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Tetraaquabis[4-(4*H*-1,2,4-triazol-4-yl)-benzoato-κN^1]nickel(II) decahydrate

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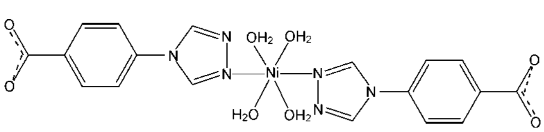
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.049; wR factor = 0.119; data-to-parameter ratio = 12.9.

In the title compound, $[Ni(C_9H_6N_3O_2)_2(H_2O)_4]\cdot10H_2O$, the Ni^{II} ion lies on a twofold rotation axis and displays a slightly distorted octahedral geometry defined by two N atoms from two monodentate 4-(1,2,4-triazol-4-yl)benzoate ligands and four water molecules, two of which also lie on the twofold rotation axis. In the crystal, the complex molecules and uncoordinated water molecules are linked *via* intermolecular O—H···N and O—H···O hydrogen bonds, forming a three-dimensional supramolecular network. π–π interactions between the benzene rings provide additional stability of the crystal packing [centroid–centroid distance = 3.792 (2) Å].

Related literature

For general background to the applications and structures of metal coordination polymers, see: Rowsell & Yaghi (2005); Su *et al.* (2010); Wang *et al.* (2009); Zhang & Chen (2008). For a related structure, see: Cui & Zhao (2011).



Experimental

Crystal data

$[Ni(C_9H_6N_3O_2)_2(H_2O)_4]\cdot10H_2O$
M_r = 687.25
Monoclinic, $C2/c$
a = 25.840 (3) Å
b = 7.8664 (8) Å
c = 16.8013 (17) Å
β = 112.712 (1)°
V = 3150.3 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.70 mm^{-1}
T = 293 K
0.22 × 0.20 × 0.19 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.83, T_{max} = 0.90
8290 measured reflections
3079 independent reflections
2273 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.119
S = 1.04
3079 reflections
238 parameters
14 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O1^{i}	0.84 (2)	1.93 (2)	2.751 (3)	167 (4)
O4—H4A···O1^{ii}	0.84 (2)	1.86 (2)	2.692 (3)	172 (4)
O5—H5A···O8	0.82 (2)	1.94 (2)	2.752 (3)	169 (4)
O5—H5B···O7	0.83 (2)	1.84 (2)	2.670 (3)	171 (4)
O6—H6A···O7	0.82 (2)	1.95 (2)	2.773 (4)	178 (4)
O6—H6B···O10	0.84 (2)	1.91 (3)	2.747 (4)	177 (6)
O7—H7A···O2^{iii}	0.84 (2)	1.84 (2)	2.674 (3)	170 (4)
O7—H7B···O9^{iv}	0.84 (2)	1.88 (2)	2.715 (4)	171 (4)
O8—H8A···N3^{v}	0.82 (2)	2.16 (2)	2.943 (3)	160 (4)
O8—H8B···O2^{vi}	0.85 (2)	1.92 (2)	2.763 (3)	175 (4)
O9—H9A···O1^{ii}	0.84 (2)	1.93 (2)	2.751 (3)	169 (4)
O9—H9B···O8	0.85 (2)	1.93 (2)	2.757 (3)	164 (4)

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

Data collection: *APEX2* (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: HY2491).

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supplementary materials

Acta Cryst. (2012). E**68**, m10 [**doi:10.1107/S1600536811051063**]

Tetraaquabis[4-(4*H*-1,2,4-triazol-4-yl)benzoato-κN^1]nickel(II) decahydrate

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Comment

Recently, the chemists have devoted themselves to design and synthesize coordination polymers, not only due to their potential applications in the realm of gas adsorption and separation, catalysis, magnetism, luminescence, host–guest chemistry *etc*, but also for their aesthetic and often complicated architectures and topologies (Su *et al.*, 2010; Wang *et al.*, 2009). It is well known that carboxylic acids are excellent building blocks for the construction of coordination polymers because the carboxylate groups may induce core aggregation and link these discrete clusters into an extended framework by virtue of its bridging ability (Rowsell & Yaghi, 2005; Zhang & Chen, 2008). Taking these into account, we chose a carboxylate ligand, 4-(1,2,4-triazol-4-yl)benzoic acid, generating the title compound, which is reported here.

In the title compound, the Ni^{II} ion lies on a twofold rotation axis and displays a slightly distorted octahedral geometry defined by two N atoms from two 4-(1,2,4-triazol-4-yl)benzoate ligands and four water molecules, two of which lie on the twofold rotation axis (Fig. 1). The bond lengths and angles are in a normal range (Cui & Zhao, 2011). In the crystal, the complex molecules and uncoordinated water molecules are linked *via* intermolecular O—H···N and O—H···O hydrogen bonds, forming a three-dimensional supramolecular network (Fig. 2). π–π interactions between the benzene rings, with a centroid–centroid distance of 3.792 (2) Å, provide additional stability of the crystal packing.

Experimental

The synthesis was performed under hydrothermal conditions. A mixture of $Ni(CH_3COO)_2.4H_2O$ (0.2 mmol, 0.050 g), 4-(1,2,4-triazol-4-yl)benzoic acid (0.4 mmol, 0.075 g), NaOH (0.4 mmol, 0.016 g) and H_2O (15 ml) in a 25 ml stainless steel reactor with a Teflon liner was heated from 293 to 443 K in 2 h and a constant temperature was maintained at 443 K for 72 h. After the mixture was cooled to 298 K, pink crystals of the title compound were obtained from the reaction.

Refinement

H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms bonded to O atoms were located in a difference Fourier map and refined with O—H distance restraints of 0.85 (2) Å and with $U_{iso}(H) = 0.054$ Å^2.

Figures

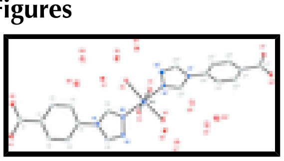

Fig. 1. The molecular structute of the title compound. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry code: (i) 1-*x*, *y*, 3/2-*z*.]

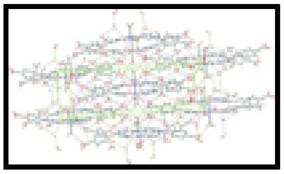

Fig. 2. View of the three-dimensional structure of the title compound built by hydrogen bonds (dashed lines).

Tetraaquabis[4-(4*H*-1,2,4-triazol-4-yl)benzoato-κN^1]nickel(II) decahydrate

Crystal data

$[Ni(C_9H_6N_3O_2)_2(H_2O)_4]\cdot 10H_2O$	$F(000) = 1448$
$M_r = 687.25$	$D_x = 1.449$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 3079 reflections
$a = 25.840$ (3) Å	$\theta = 1.0$–$25.9°$
$b = 7.8664$ (8) Å	$\mu = 0.70$ mm^{-1}
$c = 16.8013$ (17) Å	$T = 293$ K
$\beta = 112.712$ (1)°	Block, pink
$V = 3150.3$ (6) Å^3	$0.22 \times 0.20 \times 0.19$ mm
$Z = 4$	

Data collection

Bruker APEXII CCD diffractometer	3079 independent reflections
Radiation source: fine-focus sealed tube	2273 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.057$
φ and ω scans	$\theta_{max} = 25.9°$, $\theta_{min} = 2.5°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)	$h = -31 \rightarrow 31$
$T_{min} = 0.83$, $T_{max} = 0.90$	$k = -6 \rightarrow 9$
8290 measured reflections	$l = -20 \rightarrow 17$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.049$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.119$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.04$	$w = 1/[\sigma^2(F_o^2) + (0.0451P)^2 + 2.4003P]$ where $P = (F_o^2 + 2F_c^2)/3$
3079 reflections	$(\Delta/\sigma)_{max} < 0.001$
238 parameters	$\Delta\rho_{max} = 0.55$ e Å^{-3}
14 restraints	$\Delta\rho_{min} = -0.63$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.5000	0.59822 (8)	0.7500	0.01918 (19)
C1	0.83480 (12)	0.4306 (4)	1.04342 (19)	0.0186 (7)
C2	0.79863 (12)	0.3835 (4)	0.96082 (19)	0.0200 (7)
H2	0.8126	0.3236	0.9257	0.024*
C3	0.74225 (13)	0.4242 (4)	0.93015 (19)	0.0205 (7)
H3	0.7182	0.3890	0.8755	0.025*
C4	0.72201 (12)	0.5180 (4)	0.98169 (19)	0.0163 (7)
C5	0.75769 (13)	0.5702 (4)	1.0635 (2)	0.0209 (7)
H5	0.7441	0.6351	1.0975	0.025*
C6	0.81360 (12)	0.5246 (4)	1.0939 (2)	0.0194 (7)
H6	0.8374	0.5575	1.1491	0.023*
C7	0.89538 (13)	0.3748 (4)	1.0778 (2)	0.0196 (7)
C8	0.62534 (12)	0.5537 (4)	0.86818 (19)	0.0192 (7)
H8	0.6334	0.5222	0.8209	0.023*
C9	0.63313 (13)	0.6112 (4)	0.9971 (2)	0.0231 (7)
H9	0.6480	0.6275	1.0565	0.028*
N1	0.66358 (10)	0.5587 (3)	0.95053 (15)	0.0170 (6)
N2	0.57580 (10)	0.5986 (3)	0.86385 (15)	0.0193 (6)
N3	0.58082 (11)	0.6353 (4)	0.94733 (16)	0.0230 (7)
O1	0.92384 (9)	0.3974 (3)	1.15821 (13)	0.0218 (5)
O2	0.91424 (9)	0.3070 (3)	1.02773 (14)	0.0302 (6)
O3	0.5000	0.8594 (4)	0.7500	0.0294 (8)
O4	0.5000	0.3349 (4)	0.7500	0.0228 (7)
O5	0.54970 (9)	0.5800 (3)	0.67831 (14)	0.0211 (5)
O6	0.70477 (12)	0.6665 (4)	0.74921 (19)	0.0430 (7)
O7	0.60752 (10)	0.8271 (3)	0.64103 (15)	0.0280 (6)
O8	0.52147 (10)	0.3127 (3)	0.56372 (15)	0.0255 (6)
O9	0.60244 (10)	0.1461 (3)	0.69923 (16)	0.0315 (6)
O10	0.69525 (11)	0.3274 (4)	0.70686 (17)	0.0363 (7)
H3A	0.5254 (13)	0.921 (4)	0.784 (2)	0.054*
H4A	0.5231 (14)	0.265 (4)	0.783 (2)	0.054*
H5A	0.5411 (17)	0.510 (4)	0.639 (2)	0.054*
H5B	0.5653 (16)	0.656 (4)	0.661 (3)	0.054*
H6A	0.6758 (12)	0.715 (5)	0.718 (2)	0.054*
H6B	0.7026 (18)	0.562 (3)	0.738 (3)	0.054*
H7A	0.6022 (17)	0.833 (5)	0.5885 (14)	0.054*
H7B	0.6041 (18)	0.929 (3)	0.654 (3)	0.054*
H8A	0.5304 (17)	0.319 (6)	0.5218 (19)	0.054*
H8B	0.4879 (10)	0.279 (5)	0.550 (3)	0.054*
H9A	0.5962 (17)	0.146 (6)	0.7445 (18)	0.054*
H9B	0.5732 (12)	0.191 (5)	0.662 (2)	0.054*
H10A	0.7237 (12)	0.268 (5)	0.727 (2)	0.054*
H10B	0.6695 (14)	0.275 (5)	0.712 (3)	0.054*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0147 (3)	0.0216 (3)	0.0196 (3)	0.000	0.0049 (2)	0.000
C1	0.0117 (15)	0.0238 (18)	0.0189 (16)	0.0005 (13)	0.0044 (13)	0.0017 (14)
C2	0.0179 (17)	0.0281 (19)	0.0144 (16)	0.0013 (14)	0.0069 (13)	−0.0005 (14)
C3	0.0155 (16)	0.0305 (19)	0.0121 (15)	−0.0005 (14)	0.0014 (12)	0.0006 (14)
C4	0.0105 (15)	0.0197 (16)	0.0172 (16)	0.0021 (13)	0.0035 (13)	0.0023 (14)
C5	0.0188 (17)	0.0258 (19)	0.0174 (16)	0.0041 (14)	0.0062 (13)	−0.0042 (14)
C6	0.0153 (16)	0.0223 (17)	0.0170 (16)	−0.0007 (13)	0.0024 (13)	−0.0029 (14)
C7	0.0145 (16)	0.0217 (18)	0.0214 (17)	0.0004 (13)	0.0057 (14)	0.0031 (15)
C8	0.0144 (16)	0.0263 (18)	0.0148 (15)	0.0000 (13)	0.0034 (13)	−0.0012 (14)
C9	0.0170 (17)	0.037 (2)	0.0146 (16)	0.0034 (15)	0.0055 (13)	−0.0029 (15)
N1	0.0123 (13)	0.0229 (15)	0.0136 (13)	0.0014 (11)	0.0026 (10)	−0.0014 (11)
N2	0.0151 (13)	0.0272 (15)	0.0155 (13)	−0.0008 (12)	0.0058 (11)	−0.0021 (12)
N3	0.0144 (14)	0.0370 (17)	0.0149 (14)	0.0017 (12)	0.0026 (11)	−0.0043 (13)
O1	0.0167 (11)	0.0254 (12)	0.0180 (11)	0.0023 (10)	0.0010 (9)	0.0010 (10)
O2	0.0169 (13)	0.0498 (17)	0.0221 (13)	0.0123 (12)	0.0056 (10)	0.0020 (12)
O3	0.0210 (19)	0.0179 (18)	0.032 (2)	0.000	−0.0087 (15)	0.000
O4	0.0194 (18)	0.0150 (17)	0.0248 (19)	0.000	−0.0015 (14)	0.000
O5	0.0195 (12)	0.0248 (13)	0.0213 (12)	−0.0055 (10)	0.0106 (10)	−0.0034 (10)
O6	0.0341 (17)	0.0381 (17)	0.0489 (18)	0.0012 (14)	0.0073 (14)	0.0007 (15)
O7	0.0318 (14)	0.0289 (14)	0.0249 (13)	−0.0017 (12)	0.0126 (12)	0.0015 (12)
O8	0.0190 (13)	0.0378 (15)	0.0209 (12)	−0.0077 (11)	0.0090 (10)	−0.0023 (11)
O9	0.0255 (14)	0.0388 (15)	0.0315 (15)	0.0064 (12)	0.0123 (12)	0.0047 (13)
O10	0.0282 (16)	0.0390 (17)	0.0373 (16)	−0.0016 (12)	0.0080 (13)	0.0061 (13)

Geometric parameters (Å, °)

Ni1—O3	2.054 (3)	C8—H8	0.9300
Ni1—O4	2.071 (3)	C9—N3	1.300 (4)
Ni1—O5	2.077 (2)	C9—N1	1.370 (4)
Ni1—N2	2.145 (2)	C9—H9	0.9300
C1—C6	1.387 (4)	N2—N3	1.388 (3)
C1—C2	1.391 (4)	O3—H3A	0.836 (18)
C1—C7	1.510 (4)	O4—H4A	0.840 (18)
C2—C3	1.382 (4)	O5—H5A	0.822 (19)
C2—H2	0.9300	O5—H5B	0.835 (19)
C3—C4	1.385 (4)	O6—H6A	0.824 (19)
C3—H3	0.9300	O6—H6B	0.838 (19)
C4—C5	1.389 (4)	O7—H7A	0.840 (18)
C4—N1	1.430 (4)	O7—H7B	0.844 (19)
C5—C6	1.381 (4)	O8—H8A	0.823 (18)
C5—H5	0.9300	O8—H8B	0.848 (19)
C6—H6	0.9300	O9—H9A	0.836 (19)
C7—O2	1.243 (4)	O9—H9B	0.847 (19)
C7—O1	1.277 (4)	O10—H10A	0.824 (19)
C8—N2	1.303 (4)	O10—H10B	0.817 (19)

C8—N1	1.355 (4)		
O3—Ni1—O4	180.000 (2)	C5—C6—C1	121.1 (3)
O3—Ni1—O5^{i}	93.97 (6)	C5—C6—H6	119.5
O4—Ni1—O5^{i}	86.03 (7)	C1—C6—H6	119.5
O3—Ni1—O5	93.97 (7)	O2—C7—O1	124.0 (3)
O4—Ni1—O5	86.03 (7)	O2—C7—C1	119.0 (3)
O5^{i}—Ni1—O5	172.07 (13)	O1—C7—C1	116.9 (3)
O3—Ni1—N2	89.93 (7)	N2—C8—N1	111.3 (3)
O4—Ni1—N2	90.07 (7)	N2—C8—H8	124.4
O5^{i}—Ni1—N2	92.24 (9)	N1—C8—H8	124.4
O5—Ni1—N2	87.77 (9)	N3—C9—N1	111.2 (3)
O3—Ni1—N2^{i}	89.93 (7)	N3—C9—H9	124.4
O4—Ni1—N2^{i}	90.07 (7)	N1—C9—H9	124.4
O5^{i}—Ni1—N2^{i}	87.77 (9)	C8—N1—C9	103.8 (3)
O5—Ni1—N2^{i}	92.24 (9)	C8—N1—C4	128.2 (3)
N2—Ni1—N2^{i}	179.85 (16)	C9—N1—C4	128.1 (2)
C6—C1—C2	118.7 (3)	C8—N2—N3	107.1 (2)
C6—C1—C7	121.1 (3)	C8—N2—Ni1	126.1 (2)
C2—C1—C7	120.1 (3)	N3—N2—Ni1	126.73 (18)
C3—C2—C1	121.0 (3)	C9—N3—N2	106.7 (2)
C3—C2—H2	119.5	Ni1—O3—H3A	125 (3)
C1—C2—H2	119.5	Ni1—O4—H4A	131 (3)
C2—C3—C4	119.3 (3)	Ni1—O5—H5A	118 (3)
C2—C3—H3	120.4	Ni1—O5—H5B	130 (3)
C4—C3—H3	120.4	H5A—O5—H5B	103 (4)
C3—C4—C5	120.6 (3)	H6A—O6—H6B	110 (4)
C3—C4—N1	119.4 (3)	H7A—O7—H7B	103 (4)
C5—C4—N1	120.0 (3)	H8A—O8—H8B	112 (4)
C6—C5—C4	119.3 (3)	H9A—O9—H9B	103 (4)
C6—C5—H5	120.4	H10A—O10—H10B	108 (4)
C4—C5—H5	120.4		
C6—C1—C2—C3	−2.1 (5)	C3—C4—N1—C8	−17.2 (5)
C7—C1—C2—C3	175.9 (3)	C5—C4—N1—C8	163.8 (3)
C1—C2—C3—C4	2.0 (5)	C3—C4—N1—C9	162.5 (3)
C2—C3—C4—C5	−0.3 (5)	C5—C4—N1—C9	−16.5 (5)
C2—C3—C4—N1	−179.3 (3)	N1—C8—N2—N3	−0.1 (4)
C3—C4—C5—C6	−1.3 (5)	N1—C8—N2—Ni1	−176.2 (2)
N1—C4—C5—C6	177.7 (3)	O3—Ni1—N2—C8	−109.7 (3)
C4—C5—C6—C1	1.2 (5)	O4—Ni1—N2—C8	70.3 (3)
C2—C1—C6—C5	0.4 (5)	O5^{i}—Ni1—N2—C8	156.4 (3)
C7—C1—C6—C5	−177.5 (3)	O5—Ni1—N2—C8	−15.7 (3)
C6—C1—C7—O2	−172.3 (3)	O3—Ni1—N2—N3	75.0 (2)
C2—C1—C7—O2	9.8 (5)	O4—Ni1—N2—N3	−105.0 (2)
C6—C1—C7—O1	9.3 (5)	O5^{i}—Ni1—N2—N3	−19.0 (3)
C2—C1—C7—O1	−168.6 (3)	O5—Ni1—N2—N3	169.0 (3)
N2—C8—N1—C9	−0.1 (4)	N1—C9—N3—N2	−0.4 (4)

N2—C8—N1—C4	179.7 (3)	C8—N2—N3—C9	0.3 (4)
N3—C9—N1—C8	0.3 (4)	Ni1—N2—N3—C9	176.4 (2)
N3—C9—N1—C4	−179.5 (3)		

Symmetry codes: (i) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3A···O1^{ii}	0.84 (2)	1.93 (2)	2.751 (3)	167 (4)
O4—H4A···O1^{iii}	0.84 (2)	1.86 (2)	2.692 (3)	172 (4)
O5—H5A···O8	0.82 (2)	1.94 (2)	2.752 (3)	169 (4)
O5—H5B···O7	0.83 (2)	1.84 (2)	2.670 (3)	171 (4)
O6—H6A···O7	0.82 (2)	1.95 (2)	2.773 (4)	178 (4)
O6—H6B···O10	0.84 (2)	1.91 (3)	2.747 (4)	177 (6)
O7—H7A···O2^{iv}	0.84 (2)	1.84 (2)	2.674 (3)	170 (4)
O7—H7B···O9^{v}	0.84 (2)	1.88 (2)	2.715 (4)	171 (4)
O8—H8A···N3^{vi}	0.82 (2)	2.16 (2)	2.943 (3)	160 (4)
O8—H8B···O2^{vii}	0.85 (2)	1.92 (2)	2.763 (3)	175 (4)
O9—H9A···O1^{iii}	0.84 (2)	1.93 (2)	2.751 (3)	169 (4)
O9—H9B···O8	0.85 (2)	1.93 (2)	2.757 (3)	164 (4)

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

Fig. 1

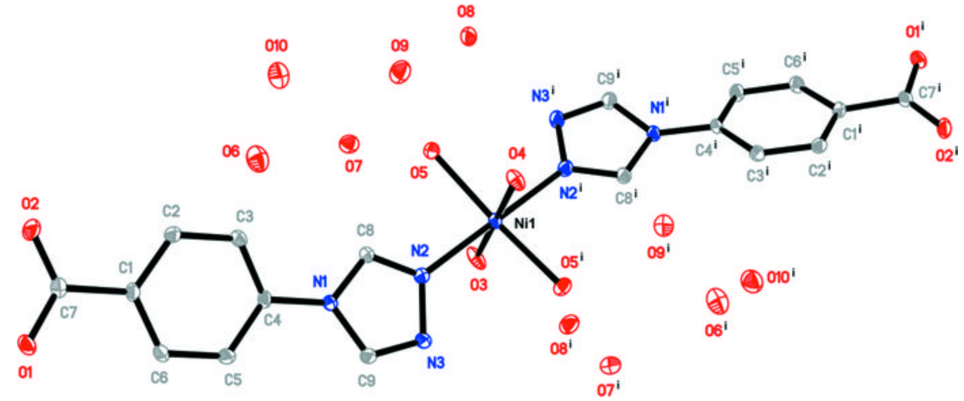
O8
O10
O9
O1i
O6
O7
O5
O4
N3i
C9i
N1i
C5i
C6i
C7i
C1i
C4i
C3i
C2i
O2i
N2i
C8i
O2
C2
C3
C8
N2
Ni1
O9i
C1
N1
O3
O5i
O10i
C7
C4
O6i
O1
C6
C5
C9
N3
O8i
O7i

Fig. 2