K., Maltey-Fanton, I., Delaire, J. A. & Aukauloo, A. (1999). *Chem. Mater.* **11**, 995–1002.
Bruker (2000). *SMART* (Version 5.625), *SAINT* (Version 6.01). *SHELXTL* (Version 6.10) and *SADABS* (Version 2.03). Bruker AXS Inc., Madison, Wisconsin, USA.
Di Bella, S., Fragalá, I., Ledoux, I., Diaz-Garcia, M. A., Lacroix, P. G. & Marks, T. J. (1994). *Chem. Mater.* **6**, 881–883.
Fun, H.-K., Chantrapromma, S., Razak, I. A., Usman, A., Tang, Y. W., Ma, W., Wu, J. Y. & Tian, Y. P. (2001). *Acta Cryst.* E**57**, m519–m521.

 doi:10.1107/S1600536807055092

Gomes, L., Sousa, C., Freire, C. & de Castro, B. (2000). *Acta Cryst.* C**56**, 1201–1203.
Lacroix, P. G., Di Bella, S. & Ledoux, I. (1996). *Chem. Mater.* **8**, 541–545.
Sarı, M., Atakol, O., Svoboda, I. & Fuess, H. (2006). *Acta Cryst.* E**62**, m563–m565.
Su, Y.-Q., Wang, P., He, Y.-F. & Liu, L.-M. (2006). *Acta Cryst.* E**62**, m2673–m2675.
Wang, F.-W. (2005). *Acta Cryst.* E**61**, m1998–m2000.
Wei, Y.-J. (2005). *Acta Cryst.* E**61**, m1088–m1089.
Zhang, S.-H., Jiang, Y.-M., Liu, Z. & Yu, K.-B. (2005). *Acta Cryst.* E**61**, m446–m448.

supplementary materials

Acta Cryst. (2007). E**63**, m2945-m2946 [**doi:10.1107/S1600536807055092**]

Diaquabis{2-[2-(isopropylammonio)ethyliminomethyl]-6-methoxyphenolato}nickel(II) dinitrate dihydrate

Y.-Z. Wang, L.-L. Li, Y.-Q. Su and C. Li

Comment

Schiff base nickel complexes have been received much attention in coordination chemistry (Di Bella *et al.*, 1994; Lacroix *et al.*, 1996; Averseng *et al.*, 1999; Wang, 2005; Fun *et al.*, 2001; Zhang *et al.*, 2005). Recently, we have reported the structure of a Schiff base nickel(II) complex (Su *et al.*, 2006). As a further investigation of the structures of such complexes, the title compound is reported here.

The complex consists of a mononuclear nickel(II) complex, with two nitrate anions and two lattice water molecules, as shown in Fig. 1. The Ni atom, lies on an inversion centre; it is chelated by the phenolic O and imine N atoms from two Schiff base ligands, and is coordinated by the O atoms from two water molecules, giving a slightly distorted octahedral geometry. The three *trans* angles at Ni are 180° by symmetry, the other angles are close to 90°, varying from 87.25 (6) to 92.75 (6)°. The Ni—O and Ni—N bond lengths are normal and comparable to those observed in other similar nickel(II) complexes (Wei, 2005; Ali *et al.*, 2004; Sarı *et al.*, 2006; Gomes *et al.*, 2000).

In the crystal structure, molecules form chains running parallel to the *a* axis through intermolecular N—H···O, O—H···O and O—H···N hydrogen bonds (Fig. 2 and Table 1).

Experimental

3-Methoxysalicylaldehyde (1.0 mmol, 152.0 mg), *N*-isopropylethane-1,2-diamine (1.0 mmol, 102.2 mg), and $Ni(NO_3)_2{\cdot}6H_2O$ (0.5 mmol, 145.3 mg) were dissolved in a 95% ethanol solution (30 ml). The mixture was stirred at room temperature for about 1 h to give a green solution. After keeping the solution in air for 12 days, green block-like crystals were formed.

Refinement

Water H atoms were located in a difference Fourier map and refined isotropically, with O—H and H···H distances restrained to 0.85 (1) Å and 1.37 (2) Å respectively. The other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

Figures

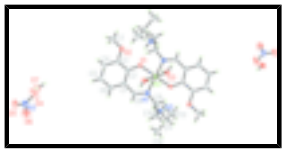


Fig. 1. The structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are at the symmetry related position (2 − *x*, −*y*, 1 − *z*).

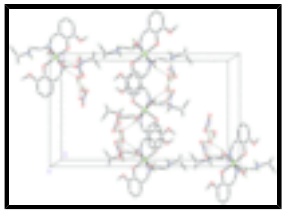


Fig. 2. The crystal packing of the title compound. Intermolecular hydrogen bonds are shown as dashed lines.

Diaquabis{2-[2-(isopropylammonio)ethyliminomethyl]-6-methoxyphenolato}nickel(II) dinitrate dihydrate

Crystal data

$[Ni(C_{13}H_{20}N_2O_2)_2(H_2O)_2](NO_3)_2\cdot 2H_2O$	$F_{000} = 1544$
$M_r = 727.39$	$D_x = 1.399$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ac 2ab	Cell parameters from 5968 reflections
$a = 14.101$ (4) Å	$\theta = 2.4$–$25.2°$
$b = 10.369$ (3) Å	$\mu = 0.63$ mm^{-1}
$c = 23.627$ (6) Å	$T = 298$ (2) K
$V = 3454.7$ (17) Å^3	Block, green
$Z = 4$	0.30 × 0.27 × 0.23 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3967 independent reflections
Radiation source: fine-focus sealed tube	3000 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.040$
$T = 298(2)$ K	$\theta_{max} = 27.5°$
ω scans	$\theta_{min} = 1.7°$
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -18\rightarrow18$
$T_{min} = 0.833$, $T_{max} = 0.868$	$k = -13\rightarrow13$
27825 measured reflections	$l = -30\rightarrow30$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.040$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.108$	$w = 1/[\sigma^2(F_o^2) + (0.0472P)^2 + 1.9738P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
3967 reflections	$\Delta\rho_{max} = 0.51$ e Å^{-3}
229 parameters	$\Delta\rho_{min} = -0.36$ e Å^{-3}

6 restraints
Primary atom site location: structure-invariant direct methods
Extinction correction: none

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 $F^2 > 2\sigma(F^2)$ 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	0.0000	0.5000	0.02925 (11)
O1	0.91529 (9)	−0.02221 (14)	0.43343 (6)	0.0370 (3)
O2	0.82723 (11)	−0.18753 (15)	0.36977 (7)	0.0468 (4)
O3	1.07598 (11)	0.14933 (15)	0.45794 (7)	0.0446 (4)
O4	0.18849 (17)	0.3220 (2)	0.33180 (15)	0.1183 (11)
O5	0.04457 (13)	0.29566 (19)	0.35709 (9)	0.0711 (6)
O6	0.11196 (19)	0.4802 (2)	0.36353 (12)	0.0932 (8)
O7	0.19608 (13)	0.07169 (17)	0.37196 (9)	0.0592 (5)
N1	0.90533 (12)	0.13969 (15)	0.52859 (7)	0.0324 (4)
N2	0.96617 (12)	0.09622 (16)	0.64619 (7)	0.0355 (4)
H2A	1.0180	0.0796	0.6252	0.043*
H2B	0.9235	0.0338	0.6389	0.043*
N3	0.11452 (15)	0.3664 (2)	0.35155 (9)	0.0530 (5)
C1	0.77137 (14)	0.0516 (2)	0.47669 (9)	0.0354 (4)
C2	0.82259 (14)	−0.02761 (19)	0.43900 (8)	0.0320 (4)
C3	0.77055 (14)	−0.1139 (2)	0.40424 (9)	0.0368 (5)
C4	0.67340 (16)	−0.1185 (2)	0.40649 (10)	0.0458 (5)
H4	0.6406	−0.1768	0.3839	0.055*
C5	0.62353 (16)	−0.0365 (3)	0.44243 (11)	0.0527 (6)
H5	0.5576	−0.0383	0.4429	0.063*
C6	0.67153 (15)	0.0466 (3)	0.47693 (10)	0.0466 (5)
H6	0.6378	0.1008	0.5010	0.056*
C7	0.7837 (2)	−0.2852 (2)	0.33677 (11)	0.0584 (7)
H7A	0.7463	−0.3399	0.3608	0.088*
H7B	0.8317	−0.3357	0.3184	0.088*
H7C	0.7435	−0.2462	0.3088	0.088*
C8	0.81822 (15)	0.1435 (2)	0.51351 (9)	0.0372 (5)
H8	0.7818	0.2112	0.5274	0.045*
C9	0.93993 (15)	0.24570 (19)	0.56478 (9)	0.0390 (5)
H9A	0.9073	0.3245	0.5543	0.047*

H9B	1.0070	0.2584	0.5576	0.047*
C10	0.92553 (16)	0.2217 (2)	0.62739 (9)	0.0422 (5)
H10A	0.9550	0.2910	0.6487	0.051*
H10B	0.8582	0.2229	0.6357	0.051*
C11	0.99340 (16)	0.0882 (2)	0.70763 (9)	0.0445 (5)
H11	1.0343	0.1620	0.7163	0.053*
C12	0.9065 (2)	0.0974 (4)	0.74436 (11)	0.0773 (9)
H12A	0.8737	0.1764	0.7363	0.116*
H12B	0.9250	0.0961	0.7835	0.116*
H12C	0.8655	0.0257	0.7367	0.116*
C13	1.0501 (3)	−0.0329 (3)	0.71657 (12)	0.0756 (9)
H13A	1.0114	−0.1066	0.7080	0.113*
H13B	1.0704	−0.0374	0.7553	0.113*
H13C	1.1045	−0.0322	0.6922	0.113*
H3A	1.1215 (14)	0.117 (3)	0.4393 (11)	0.080*
H3B	1.0443 (17)	0.195 (3)	0.4351 (10)	0.080*
H7D	0.195 (2)	0.1423 (17)	0.3541 (12)	0.080*
H7E	0.2499 (11)	0.038 (2)	0.3686 (13)	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.02767 (19)	0.02977 (19)	0.03031 (19)	0.00044 (14)	−0.00154 (14)	−0.00484 (14)
O1	0.0275 (7)	0.0491 (9)	0.0345 (7)	0.0027 (6)	−0.0017 (6)	−0.0104 (6)
O2	0.0431 (8)	0.0485 (9)	0.0488 (9)	−0.0050 (7)	−0.0034 (7)	−0.0174 (7)
O3	0.0473 (9)	0.0403 (9)	0.0461 (9)	−0.0027 (7)	0.0043 (7)	0.0002 (7)
O4	0.0653 (14)	0.0643 (14)	0.225 (3)	0.0072 (12)	0.0497 (18)	0.0195 (18)
O5	0.0448 (10)	0.0706 (13)	0.0980 (16)	−0.0061 (9)	−0.0065 (10)	0.0168 (11)
O6	0.1038 (19)	0.0531 (13)	0.123 (2)	−0.0006 (12)	0.0109 (16)	−0.0196 (13)
O7	0.0506 (10)	0.0472 (10)	0.0798 (13)	0.0028 (8)	0.0140 (10)	0.0007 (9)
N1	0.0364 (9)	0.0298 (8)	0.0311 (8)	0.0021 (7)	−0.0024 (7)	−0.0023 (7)
N2	0.0376 (9)	0.0361 (9)	0.0329 (9)	0.0005 (7)	0.0028 (7)	−0.0068 (7)
N3	0.0467 (12)	0.0479 (12)	0.0643 (13)	0.0041 (10)	−0.0029 (10)	0.0125 (10)
C1	0.0298 (10)	0.0415 (11)	0.0350 (10)	0.0065 (9)	−0.0043 (8)	0.0004 (9)
C2	0.0293 (9)	0.0350 (10)	0.0318 (10)	0.0025 (8)	−0.0028 (8)	0.0032 (8)
C3	0.0368 (11)	0.0376 (11)	0.0361 (11)	−0.0016 (9)	−0.0045 (8)	0.0021 (9)
C4	0.0385 (12)	0.0497 (13)	0.0491 (13)	−0.0087 (10)	−0.0110 (10)	0.0021 (11)
C5	0.0286 (11)	0.0681 (16)	0.0613 (16)	−0.0003 (11)	−0.0040 (11)	0.0038 (13)
C6	0.0332 (11)	0.0588 (14)	0.0479 (13)	0.0095 (10)	−0.0006 (10)	−0.0021 (11)
C7	0.0668 (17)	0.0509 (14)	0.0574 (15)	−0.0103 (12)	−0.0109 (13)	−0.0141 (12)
C8	0.0378 (11)	0.0377 (11)	0.0361 (11)	0.0097 (9)	0.0019 (8)	−0.0022 (9)
C9	0.0467 (12)	0.0281 (10)	0.0422 (11)	0.0032 (9)	−0.0033 (9)	−0.0052 (9)
C10	0.0475 (12)	0.0386 (11)	0.0404 (12)	0.0082 (10)	−0.0002 (10)	−0.0109 (9)
C11	0.0512 (13)	0.0503 (13)	0.0320 (11)	−0.0018 (11)	−0.0031 (9)	−0.0079 (10)
C12	0.077 (2)	0.118 (3)	0.0371 (14)	−0.0082 (19)	0.0125 (13)	−0.0068 (16)
C13	0.113 (3)	0.0651 (18)	0.0485 (16)	0.0218 (18)	−0.0159 (17)	0.0013 (13)

Geometric parameters (Å, °)

Ni1—O1^{i}	1.9884 (14)	C2—C3	1.419 (3)
Ni1—O1	1.9884 (14)	C3—C4	1.372 (3)
Ni1—N1	2.0824 (16)	C4—C5	1.393 (3)
Ni1—N1^{i}	2.0824 (16)	C4—H4	0.9300
Ni1—O3	2.1291 (16)	C5—C6	1.366 (4)
Ni1—O3^{i}	2.1291 (16)	C5—H5	0.9300
O1—C2	1.315 (2)	C6—H6	0.9300
O2—C3	1.373 (3)	C7—H7A	0.9600
O2—C7	1.418 (3)	C7—H7B	0.9600
O3—H3A	0.85 (3)	C7—H7C	0.9600
O3—H3B	0.85 (3)	C8—H8	0.9300
O4—N3	1.232 (3)	C9—C10	1.514 (3)
O5—N3	1.236 (3)	C9—H9A	0.9700
O6—N3	1.214 (3)	C9—H9B	0.9700
O7—H7D	0.845 (10)	C10—H10A	0.9700
O7—H7E	0.840 (10)	C10—H10B	0.9700
N1—C8	1.279 (3)	C11—C12	1.504 (3)
N1—C9	1.476 (2)	C11—C13	1.504 (4)
N2—C10	1.490 (3)	C11—H11	0.9800
N2—C11	1.504 (3)	C12—H12A	0.9600
N2—H2A	0.9000	C12—H12B	0.9600
N2—H2B	0.9000	C12—H12C	0.9600
C1—C6	1.409 (3)	C13—H13A	0.9600
C1—C2	1.410 (3)	C13—H13B	0.9600
C1—C8	1.450 (3)	C13—H13C	0.9600
O1^{i}—Ni1—O1	180.0	C6—C5—C4	119.9 (2)
O1^{i}—Ni1—N1	92.75 (6)	C6—C5—H5	120.0
O1—Ni1—N1	87.25 (6)	C4—C5—H5	120.0
O1^{i}—Ni1—N1^{i}	87.25 (6)	C5—C6—C1	121.1 (2)
O1—Ni1—N1^{i}	92.75 (6)	C5—C6—H6	119.5
N1—Ni1—N1^{i}	180.00 (8)	C1—C6—H6	119.5
O1^{i}—Ni1—O3	89.01 (6)	O2—C7—H7A	109.5
O1—Ni1—O3	90.99 (6)	O2—C7—H7B	109.5
N1—Ni1—O3	88.18 (7)	H7A—C7—H7B	109.5
N1^{i}—Ni1—O3	91.82 (7)	O2—C7—H7C	109.5
O1^{i}—Ni1—O3^{i}	90.99 (6)	H7A—C7—H7C	109.5
O1—Ni1—O3^{i}	89.01 (6)	H7B—C7—H7C	109.5
N1—Ni1—O3^{i}	91.82 (7)	N1—C8—C1	125.74 (19)
N1^{i}—Ni1—O3^{i}	88.18 (7)	N1—C8—H8	117.1
O3—Ni1—O3^{i}	180.0	C1—C8—H8	117.1
C2—O1—Ni1	121.53 (13)	N1—C9—C10	113.55 (17)
C3—O2—C7	118.10 (18)	N1—C9—H9A	108.9
Ni1—O3—H3A	110 (2)	C10—C9—H9A	108.9

Ni1—O3—H3B	116 (2)	N1—C9—H9B	108.9
H3A—O3—H3B	107 (2)	C10—C9—H9B	108.9
H7D—O7—H7E	109 (2)	H9A—C9—H9B	107.7
C8—N1—C9	117.10 (17)	N2—C10—C9	112.53 (17)
C8—N1—Ni1	123.15 (14)	N2—C10—H10A	109.1
C9—N1—Ni1	119.61 (13)	C9—C10—H10A	109.1
C10—N2—C11	115.72 (16)	N2—C10—H10B	109.1
C10—N2—H2A	108.4	C9—C10—H10B	109.1
C11—N2—H2A	108.4	H10A—C10—H10B	107.8
C10—N2—H2B	108.4	N2—C11—C12	110.22 (19)
C11—N2—H2B	108.4	N2—C11—C13	108.50 (19)
H2A—N2—H2B	107.4	C12—C11—C13	113.9 (2)
O6—N3—O4	118.5 (2)	N2—C11—H11	108.0
O6—N3—O5	121.9 (2)	C12—C11—H11	108.0
O4—N3—O5	119.6 (2)	C13—C11—H11	108.0
C6—C1—C2	119.5 (2)	C11—C12—H12A	109.5
C6—C1—C8	118.5 (2)	C11—C12—H12B	109.5
C2—C1—C8	121.90 (18)	H12A—C12—H12B	109.5
O1—C2—C1	123.19 (18)	C11—C12—H12C	109.5
O1—C2—C3	118.87 (18)	H12A—C12—H12C	109.5
C1—C2—C3	117.90 (18)	H12B—C12—H12C	109.5
C4—C3—O2	125.8 (2)	C11—C13—H13A	109.5
C4—C3—C2	121.0 (2)	C11—C13—H13B	109.5
O2—C3—C2	113.14 (17)	H13A—C13—H13B	109.5
C3—C4—C5	120.5 (2)	C11—C13—H13C	109.5
C3—C4—H4	119.8	H13A—C13—H13C	109.5
C5—C4—H4	119.8	H13B—C13—H13C	109.5

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O1^{i}	0.90	1.78	2.631 (2)	158
N2—H2A···O2^{i}	0.90	2.46	3.086 (2)	127
N2—H2B···O7^{ii}	0.90	2.03	2.907 (3)	166
O3—H3A···O7^{iii}	0.85 (3)	1.965 (15)	2.765 (2)	157 (3)
O3—H3B···O5^{iii}	0.85 (3)	2.118 (18)	2.859 (3)	146 (2)
O7—H7D···O4	0.85 (3)	1.939 (12)	2.765 (3)	166 (3)
O7—H7D···N3	0.85 (3)	2.588 (18)	3.300 (3)	143 (3)
O7—H7D···O5	0.85 (3)	2.65 (2)	3.175 (3)	121 (2)
O7—H7E···O6^{iv}	0.84 (3)	2.041 (11)	2.875 (3)	172 (3)
O7—H7E···O4^{iv}	0.84 (3)	2.55 (2)	3.202 (3)	135 (3)
O7—H7E···N3^{iv}	0.84 (3)	2.641 (13)	3.449 (3)	162 (3)

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

Fig. 1

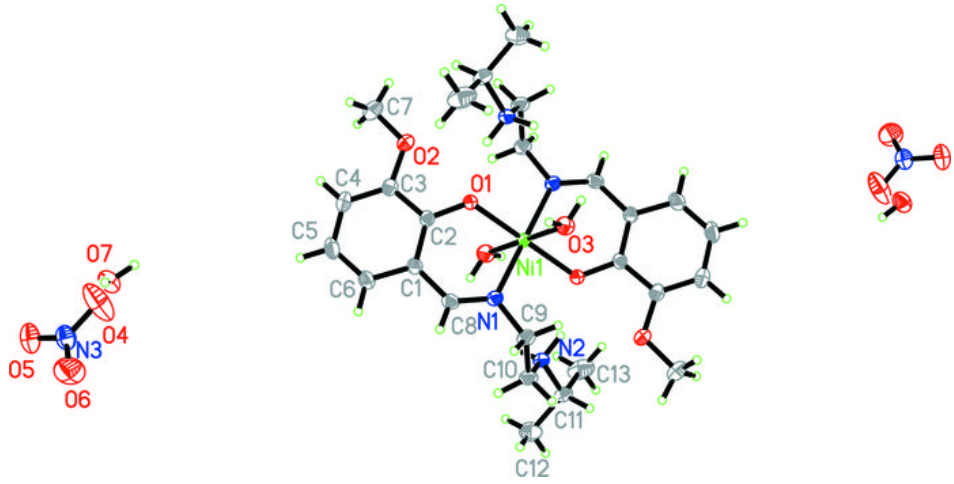

O7
O4
N3
O5
O6
C7
O2
C4
C3
O1
C5
C2
O3
Ni1
C6
C1
C8
N1
C9
N2
C10
C13
C11
C12

Fig. 2