Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Hexaaquanickel(II) bis[(4-nitrophenoxy)-acetate] pentahydrate

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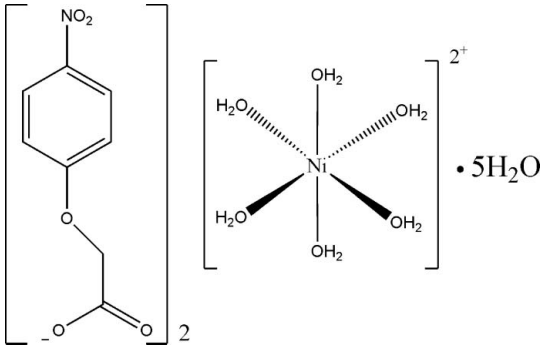
Received 21 April 2007; accepted 22 April 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.038; wR factor = 0.130; data-to-parameter ratio = 16.5.

In the ionic title compound, $[Ni(H_2O)_6](C_8H_6NO_5)_2\cdot 5H_2O$, the $[Co(H_2O)_6]^{2+}$ cation, (4-nitrophenoxy)acetate anions and water molecules engage in O—H···O hydrogen bonding, generating a three-dimensional hydrogen-bonded network.

Related literature

For related literature, see: Gao *et al.* (2006); Mirci (1990); Prout *et al.* (1975); Tian *et al.* (2006).



Experimental

Crystal data

$[Ni(H_2O)_6](C_8H_6NO_5)_2\cdot 5H_2O$
M_r = 649.14
Triclinic, $P\overline{1}$
a = 7.0096 (14) Å
b = 10.661 (2) Å
c = 18.313 (4) Å
α = 87.89 (3)°
β = 87.83 (3)°
γ = 84.17 (3)°
V = 1359.7 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.81 mm^{-1}
T = 293 (2) K
0.38 × 0.21 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.751, T_{max} = 0.864
12966 measured reflections
5939 independent reflections
4930 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.130
S = 1.14
5939 reflections
361 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 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
O11—H13···O1	0.85	1.87	2.706 (3)	167
O11—H14···O19	0.85	1.84	2.687 (3)	176
O12—H15···O18	0.85	1.94	2.739 (3)	156
O12—H16···O7^{i}	0.85	1.79	2.640 (3)	173
O13—H17···O2^{ii}	0.85	1.80	2.652 (3)	179
O13—H18···O12^{iii}	0.85	2.01	2.859 (3)	173
O14—H19···O6^{ii}	0.85	1.97	2.814 (3)	171
O14—H20···O17^{iv}	0.85	1.93	2.749 (3)	161
O15—H21···O7^{v}	0.85	1.88	2.719 (3)	168
O15—H22···O20	0.85	1.94	2.779 (3)	169
O16—H23···O1^{ii}	0.85	2.04	2.831 (3)	154
O16—H24···O6^{i}	0.85	1.93	2.762 (3)	168
O17—H25···O1	0.85	2.07	2.885 (3)	160
O17—H26···O6	0.85	1.96	2.789 (3)	166
O18—H27···O21^{vi}	0.85	2.05	2.890 (4)	173
O18—H28···O11	0.85	2.23	2.881 (3)	133
O19—H29···O21	0.85	2.12	2.788 (4)	135
O19—H30···O17^{iv}	0.85	1.97	2.786 (4)	161
O20—H31···O18	0.85	2.26	3.018 (4)	148
O20—H32···O2^{vii}	0.85	1.96	2.753 (3)	156
O21—H33···O20	0.85	1.98	2.805 (4)	164
O21—H34···O10^{viii}	0.85	2.06	2.905 (3)	171

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); 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: *SHELXL97*.

The authors thank Heilongjiang University for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2257).

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 doi:10.1107/S1600536807020041

supplementary materials

Acta Cryst. (2007). E**63**, m1519 [**doi:10.1107/S1600536807020041**]

Hexaaquanickel(II) bis[(4-nitrophenoxy)acetate] pentahydrate

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Comment

Complexes of 4-nitrophenoxyacetic acid and metal ions (*M*= Cu and Sn) have been structurally characterized (Prout *et al.*, 1975; Tian *et al.*, 2006). Recently, we reported the cobalt derivative (Gao *et al.*, 2006); following this study, we report the nickel complex (I), which consists of a hexaaquanickel(II) cation, two 4-nitrophenoxyacetate anions and five lattice water molecules (Fig.1). The Ni(II) atom is six-coordinated in an octahedral environment. The two anions are approximately parallel. The cation, anion and lattice water molecules are linked by O—H···O hydrogen bonds into a three-dimensional network structure. (Table 1).

Experimental

4-nitrophenoxy acetic acid was prepared by nucleophilic reaction of chloroacetic acid and 4-nitrophenol under basic conditions. (Mirci, 1990). Nickel nitrate hexahydrate (0.582 g, 2 mmol) and 4-nitrophenoxy acetic acid (0.394 g, 2 mmol) were dissolved in water and the pH was adjusted to 6 with 0.01*M* sodium hydroxide; green crystals separated from the filtered solution after several days.

Refinement

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, withwith C—H = 0.93 Å (aromatic C) or C—H = 0.93 Å (methylene C), and with U_{iso}(H) = 1.2Ueq(C). Water H atoms were initially located in a difference Fourier map but they were treated as riding on their parent atoms with O—H = 0.85 Å and with U_{iso}(H) = 1.5Ueq(O).

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); 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: *SHELXL97*.

Figures

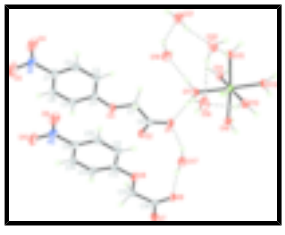


Fig. 1. The molecular structure of (I), showing displacement ellipsoids at the 30% probability level for non-H atoms. Dashed lines indicate the intermolecular O—H···O hydrogen bonding interactions.

Hexaaquanickel(II) bis[(4-nitrophenoxy)acetate] pentahydrate

Crystal data

$[Ni(H_2O)_6](C_8H_6NO_5)_2 \cdot 5H_2O$	$Z = 2$
$M_r = 649.14$	$F_{000} = 680$
Triclinic, $P\overline{1}$	$D_x = 1.586$ Mg m^{-3}
Hall symbol: -p 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.0096$ (14) Å	Cell parameters from 10904 reflections
$b = 10.661$ (2) Å	$\theta = 6.2$–55.0º
$c = 18.313$ (4) Å	$\mu = 0.81$ mm^{-1}
$\alpha = 87.89$ (3)º	$T = 293$ (2) K
$\beta = 87.83$ (3)º	Block, green
$\gamma = 84.17$ (3)º	0.38 × 0.21 × 0.19 mm
$V = 1359.7$ (5) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	5939 independent reflections
Radiation source: fine-focus sealed tube	4930 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.030$
$T = 293$(2) K	$\theta_{max} = 27.5$º
ω scans	$\theta_{min} = 3.1$º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -9 \rightarrow 8$
$T_{min} = 0.751$, $T_{max} = 0.864$	$k = -13 \rightarrow 13$
12966 measured reflections	$l = -23 \rightarrow 23$

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0599P)^2 + 1.1083P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.038$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.130$	$\Delta\rho_{max} = 0.44$ e Å^{-3}
$S = 1.14$	$\Delta\rho_{min} = -0.36$ e Å^{-3}
5939 reflections	Extinction correction: none
361 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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}
C1	0.3512 (4)	0.7403 (3)	−0.02246 (15)	0.0366 (6)
C2	0.3458 (5)	0.6281 (3)	0.01720 (16)	0.0386 (7)
H1	0.3237	0.5549	−0.0059	0.046*
C3	0.3733 (4)	0.6255 (3)	0.09147 (15)	0.0351 (6)
H2	0.3701	0.5505	0.1189	0.042*
C4	0.4058 (4)	0.7355 (3)	0.12483 (14)	0.0298 (5)
C5	0.4065 (4)	0.8493 (3)	0.08428 (16)	0.0364 (6)
H3	0.4245	0.9234	0.1073	0.044*
C6	0.3803 (4)	0.8511 (3)	0.01020 (16)	0.0388 (7)
H4	0.3821	0.9259	−0.0175	0.047*
C7	0.4567 (4)	0.6321 (2)	0.24160 (14)	0.0305 (6)
H5	0.5515	0.5711	0.2194	0.037*
H6	0.3357	0.5954	0.2467	0.037*
C8	0.5208 (4)	0.6657 (2)	0.31593 (14)	0.0283 (5)
C9	0.8907 (4)	0.7552 (3)	0.07108 (15)	0.0330 (6)
C10	0.8987 (4)	0.6425 (3)	0.11133 (17)	0.0383 (6)
H7	0.8835	0.5674	0.0890	0.046*
C11	0.9297 (4)	0.6437 (3)	0.18487 (16)	0.0363 (6)
H8	0.9351	0.5689	0.2128	0.044*
C12	0.9529 (4)	0.7571 (3)	0.21773 (14)	0.0299 (5)
C13	0.9400 (4)	0.8693 (3)	0.17696 (15)	0.0346 (6)
H9	0.9511	0.9451	0.1992	0.041*
C14	0.9106 (4)	0.8677 (3)	0.10312 (16)	0.0361 (6)
H10	0.9043	0.9423	0.0750	0.043*
C15	1.0254 (4)	0.8571 (3)	0.32586 (14)	0.0315 (6)
H11	0.9097	0.9153	0.3267	0.038*
H12	1.1259	0.8982	0.2997	0.038*
C16	1.0844 (4)	0.8230 (3)	0.40322 (14)	0.0286 (5)
N1	0.3258 (5)	0.7421 (3)	−0.10114 (15)	0.0526 (7)
N2	0.8634 (4)	0.7544 (3)	−0.00673 (14)	0.0424 (6)
Ni1	0.43587 (5)	0.23562 (3)	0.447639 (17)	0.02541 (11)
O1	0.5651 (3)	0.57280 (19)	0.35882 (11)	0.0368 (5)
O2	0.5224 (4)	0.77804 (19)	0.33005 (11)	0.0419 (5)

O3	0.4351 (3)	0.74521 (19)	0.19680 (11)	0.0375 (5)
O4	0.2948 (6)	0.6455 (3)	−0.12972 (15)	0.0807 (10)
O5	0.3377 (6)	0.8428 (3)	−0.13473 (15)	0.0918 (12)
O6	1.0903 (3)	0.71016 (18)	0.42585 (10)	0.0336 (4)
O7	1.1241 (3)	0.91283 (19)	0.43944 (11)	0.0385 (5)
O8	0.9915 (3)	0.74599 (19)	0.28957 (10)	0.0362 (5)
O9	0.8414 (5)	0.6555 (3)	−0.03502 (14)	0.0660 (8)
O10	0.8628 (4)	0.8548 (3)	−0.04213 (13)	0.0611 (7)
O11	0.4960 (3)	0.32888 (18)	0.34959 (10)	0.0319 (4)
H13	0.5356	0.4016	0.3504	0.048*
H14	0.4044	0.3402	0.3202	0.048*
O12	0.6910 (3)	0.11685 (18)	0.43716 (10)	0.0333 (4)
H15	0.7593	0.1223	0.3980	0.050*
H16	0.7595	0.1067	0.4747	0.050*
O13	0.3710 (3)	0.14336 (18)	0.54341 (10)	0.0345 (4)
H17	0.4062	0.1693	0.5836	0.052*
H18	0.3631	0.0644	0.5483	0.052*
O14	0.1887 (3)	0.3503 (2)	0.46768 (11)	0.0389 (5)
H19	0.1123	0.3350	0.5033	0.058*
H20	0.1258	0.3797	0.4310	0.058*
O15	0.2963 (3)	0.1171 (2)	0.38772 (11)	0.0401 (5)
H21	0.2280	0.0609	0.4052	0.060*
H22	0.3638	0.0848	0.3523	0.060*
O16	0.5789 (3)	0.36211 (17)	0.49962 (10)	0.0322 (4)
H23	0.5090	0.3960	0.5339	0.048*
H24	0.6880	0.3369	0.5165	0.048*
O17	0.9698 (3)	0.4941 (2)	0.36813 (13)	0.0447 (5)
H25	0.8479	0.4993	0.3709	0.067*
H26	0.9998	0.5661	0.3793	0.067*
O18	0.8077 (4)	0.1571 (3)	0.29453 (13)	0.0583 (7)
H27	0.9014	0.1539	0.2636	0.087*
H28	0.7297	0.2213	0.2847	0.087*
O19	0.2034 (4)	0.3774 (2)	0.25875 (15)	0.0573 (6)
H29	0.1448	0.3378	0.2286	0.086*
H30	0.1123	0.4045	0.2878	0.086*
O20	0.4729 (4)	0.0133 (2)	0.26230 (13)	0.0479 (6)
H31	0.5790	0.0442	0.2540	0.072*
H32	0.4932	−0.0659	0.2703	0.072*
O21	0.1491 (4)	0.1463 (2)	0.20047 (13)	0.0542 (6)
H33	0.2577	0.1190	0.2170	0.081*
H34	0.1573	0.1398	0.1543	0.081*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0371 (15)	0.0458 (17)	0.0261 (14)	−0.0008 (13)	−0.0022 (11)	0.0009 (12)
C2	0.0471 (17)	0.0356 (15)	0.0338 (15)	−0.0044 (13)	−0.0062 (12)	−0.0046 (12)
C3	0.0436 (16)	0.0297 (14)	0.0324 (14)	−0.0058 (12)	−0.0057 (12)	0.0036 (11)

C4	0.0302 (13)	0.0332 (14)	0.0254 (12)	−0.0012 (11)	−0.0030 (10)	0.0015 (10)
C5	0.0443 (17)	0.0327 (15)	0.0320 (14)	−0.0026 (13)	−0.0049 (12)	0.0001 (11)
C6	0.0429 (17)	0.0404 (16)	0.0324 (15)	−0.0034 (13)	−0.0029 (12)	0.0088 (12)
C7	0.0390 (15)	0.0247 (13)	0.0276 (13)	−0.0018 (11)	−0.0040 (11)	0.0018 (10)
C8	0.0308 (13)	0.0267 (13)	0.0273 (13)	−0.0036 (11)	0.0001 (10)	0.0013 (10)
C9	0.0301 (14)	0.0423 (16)	0.0266 (13)	−0.0021 (12)	−0.0053 (10)	−0.0006 (11)
C10	0.0417 (16)	0.0354 (15)	0.0393 (16)	−0.0088 (13)	−0.0080 (12)	−0.0035 (12)
C11	0.0435 (16)	0.0310 (14)	0.0352 (15)	−0.0077 (13)	−0.0062 (12)	0.0053 (11)
C12	0.0275 (13)	0.0353 (14)	0.0267 (13)	−0.0023 (11)	−0.0026 (10)	0.0016 (10)
C13	0.0416 (16)	0.0301 (14)	0.0320 (14)	−0.0026 (12)	−0.0047 (11)	0.0006 (11)
C14	0.0406 (16)	0.0348 (15)	0.0320 (14)	−0.0001 (12)	−0.0062 (11)	0.0057 (11)
C15	0.0382 (15)	0.0276 (13)	0.0286 (13)	−0.0032 (11)	−0.0036 (11)	0.0007 (10)
C16	0.0273 (13)	0.0319 (14)	0.0263 (12)	−0.0033 (11)	−0.0001 (10)	0.0012 (10)
N1	0.066 (2)	0.062 (2)	0.0296 (14)	−0.0051 (16)	−0.0069 (13)	−0.0001 (13)
N2	0.0426 (15)	0.0536 (17)	0.0313 (13)	−0.0041 (13)	−0.0057 (10)	−0.0020 (12)
Ni1	0.0323 (2)	0.02138 (18)	0.02258 (17)	−0.00295 (13)	−0.00290 (12)	0.00103 (11)
O1	0.0508 (12)	0.0290 (10)	0.0304 (10)	−0.0026 (9)	−0.0093 (9)	0.0054 (8)
O2	0.0696 (15)	0.0280 (10)	0.0289 (10)	−0.0054 (10)	−0.0109 (10)	0.0005 (8)
O3	0.0586 (13)	0.0275 (10)	0.0267 (10)	−0.0044 (9)	−0.0091 (9)	0.0023 (7)
O4	0.132 (3)	0.076 (2)	0.0369 (14)	−0.013 (2)	−0.0194 (16)	−0.0112 (14)
O5	0.164 (4)	0.079 (2)	0.0340 (14)	−0.025 (2)	−0.0150 (18)	0.0167 (14)
O6	0.0386 (11)	0.0306 (10)	0.0319 (10)	−0.0053 (8)	−0.0062 (8)	0.0043 (8)
O7	0.0519 (13)	0.0333 (11)	0.0315 (10)	−0.0080 (9)	−0.0055 (9)	−0.0006 (8)
O8	0.0515 (12)	0.0317 (10)	0.0262 (9)	−0.0066 (9)	−0.0075 (8)	0.0026 (8)
O9	0.101 (2)	0.0585 (17)	0.0417 (14)	−0.0133 (15)	−0.0179 (14)	−0.0121 (12)
O10	0.092 (2)	0.0599 (16)	0.0318 (12)	−0.0096 (15)	−0.0137 (12)	0.0096 (11)
O11	0.0417 (11)	0.0256 (9)	0.0287 (9)	−0.0056 (8)	−0.0046 (8)	0.0033 (7)
O12	0.0388 (11)	0.0304 (10)	0.0298 (10)	0.0007 (8)	−0.0025 (8)	−0.0009 (7)
O13	0.0523 (12)	0.0269 (10)	0.0255 (9)	−0.0094 (9)	−0.0052 (8)	0.0033 (7)
O14	0.0370 (11)	0.0419 (12)	0.0352 (11)	0.0039 (9)	0.0029 (8)	0.0104 (9)
O15	0.0539 (13)	0.0366 (11)	0.0329 (10)	−0.0183 (10)	−0.0034 (9)	−0.0038 (8)
O16	0.0359 (10)	0.0279 (10)	0.0329 (10)	−0.0005 (8)	−0.0074 (8)	−0.0039 (7)
O17	0.0460 (13)	0.0330 (11)	0.0542 (14)	0.0022 (10)	−0.0104 (10)	0.0004 (9)
O18	0.0687 (17)	0.0573 (15)	0.0441 (14)	0.0093 (13)	0.0108 (12)	0.0067 (11)
O19	0.0625 (16)	0.0543 (15)	0.0564 (15)	−0.0053 (13)	−0.0182 (12)	−0.0036 (12)
O20	0.0582 (14)	0.0338 (12)	0.0510 (14)	−0.0048 (10)	0.0032 (11)	0.0049 (10)
O21	0.0668 (16)	0.0596 (16)	0.0365 (12)	−0.0064 (13)	−0.0066 (11)	−0.0021 (11)

Geometric parameters (Å, °)

C1—C2	1.379 (4)	C16—O7	1.245 (3)
C1—C6	1.380 (4)	C16—O6	1.255 (3)
C1—N1	1.458 (4)	N1—O4	1.214 (4)
C2—C3	1.380 (4)	N1—O5	1.226 (4)
C2—H1	0.9300	N2—O9	1.218 (4)
C3—C4	1.385 (4)	N2—O10	1.230 (4)
C3—H2	0.9300	Ni1—O13	2.038 (2)
C4—O3	1.351 (3)	Ni1—O16	2.042 (2)
C4—C5	1.400 (4)	Ni1—O14	2.045 (2)

C5—C6	1.375 (4)	Ni1—O15	2.048 (2)
C5—H3	0.9300	Ni1—O11	2.070 (2)
C6—H4	0.9300	Ni1—O12	2.091 (2)
C7—O3	1.431 (3)	O11—H13	0.8500
C7—C8	1.516 (4)	O11—H14	0.8500
C7—H5	0.9700	O12—H15	0.8499
C7—H6	0.9700	O12—H16	0.8501
C8—O2	1.236 (3)	O13—H17	0.8502
C8—O1	1.262 (3)	O13—H18	0.8500
C9—C14	1.375 (4)	O14—H19	0.8500
C9—C10	1.384 (4)	O14—H20	0.8501
C9—N2	1.445 (4)	O15—H21	0.8500
C10—C11	1.373 (4)	O15—H22	0.8500
C10—H7	0.9300	O16—H23	0.8499
C11—C12	1.398 (4)	O16—H24	0.8499
C11—H8	0.9300	O17—H25	0.8501
C12—O8	1.352 (3)	O17—H26	0.8501
C12—C13	1.383 (4)	O18—H27	0.8499
C13—C14	1.377 (4)	O18—H28	0.8500
C13—H9	0.9300	O19—H29	0.8500
C14—H10	0.9300	O19—H30	0.8500
C15—O8	1.424 (3)	O20—H31	0.8500
C15—C16	1.512 (4)	O20—H32	0.8500
C15—H11	0.9700	O21—H33	0.8499
C15—H12	0.9700	O21—H34	0.8501
C2—C1—C6	121.9 (3)	H11—C15—H12	108.2
C2—C1—N1	119.2 (3)	O7—C16—O6	125.4 (3)
C6—C1—N1	118.9 (3)	O7—C16—C15	115.2 (2)
C1—C2—C3	119.4 (3)	O6—C16—C15	119.4 (2)
C1—C2—H1	120.3	O4—N1—O5	123.8 (3)
C3—C2—H1	120.3	O4—N1—C1	119.1 (3)
C2—C3—C4	119.4 (3)	O5—N1—C1	117.2 (3)
C2—C3—H2	120.3	O9—N2—O10	122.3 (3)
C4—C3—H2	120.3	O9—N2—C9	119.4 (3)
O3—C4—C3	125.1 (2)	O10—N2—C9	118.3 (3)
O3—C4—C5	114.3 (2)	O13—Ni1—O16	92.38 (8)
C3—C4—C5	120.7 (3)	O13—Ni1—O14	86.00 (9)
C6—C5—C4	119.6 (3)	O16—Ni1—O14	87.80 (9)
C6—C5—H3	120.2	O13—Ni1—O15	92.31 (9)
C4—C5—H3	120.2	O16—Ni1—O15	175.30 (8)
C5—C6—C1	119.1 (3)	O14—Ni1—O15	92.18 (9)
C5—C6—H4	120.5	O13—Ni1—O11	178.78 (8)
C1—C6—H4	120.5	O16—Ni1—O11	88.57 (8)
O3—C7—C8	108.2 (2)	O14—Ni1—O11	93.25 (8)
O3—C7—H5	110.1	O15—Ni1—O11	86.74 (8)
C8—C7—H5	110.1	O13—Ni1—O12	89.70 (9)
O3—C7—H6	110.1	O16—Ni1—O12	89.70 (8)
C8—C7—H6	110.1	O14—Ni1—O12	174.93 (8)
H5—C7—H6	108.4	O15—Ni1—O12	90.67 (9)

O2—C8—O1	125.9 (3)	O11—Ni1—O12	91.09 (8)
O2—C8—C7	119.0 (2)	C4—O3—C7	118.5 (2)
O1—C8—C7	115.1 (2)	C12—O8—C15	117.9 (2)
C14—C9—C10	121.6 (3)	Ni1—O11—H13	119.0
C14—C9—N2	119.2 (3)	Ni1—O11—H14	115.7
C10—C9—N2	119.1 (3)	H13—O11—H14	102.9
C11—C10—C9	118.7 (3)	Ni1—O12—H15	118.6
C11—C10—H7	120.6	Ni1—O12—H16	116.5
C9—C10—H7	120.6	H15—O12—H16	111.7
C10—C11—C12	120.1 (3)	Ni1—O13—H17	119.9
C10—C11—H8	120.0	Ni1—O13—H18	124.8
C12—C11—H8	120.0	H17—O13—H18	108.3
O8—C12—C13	124.8 (3)	Ni1—O14—H19	121.5
O8—C12—C11	114.8 (2)	Ni1—O14—H20	117.5
C13—C12—C11	120.4 (3)	H19—O14—H20	110.1
C14—C13—C12	119.4 (3)	Ni1—O15—H21	125.6
C14—C13—H9	120.3	Ni1—O15—H22	113.9
C12—C13—H9	120.3	H21—O15—H22	107.0
C9—C14—C13	119.8 (3)	Ni1—O16—H23	110.7
C9—C14—H10	120.1	Ni1—O16—H24	118.2
C13—C14—H10	120.1	H23—O16—H24	108.2
O8—C15—C16	109.7 (2)	H25—O17—H26	105.8
O8—C15—H11	109.7	H27—O18—H28	109.3
C16—C15—H11	109.7	H29—O19—H30	101.7
O8—C15—H12	109.7	H31—O20—H32	109.7
C16—C15—H12	109.7	H33—O21—H34	107.3

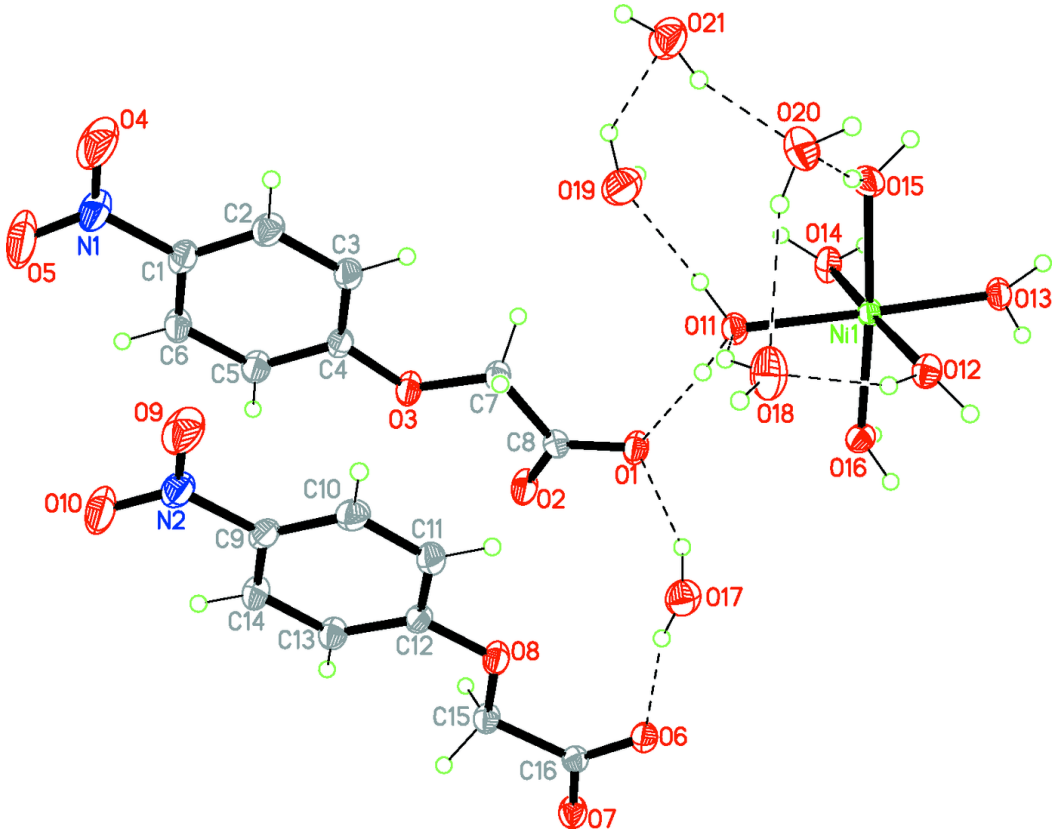
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O11—H13···O1	0.85	1.87	2.706 (3)	167
O11—H14···O19	0.85	1.84	2.687 (3)	176
O12—H15···O18	0.85	1.94	2.739 (3)	156
O12—H16···O7^{i}	0.85	1.79	2.640 (3)	173
O13—H17···O2^{ii}	0.85	1.80	2.652 (3)	179
O13—H18···O12^{iii}	0.85	2.01	2.859 (3)	173
O14—H19···O6^{ii}	0.85	1.97	2.814 (3)	171
O14—H20···O17^{iv}	0.85	1.93	2.749 (3)	161
O15—H21···O7^{v}	0.85	1.88	2.719 (3)	168
O15—H22···O20	0.85	1.94	2.779 (3)	169
O16—H23···O1^{ii}	0.85	2.04	2.831 (3)	154
O16—H24···O6^{i}	0.85	1.93	2.762 (3)	168
O17—H25···O1	0.85	2.07	2.885 (3)	160
O17—H26···O6	0.85	1.96	2.789 (3)	166
O18—H27···O21^{vi}	0.85	2.05	2.890 (4)	173
O18—H28···O11	0.85	2.23	2.881 (3)	133
O19—H29···O21	0.85	2.12	2.788 (4)	135

O19—H30···O17^{iv}	0.85	1.97	2.786 (4)	161
O20—H31···O18	0.85	2.26	3.018 (4)	148
O20—H32···O2^{vii}	0.85	1.96	2.753 (3)	156
O21—H33···O20	0.85	1.98	2.805 (4)	164
O21—H34···O10^{viii}	0.85	2.06	2.905 (3)	171

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

Fig. 1


O21
O20
O19
O15
O4
N1
O5
C2
C3
C1
O14
O13
O11
Ni1
C6
C5
C4
O3
C7
O12
O18
C8
O1
O16
O9
O10
N2
C10
C11
C9
O17
C14
C13
C12
O8
C15
O6
C16
O7