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## Aquabis(1*H*-imidazole- $\kappa$ N<sup>3</sup>)bis(4-methylbenzoato)- $\kappa$ O; $\kappa$ O,*O'*-nickel(II)

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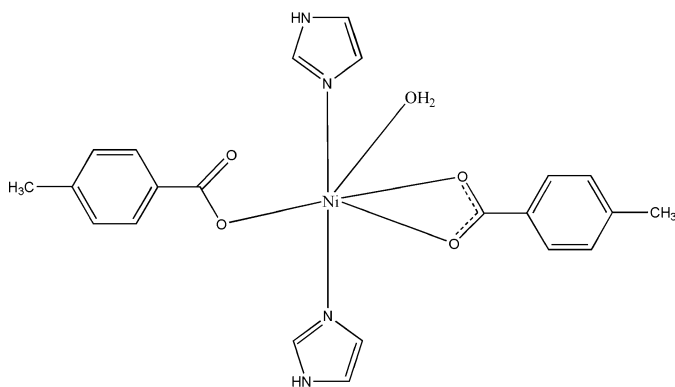
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å;  $R$  factor = 0.061;  $wR$  factor = 0.171; data-to-parameter ratio = 12.7.

In the mononuclear title compound,  $[\text{Ni}(\text{C}_8\text{H}_7\text{O}_2)_2(\text{C}_3\text{H}_4\text{N}_2)_2(\text{H}_2\text{O})]$ , the  $\text{Ni}^{\text{II}}$  atom is coordinated by three carboxylate O atoms (from a bidentate 4-methylbenzoate ligand and a monodentate 4-methylbenzoate ligand), two N atoms (from two imidazole ligands) and a water molecule in an octahedral geometry. Intermolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen-bonding interactions lead to infinite chains, which are further self-assembled into a supramolecular network through intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen-bonding interactions and  $\pi-\pi$  stacking [centroid-centroid distance = 3.717 (2) Å].

### Related literature

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



### Experimental

#### Crystal data

$[\text{Ni}(\text{C}_8\text{H}_7\text{O}_2)_2(\text{C}_3\text{H}_4\text{N}_2)_2(\text{H}_2\text{O})]$   
 $M_r = 483.16$   
 Monoclinic,  $P2_1/n$   
 $a = 18.9456$  (12) Å  
 $b = 5.8755$  (4) Å  
 $c = 20.3209$  (14) Å  
 $\beta = 101.813$  (4)°

$V = 2214.1$  (3) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.92$  mm<sup>-1</sup>  
 $T = 296$  (2) K  
 $0.30 \times 0.26 \times 0.25$  mm

#### Data collection

Bruker APEXII area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\text{min}} = 0.770$ ,  $T_{\text{max}} = 0.803$

20580 measured reflections  
 3776 independent reflections  
 2815 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.077$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.060$   
 $wR(F^2) = 0.171$   
 $S = 1.07$   
 3776 reflections  
 297 parameters  
 3 restraints

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}} = 1.02$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.71$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1W}-\text{H1W}\cdots\text{O3}^{\text{i}}$	0.826 (10)	2.31 (4)	2.782 (4)	116 (4)
$\text{O1W}-\text{H1W}\cdots\text{O2}^{\text{i}}$	0.826 (10)	2.21 (3)	2.772 (4)	126 (3)
$\text{N2}-\text{H2}\cdots\text{O2}^{\text{ii}}$	0.86	1.96	2.816 (5)	175
$\text{N4}-\text{H22}\cdots\text{O4}^{\text{iii}}$	0.86	2.02	2.865 (4)	167

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

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: XP in SHELXTL (Sheldrick, 2008); 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: NG2442).

### References

- Bruker (2004). APEX2 and SAINT. Bruker AXS Inc, Madison, Wisconsin, USA.  
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.  
 Sheldrick, G. M. (2008). Acta Cryst. A64, 112–122.  
 Song, W.-D., Gu, C.-S., Hao, X.-M. & Liu, J.-W. (2007). Acta Cryst. E63, m1023–m1024.

**supplementary materials**

*Acta Cryst.* (2008). E64, m648 [ doi:10.1107/S1600536808009471 ]

## Aquabis(1*H*-imidazole- $\kappa$ N<sup>3</sup>)bis(4-methylbenzoato)- $\kappa$ O; $\kappa$ O,*O'*-nickel(II)

W.-D. Song, R.-Z. Fan and H.-M. Wu

### Comment

In the structural investigation of 4-methylbenzoate complexes, it has been found that the 4-methylbenzoic acid functions as a multidentate ligand [Song *et al.* (2007)], with versatile binding and coordination modes. In this paper, we report the crystal structure of the title compound, (I), a new Ni complex obtained by the reaction of 4-methylbenzoic acid, imidazole and nickel chloride in alkaline aqueous solution.

As illustrated in Figure 1, the Ni<sup>II</sup> atom exists in a disordered octahedral environment, defined by three carboxyl O atoms from one bidentate 4-methylbenzoate ligand and one monodentate 4-methylbenzoate ligand, two N atoms from two imidazole ligands and one water molecule. Intermolecular O—H $\cdots$ O hydrogen bonding interactions (Table 1) form infinite chains involving the coordinating water molecule as donors and O atoms of 4-methylbenzoate ligands as acceptors, which are further self-assembled into a supramolecular network through intermolecular N—H $\cdots$ O hydrogen bonding interactions and  $\pi$ - $\pi$  stacking interactions of neighboring complexes, with a centroid-centroid distance of 3.717 (2) Å. (Fig. 2).

### Experimental

A mixture of nickel chloride(1 mmol), 4-methylbenzoic acid (1 mmol), imidazole(1 mmol), NaOH (1.5 mmol) and H<sub>2</sub>O (12 ml) was placed in a 23 ml Teflon reactor, which was heated to 433 K for three days and then cooled to room temperature at a rate of 10 K h<sup>-1</sup>. The crystals obtained were washed with water and dried in air.

### Refinement

H atoms were placed at calculated positions and were treated as riding on the parent C atoms with C—H = 0.93 - 0.97 Å, N—H = 0.86 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C}, \text{N})$ .

### Figures

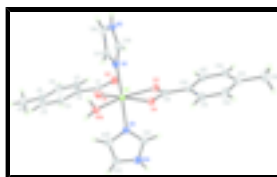


Fig. 1. The structure of (I), showing the atomic numbering scheme. Non-H atoms are shown as 30% probability displacement ellipsoids.

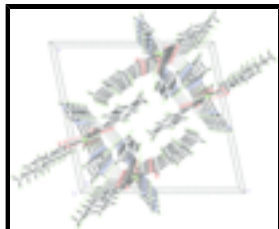


Fig. 2. The packing of structure (I).

## Aquabis(1H-imidazole- $\kappa\text{N}^3$ )bis(4-methylbenzoato)- $\kappa\text{O};\kappa\text{O},\text{O}'$ -nickel(II)

### Crystal data

$[\text{Ni}(\text{C}_8\text{H}_7\text{O}_2)_2(\text{C}_3\text{H}_4\text{N}_2)_2(\text{H}_2\text{O})]$

$M_r = 483.16$

Monoclinic,  $P2_1/n$

Hall symbol:  $-P\ 2yn$

$a = 18.9456\ (12)\ \text{\AA}$

$b = 5.8755\ (4)\ \text{\AA}$

$c = 20.3209\ (14)\ \text{\AA}$

$\beta = 101.813\ (4)^\circ$

$V = 2214.1\ (3)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 1008$

$D_x = 1.449\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3600 reflections

$\theta = 1.4\text{--}28^\circ$

$\mu = 0.92\ \text{mm}^{-1}$

$T = 296\ (2)\ \text{K}$

Block, blue

$0.30 \times 0.26 \times 0.25\ \text{mm}$

### Data collection

Bruker APEXII area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 296\ (2)\ \text{K}$

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(SADABS; Sheldrick, 1996)

$T_{\min} = 0.770$ ,  $T_{\max} = 0.803$

20580 measured reflections

3776 independent reflections

2815 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.077$

$\theta_{\max} = 25.2^\circ$

$\theta_{\min} = 1.7^\circ$

$h = -22 \rightarrow 22$

$k = -7 \rightarrow 7$

$l = -22 \rightarrow 21$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.060$

$wR(F^2) = 0.171$

$S = 1.07$

3776 reflections

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

$w = 1/[\sigma^2(F_o^2) + (0.1064P)^2 + 0.0659P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 1.02\ \text{e \AA}^{-3}$

297 parameters

$$\Delta\rho_{\min} = -0.71 \text{ e } \text{\AA}^{-3}$$

3 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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.68032 (18)	0.0732 (7)	0.9997 (2)	0.0328 (10)
C2	0.72717 (19)	0.1141 (7)	1.0678 (2)	0.0318 (10)
C3	0.7618 (2)	0.3198 (8)	1.0827 (2)	0.0434 (12)
H3	0.7552	0.4352	1.0507	0.052*
C4	0.8066 (2)	0.3558 (9)	1.1451 (3)	0.0515 (13)
H4	0.8302	0.4949	1.1538	0.062*
C5	0.8171 (2)	0.1911 (9)	1.1943 (3)	0.0450 (12)
C6	0.7816 (2)	-0.0143 (9)	1.1796 (3)	0.0532 (13)
H6	0.7875	-0.1286	1.2119	0.064*
C7	0.7377 (2)	-0.0515 (8)	1.1177 (3)	0.0473 (12)
H7	0.7144	-0.1910	1.1090	0.057*
C8	0.8676 (3)	0.2326 (11)	1.2602 (3)	0.0676 (17)
H8A	0.9136	0.1655	1.2593	0.101*
H8B	0.8482	0.1655	1.2957	0.101*
H8C	0.8733	0.3935	1.2677	0.101*
C9	0.56235 (18)	0.1063 (7)	0.7571 (2)	0.0291 (9)
C10	0.51866 (17)	0.0039 (6)	0.6958 (2)	0.0282 (9)
C11	0.5069 (2)	0.1198 (8)	0.6345 (2)	0.0402 (11)
H11	0.5271	0.2633	0.6325	0.048*
C12	0.4665 (2)	0.0269 (8)	0.5775 (2)	0.0463 (12)
H12	0.4593	0.1088	0.5375	0.056*
C13	0.4360 (2)	-0.1874 (8)	0.5782 (3)	0.0442 (12)
C14	0.4474 (2)	-0.3059 (8)	0.6384 (3)	0.0406 (12)
H14	0.4271	-0.4496	0.6398	0.049*
C15	0.4884 (2)	-0.2135 (7)	0.6964 (2)	0.0351 (11)
H15	0.4960	-0.2964	0.7362	0.042*
C16	0.3904 (3)	-0.2924 (10)	0.5148 (3)	0.0693 (17)
H16A	0.4187	-0.3031	0.4807	0.104*
H16B	0.3490	-0.1985	0.4989	0.104*

## supplementary materials

H16C	0.3750	-0.4417	0.5249	0.104*
C17	0.49535 (19)	0.5721 (7)	0.8861 (2)	0.0373 (11)
H17	0.5079	0.7042	0.8660	0.045*
C18	0.4381 (2)	0.5510 (8)	0.9164 (2)	0.0433 (12)
H18	0.4047	0.6627	0.9210	0.052*
C19	0.4959 (2)	0.2304 (8)	0.9211 (3)	0.0411 (12)
H19	0.5083	0.0787	0.9301	0.049*
C20	0.7912 (2)	0.2900 (8)	0.8792 (3)	0.0495 (14)
H20	0.7947	0.3948	0.9140	0.059*
C21	0.7474 (2)	0.0663 (7)	0.7991 (2)	0.0420 (11)
H21	0.7152	-0.0160	0.7671	0.050*
N4	0.81940 (17)	0.0528 (6)	0.8074 (2)	0.0467 (10)
H22	0.8430	-0.0306	0.7846	0.056*
N1	0.53185 (15)	0.3705 (6)	0.88955 (18)	0.0333 (8)
N2	0.43972 (17)	0.3329 (7)	0.93841 (19)	0.0413 (10)
H2	0.4098	0.2716	0.9598	0.050*
N3	0.72811 (16)	0.2084 (5)	0.84118 (19)	0.0322 (9)
C22	0.8477 (2)	0.1935 (9)	0.8579 (3)	0.0499 (14)
H4A	0.8964	0.2199	0.8749	0.060*
Ni1	0.62851 (2)	0.29313 (8)	0.86285 (3)	0.0263 (2)
O1	0.67349 (15)	0.2409 (5)	0.95998 (16)	0.0380 (8)
O2	0.65064 (15)	-0.1153 (5)	0.98695 (15)	0.0437 (8)
O3	0.57902 (13)	-0.0107 (4)	0.80995 (15)	0.0338 (7)
O4	0.58228 (13)	0.3134 (4)	0.75769 (15)	0.0300 (7)
O1W	0.66137 (13)	0.6312 (5)	0.87438 (15)	0.0344 (7)
H1W	0.6334 (14)	0.721 (6)	0.887 (2)	0.052*
H2W	0.7005 (9)	0.663 (7)	0.896 (2)	0.052*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0320 (19)	0.036 (2)	0.034 (3)	0.0060 (16)	0.0155 (18)	-0.002 (2)
C2	0.0314 (18)	0.038 (2)	0.027 (3)	0.0003 (17)	0.0100 (17)	0.001 (2)
C3	0.049 (2)	0.042 (3)	0.036 (3)	-0.0022 (19)	0.002 (2)	0.009 (2)
C4	0.047 (2)	0.053 (3)	0.050 (4)	-0.008 (2)	0.001 (2)	-0.005 (3)
C5	0.035 (2)	0.069 (3)	0.029 (3)	0.005 (2)	0.0035 (19)	0.002 (3)
C6	0.054 (3)	0.068 (3)	0.035 (3)	0.002 (2)	0.001 (2)	0.021 (3)
C7	0.048 (2)	0.047 (3)	0.046 (3)	-0.007 (2)	0.006 (2)	0.004 (2)
C8	0.050 (3)	0.107 (5)	0.043 (4)	0.002 (3)	0.001 (3)	0.001 (3)
C9	0.0326 (18)	0.026 (2)	0.031 (3)	0.0049 (16)	0.0122 (17)	0.001 (2)
C10	0.0306 (18)	0.030 (2)	0.026 (3)	0.0001 (15)	0.0104 (16)	0.0001 (19)
C11	0.046 (2)	0.034 (2)	0.041 (3)	-0.0007 (19)	0.011 (2)	-0.002 (2)
C12	0.057 (3)	0.048 (3)	0.032 (3)	0.003 (2)	0.005 (2)	0.004 (2)
C13	0.036 (2)	0.055 (3)	0.042 (3)	-0.0048 (19)	0.008 (2)	-0.012 (3)
C14	0.038 (2)	0.040 (3)	0.044 (4)	-0.0082 (17)	0.008 (2)	-0.008 (2)
C15	0.039 (2)	0.030 (2)	0.038 (3)	-0.0015 (16)	0.0107 (19)	-0.001 (2)
C16	0.070 (3)	0.079 (4)	0.057 (5)	-0.020 (3)	0.008 (3)	-0.025 (3)
C17	0.036 (2)	0.034 (2)	0.044 (3)	-0.0018 (16)	0.0125 (18)	-0.007 (2)

C18	0.036 (2)	0.052 (3)	0.045 (3)	0.0025 (19)	0.014 (2)	-0.013 (2)
C19	0.040 (2)	0.042 (3)	0.043 (3)	-0.0010 (18)	0.010 (2)	0.000 (2)
C20	0.034 (2)	0.060 (3)	0.056 (4)	-0.0034 (19)	0.013 (2)	-0.016 (3)
C21	0.043 (2)	0.036 (2)	0.049 (3)	0.0004 (18)	0.015 (2)	-0.008 (2)
N4	0.0425 (19)	0.045 (2)	0.059 (3)	0.0097 (16)	0.0251 (18)	-0.005 (2)
N1	0.0318 (16)	0.0358 (19)	0.035 (2)	-0.0025 (14)	0.0123 (14)	0.0007 (17)
N2	0.0344 (17)	0.058 (3)	0.037 (3)	-0.0090 (16)	0.0194 (16)	-0.006 (2)
N3	0.0329 (16)	0.0297 (18)	0.036 (3)	0.0001 (13)	0.0130 (15)	-0.0062 (17)
C22	0.034 (2)	0.064 (3)	0.055 (4)	0.000 (2)	0.016 (2)	-0.001 (3)
Ni1	0.0288 (3)	0.0243 (3)	0.0276 (4)	0.00023 (17)	0.0098 (2)	0.0002 (2)
O1	0.0404 (15)	0.0427 (18)	0.030 (2)	0.0005 (12)	0.0042 (13)	0.0050 (14)
O2	0.0580 (17)	0.0408 (18)	0.035 (2)	-0.0158 (15)	0.0168 (14)	-0.0062 (16)
O3	0.0400 (14)	0.0276 (15)	0.032 (2)	-0.0014 (11)	0.0030 (12)	0.0030 (14)
O4	0.0374 (14)	0.0249 (15)	0.0286 (19)	-0.0026 (11)	0.0090 (12)	0.0007 (13)
O1W	0.0316 (13)	0.0292 (15)	0.044 (2)	-0.0014 (12)	0.0124 (13)	-0.0067 (14)

*Geometric parameters (Å, °)*

C1—O2	1.245 (5)	C15—H15	0.9300
C1—O1	1.264 (5)	C16—H16A	0.9600
C1—C2	1.503 (6)	C16—H16B	0.9600
C2—C3	1.379 (6)	C16—H16C	0.9600
C2—C7	1.389 (6)	C17—C18	1.359 (6)
C3—C4	1.391 (6)	C17—N1	1.366 (5)
C3—H3	0.9300	C17—H17	0.9300
C4—C5	1.376 (7)	C18—N2	1.356 (6)
C4—H4	0.9300	C18—H18	0.9300
C5—C6	1.384 (7)	C19—N1	1.315 (5)
C5—C8	1.497 (7)	C19—N2	1.333 (5)
C6—C7	1.376 (6)	C19—H19	0.9300
C6—H6	0.9300	C20—C22	1.359 (6)
C7—H7	0.9300	C20—N3	1.370 (5)
C8—H8A	0.9600	C20—H20	0.9300
C8—H8B	0.9600	C21—N3	1.300 (5)
C8—H8C	0.9600	C21—N4	1.342 (5)
C9—O3	1.260 (5)	C21—H21	0.9300
C9—O4	1.274 (5)	N4—C22	1.341 (6)
C9—C10	1.475 (6)	N4—H22	0.8600
C10—C11	1.396 (6)	N1—Ni1	2.065 (3)
C10—C15	1.401 (5)	N2—H2	0.8600
C11—C12	1.365 (6)	N3—Ni1	2.084 (3)
C11—H11	0.9300	C22—H4A	0.9300
C12—C13	1.387 (6)	Ni1—O1	2.007 (3)
C12—H12	0.9300	Ni1—O1W	2.081 (3)
C13—C14	1.385 (7)	Ni1—O4	2.140 (3)
C13—C16	1.526 (7)	Ni1—O3	2.193 (3)
C14—C15	1.383 (6)	O1W—H1W	0.826 (10)
C14—H14	0.9300	O1W—H2W	0.805 (10)
O2—C1—O1	125.3 (4)	H16B—C16—H16C	109.5

## supplementary materials

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O2—C1—C2	119.4 (4)	C18—C17—N1	109.9 (4)
O1—C1—C2	115.3 (4)	C18—C17—H17	125.1
C3—C2—C7	117.6 (4)	N1—C17—H17	125.1
C3—C2—C1	120.4 (4)	N2—C18—C17	105.6 (4)
C7—C2—C1	121.9 (4)	N2—C18—H18	127.2
C2—C3—C4	120.5 (4)	C17—C18—H18	127.2
C2—C3—H3	119.8	N1—C19—N2	111.5 (4)
C4—C3—H3	119.8	N1—C19—H19	124.2
C5—C4—C3	121.7 (5)	N2—C19—H19	124.2
C5—C4—H4	119.1	C22—C20—N3	109.1 (4)
C3—C4—H4	119.1	C22—C20—H20	125.4
C4—C5—C6	117.7 (4)	N3—C20—H20	125.4
C4—C5—C8	120.3 (5)	N3—C21—N4	111.7 (4)
C6—C5—C8	121.9 (5)	N3—C21—H21	124.1
C7—C6—C5	120.8 (5)	N4—C21—H21	124.1
C7—C6—H6	119.6	C22—N4—C21	107.3 (4)
C5—C6—H6	119.6	C22—N4—H22	126.4
C6—C7—C2	121.7 (4)	C21—N4—H22	126.4
C6—C7—H7	119.2	C19—N1—C17	105.1 (3)
C2—C7—H7	119.2	C19—N1—Ni1	124.4 (3)
C5—C8—H8A	109.5	C17—N1—Ni1	130.1 (3)
C5—C8—H8B	109.5	C19—N2—C18	107.8 (4)
H8A—C8—H8B	109.5	C19—N2—H2	126.1
C5—C8—H8C	109.5	C18—N2—H2	126.1
H8A—C8—H8C	109.5	C21—N3—C20	105.4 (3)
H8B—C8—H8C	109.5	C21—N3—Ni1	132.9 (3)
O3—C9—O4	119.4 (4)	C20—N3—Ni1	121.3 (3)
O3—C9—C10	119.8 (4)	N4—C22—C20	106.5 (4)
O4—C9—C10	120.8 (4)	N4—C22—H4A	126.8
C11—C10—C15	117.5 (4)	C20—C22—H4A	126.8
C11—C10—C9	120.9 (4)	O1—Ni1—N1	89.78 (13)
C15—C10—C9	121.6 (4)	O1—Ni1—O1W	88.76 (12)
C12—C11—C10	121.4 (4)	N1—Ni1—O1W	91.21 (12)
C12—C11—H11	119.3	O1—Ni1—N3	87.18 (13)
C10—C11—H11	119.3	N1—Ni1—N3	176.89 (14)
C11—C12—C13	121.1 (5)	O1W—Ni1—N3	89.37 (11)
C11—C12—H12	119.4	O1—Ni1—O4	174.26 (11)
C13—C12—H12	119.4	N1—Ni1—O4	92.66 (12)
C14—C13—C12	118.4 (4)	O1W—Ni1—O4	96.38 (11)
C14—C13—C16	120.1 (5)	N3—Ni1—O4	90.32 (12)
C12—C13—C16	121.5 (5)	O1—Ni1—O3	114.23 (12)
C15—C14—C13	120.9 (4)	N1—Ni1—O3	89.70 (12)
C15—C14—H14	119.5	O1W—Ni1—O3	157.00 (12)
C13—C14—H14	119.5	N3—Ni1—O3	90.96 (11)
C14—C15—C10	120.6 (4)	O4—Ni1—O3	60.62 (10)
C14—C15—H15	119.7	C1—O1—Ni1	135.7 (3)
C10—C15—H15	119.7	C9—O3—Ni1	88.9 (2)
C13—C16—H16A	109.5	C9—O4—Ni1	90.9 (2)
C13—C16—H16B	109.5	Ni1—O1W—H1W	116 (3)

H16A—C16—H16B	109.5	Ni1—O1W—H2W	120 (3)
C13—C16—H16C	109.5	H1W—O1W—H2W	104.8 (17)
H16A—C16—H16C	109.5		

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O1W—H1W $\cdots$ O3 <sup>i</sup>	0.826 (10)	2.31 (4)	2.782 (4)	116 (4)
O1W—H1W $\cdots$ O2 <sup>i</sup>	0.826 (10)	2.21 (3)	2.772 (4)	126 (3)
N2—H2 $\cdots$ O2 <sup>ii</sup>	0.86	1.96	2.816 (5)	175
N4—H22 $\cdots$ O4 <sup>iii</sup>	0.86	2.02	2.865 (4)	167

Symmetry codes: (i)  $x, y+1, z$ ; (ii)  $-x+1, -y, -z+2$ ; (iii)  $-x+3/2, y-1/2, -z+3/2$ .



Fig. 2

