Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetraaquabis[4-(tetrazol-1-yl)benzoato-κN^4]nickel(II) dihydrate

Shu-Ming Zhang[a]* and Jian-Long Du[b]

[a]School of Chemical Engineering and Technology, Hebei University of Technology, Tianjin 300130, People's Republic of China, and [b]College of Chemistry & Environmental Science, Hebei University, Baoding 071002, People's Republic of China
Correspondence e-mail: zsmchange@sina.com

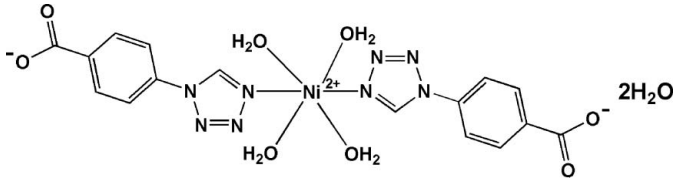
Received 14 November 2007; accepted 17 November 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.068; data-to-parameter ratio = 13.1.

In the title compound, $[Ni(C_8H_5N_4O_2)_2(H_2O)_4]\cdot 2H_2O$, the Ni^{II} ion lies on an inversion centre and is coordinated by two N atoms from two 4-(tetrazol-1-yl)benzoate ligands and four O atoms from four water molecules in a slightly distorted octahedral geometry. In addition, there are two uncoordinated water molecules in the structure. The crystal structure is stabilized by intermolecular O—H···O hydrogen bonds.

Related literature

For related literature, see: Zhang *et al.* (2007); Zou *et al.* (2005); Bronisz (2007); Dinca *et al.* (2006); Li *et al.* (2006, 2007).



Experimental

Crystal data

$[Ni(C_8H_5N_4O_2)_2(H_2O)_4]\cdot 2H_2O$
M_r = 545.13
Triclinic, $P\overline{1}$
a = 7.3830 (15) Å
b = 7.5819 (15) Å
c = 10.712 (2) Å
α = 96.90 (3)°
β = 94.62 (3)°
γ = 116.00 (3)°
V = 529.0 (2) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.99 mm^{-1}
T = 293 (2) K
0.3 × 0.3 × 0.3 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.758, T_{max} = 0.766
5651 measured reflections
2419 independent reflections
2221 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.068
S = 1.14
2419 reflections
184 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O2W	2.0252 (15)	Ni1—N1	2.0927 (15)
Ni1—O1W	2.0315 (16)		
O2W—Ni1—O1W	89.19 (7)	O1W—Ni1—N1	91.93 (7)
O2W—Ni1—N1	92.56 (7)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O1^{i}	0.79 (3)	1.92 (3)	2.704 (2)	171 (3)
O1W—H1WB···O2^{ii}	0.80 (3)	1.93 (3)	2.724 (2)	172 (3)
O2W—H2WB···O2^{iii}	0.77 (3)	2.04 (3)	2.771 (2)	160 (3)
O2W—H2WA···O3W^{iv}	0.80 (3)	1.91 (3)	2.697 (3)	168 (3)
O3W—H3WB···O1^{v}	0.74 (3)	2.21 (3)	2.917 (2)	162 (3)
O3W—H3WA···O2^{vi}	0.84 (3)	1.96 (3)	2.793 (2)	173 (3)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

The authors thank the Natural Science Foundation of Hebei Province of China (No. B2005000007) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2494).

References

Bronisz, R. (2007). *Inorg. Chem.* **46**, 6733–6739.
Bruker (1998). *SMART* (Version 5.051), *SAINT* (Version 5.01), *SADABS* (Version 2.03) and *SHELXTL* (Version 6.1). Bruker AXS Inc., Madison, Wisconsin, USA.
Dinca, M., Dailly, A., Liu, Y., Brown, C. M., Neumann, D. A. & Long, J. R. (2006). *J. Am. Chem. Soc.* **128**, 16876–16883.
Li, J.-R., Tao, Y., Yu, Q. & Bu, X.-H. (2006). *Cryst. Growth Des.* **6**, 2493–2500.
Li, J. R., Tao, Y., Yu, Q. & Bu, X. H. (2007). *Chem. Commun.* pp. 1527–1529.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Zhang, J.-Z., Pan, J.-X., Cao, W.-R. & Chen, Q.-W. (2007). *Acta Cryst.* E**63**, m1042–m1043.
Zou, R.-Q., Cai, L.-Z. & Guo, G.-C. (2005). *J. Mol. Struct.* **737**, 125–129.

supplementary materials

Acta Cryst. (2007). E**63**, m3139 [**doi:10.1107/S1600536807060138**]

Tetraaquabis[4-(tetrazol-1-yl)benzoato-κN^4]nickel(II) dihydrate

S.-M. Zhang and J.-L. Du

Comment

Metal-organic frameworks (MOFs) containing 1*H*-tetrazol and its derivatives have attracted great attentions of many research groups due to their intriguing structural diversity and potential applications in luminescence, magnetism and gas storage (Dinca, *et al.*, 2006; Li, *et al.*, 2007; Bronisz, 2007). However, there are rare reports of ligands based on tetrazol and carboxylate groups as building blocks for the construction of MOFs. So we synthesized several coordination compounds by such ligands. And here we report the structure of title compound (I).

The structure of (I) consists of discrete neutral unit $[Ni(C_8H_5N_4O_2)_2(H_2O)_2]$ and two lattice water molecules (Fig. 1), atom Ni1 occupies an inversion centre and is coordinated by two N atoms from two 4-(tetrazol-1- yl)benzoate ligands and four O atoms from four water molecules in a distorted octahedral geometry. The Ni1—N1 distance of 2.0927 (15)Å is slightly lengthened, while the distances of Ni1—O1W and Ni1—O2W bonds (Table 1) is slightly shorten compared with the values observed in related complex (Zhang *et al.*, 2007). The crystal stacking of (I) (Fig. 2) is stabilized by intermolecular O—H···O hydrogen bonds (Table 2) (Li, *et al.*, 2006), which is similar to that in related reports (Zou, *et al.*, 2005; Zhang, *et al.*, 2007).

Experimental

A solution of $NiCl_2·6H_2O$ (24 mg, 0.1 mmol) in water (5 ml) was added to a solution of 4-(tetrazol-1-yl) benzoic acid (38 mg, 0.2 mmol) and sodium hydroxide (8 mg, 0.2 mmol) in methanol (5 ml). The reaction mixture was stirred for 30 min and then filtered. Green crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation after two weeks [yield: 40%].

Refinement

H atoms bounded to C atoms were included in calculated positions and treated in the subsequent refinement as riding atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The H atoms of water was located in Fourier difference map and refined freely.

Figures

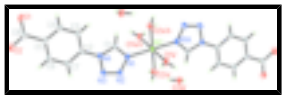


Fig. 1. The molecular structure of (I), with 40% probability displacement ellipsoids. [Symmetry code: (A) $-x + 1, -y, -z + 1$.]

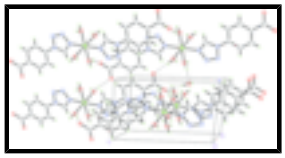


Fig. 2. A portion of the crystal stacking structure, showing the intermolecular O—H···O hydrogen bonds (dashed lines).

Tetraaquabis[4-(tetrazol-1-yl)benzoato-κN^4]nickel(II) dihydrate

Crystal data

$[Ni(C_8H_5N_4O_2)_2(H_2O)_4]\cdot 2H_2O$	$Z = 1$
$M_r = 545.13$	$F_{000} = 282$
Triclinic, $P\overline{1}$	$D_x = 1.711$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.3830$ (15) Å	Cell parameters from 5360 reflections
$b = 7.5819$ (15) Å	$\theta = 3.0$–27.8º
$c = 10.712$ (2) Å	$\mu = 0.99$ mm^{-1}
$\alpha = 96.90$ (3)º	$T = 293$ (2) K
$\beta = 94.62$ (3)º	Block, green
$\gamma = 116.00$ (3)º	0.3 × 0.3 × 0.3 mm
$V = 529.0$ (2) Å^3	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	2419 independent reflections
Radiation source: fine-focus sealed tube	2221 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.022$
$T = 293(2)$ K	$\theta_{max} = 27.5$º
φ and ω scan	$\theta_{min} = 3.0$º
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$h = -9\rightarrow 9$
$T_{min} = 0.758$, $T_{max} = 0.766$	$k = -9\rightarrow 9$
5651 measured reflections	$l = -13\rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.031$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.068$	$w = 1/[\sigma^2(F_o^2) + (0.0235P)^2 + 0.250P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.14$	$(\Delta/\sigma)_{max} < 0.001$
2419 reflections	$\Delta\rho_{max} = 0.25$ e Å^{-3}
184 parameters	$\Delta\rho_{min} = -0.27$ e Å^{-3}
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 $F^2 > \sigma(F^2)$ 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	0.5000	0.0000	0.5000	0.01921 (10)
O2W	0.7492 (2)	−0.0451 (3)	0.53264 (13)	0.0276 (3)
O3W	0.0848 (2)	0.2902 (2)	0.64256 (16)	0.0335 (3)
N1	0.5324 (2)	0.1275 (2)	0.68998 (14)	0.0241 (3)
O1W	0.6797 (2)	0.2685 (2)	0.45392 (14)	0.0298 (3)
O2	0.1970 (2)	0.3646 (2)	1.40415 (12)	0.0319 (3)
N4	0.4656 (2)	0.2020 (2)	0.87325 (13)	0.0222 (3)
O1	−0.0689 (2)	0.3363 (2)	1.27599 (13)	0.0389 (4)
N2	0.6909 (3)	0.1679 (3)	0.77918 (15)	0.0364 (4)
C1	0.3960 (3)	0.1505 (3)	0.75005 (16)	0.0270 (4)
H1A	0.2701	0.1334	0.7125	0.032*
N3	0.6530 (3)	0.2133 (3)	0.88977 (16)	0.0381 (4)
C8	0.1002 (3)	0.3386 (3)	1.29574 (17)	0.0259 (4)
C6	0.3882 (3)	0.3152 (3)	1.20129 (17)	0.0289 (4)
H6A	0.4567	0.3434	1.2835	0.035*
C4	0.1001 (3)	0.2715 (3)	1.06100 (18)	0.0287 (4)
H4A	−0.0268	0.2696	1.0481	0.034*
C2	0.3748 (3)	0.2411 (3)	0.97907 (16)	0.0222 (4)
C5	0.1985 (3)	0.3081 (3)	1.18314 (16)	0.0232 (4)
C7	0.4783 (3)	0.2814 (3)	1.09967 (17)	0.0284 (4)
H7A	0.6064	0.2857	1.1123	0.034*
C3	0.1874 (3)	0.2377 (3)	0.95800 (17)	0.0294 (4)
H3A	0.1208	0.2129	0.8757	0.035*
H1WB	0.716 (4)	0.371 (4)	0.502 (3)	0.043 (7)*
H2WB	0.741 (4)	−0.138 (4)	0.559 (3)	0.056 (9)*
H1WA	0.762 (4)	0.288 (4)	0.408 (3)	0.059 (9)*
H3WB	0.069 (4)	0.372 (4)	0.675 (3)	0.044 (8)*
H2WA	0.847 (5)	0.048 (5)	0.574 (3)	0.059 (9)*
H3WA	0.118 (5)	0.321 (5)	0.572 (3)	0.074 (10)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.02186 (18)	0.02399 (18)	0.01459 (16)	0.01276 (14)	0.00607 (12)	0.00174 (12)
O2W	0.0278 (8)	0.0313 (8)	0.0277 (7)	0.0172 (7)	0.0047 (6)	0.0034 (7)
O3W	0.0370 (8)	0.0400 (9)	0.0309 (8)	0.0228 (7)	0.0111 (7)	0.0070 (7)
N1	0.0278 (8)	0.0300 (8)	0.0179 (7)	0.0161 (7)	0.0066 (6)	0.0026 (6)
O1W	0.0365 (8)	0.0268 (8)	0.0257 (7)	0.0123 (7)	0.0152 (7)	0.0035 (6)
O2	0.0464 (9)	0.0384 (8)	0.0177 (7)	0.0247 (7)	0.0101 (6)	0.0039 (6)
N4	0.0230 (8)	0.0309 (8)	0.0158 (7)	0.0149 (7)	0.0065 (6)	0.0016 (6)
O1	0.0377 (8)	0.0605 (10)	0.0299 (8)	0.0311 (8)	0.0159 (6)	0.0067 (7)
N2	0.0298 (9)	0.0620 (12)	0.0201 (8)	0.0258 (9)	0.0048 (7)	−0.0031 (8)
C1	0.0283 (10)	0.0403 (11)	0.0168 (9)	0.0200 (9)	0.0050 (7)	0.0016 (8)
N3	0.0298 (9)	0.0673 (13)	0.0222 (8)	0.0288 (9)	0.0043 (7)	−0.0023 (8)
C8	0.0350 (11)	0.0245 (9)	0.0214 (9)	0.0151 (8)	0.0118 (8)	0.0036 (7)
C6	0.0326 (11)	0.0414 (11)	0.0163 (9)	0.0202 (9)	0.0055 (8)	0.0031 (8)
C4	0.0253 (10)	0.0427 (12)	0.0226 (9)	0.0197 (9)	0.0060 (8)	0.0029 (8)
C2	0.0272 (9)	0.0261 (9)	0.0158 (8)	0.0136 (8)	0.0086 (7)	0.0028 (7)
C5	0.0282 (10)	0.0258 (9)	0.0177 (8)	0.0135 (8)	0.0087 (7)	0.0031 (7)
C7	0.0265 (10)	0.0445 (12)	0.0198 (9)	0.0212 (9)	0.0054 (8)	0.0042 (8)
C3	0.0297 (10)	0.0463 (12)	0.0160 (9)	0.0213 (10)	0.0040 (7)	0.0025 (8)

Geometric parameters (Å, °)

Ni1—O2W^{i}	2.0252 (15)	N4—N3	1.344 (2)
Ni1—O2W	2.0252 (15)	N4—C2	1.428 (2)
Ni1—O1W	2.0315 (16)	O1—C8	1.241 (2)
Ni1—O1W^{i}	2.0315 (16)	N2—N3	1.281 (2)
Ni1—N1^{i}	2.0927 (15)	C1—H1A	0.9300
Ni1—N1	2.0927 (15)	C8—C5	1.502 (2)
O2W—H2WB	0.77 (3)	C6—C5	1.375 (3)
O2W—H2WA	0.80 (3)	C6—C7	1.376 (3)
O3W—H3WB	0.74 (3)	C6—H6A	0.9300
O3W—H3WA	0.84 (3)	C4—C3	1.375 (3)
N1—C1	1.299 (2)	C4—C5	1.378 (3)
N1—N2	1.346 (2)	C4—H4A	0.9300
O1W—H1WB	0.80 (3)	C2—C3	1.371 (3)
O1W—H1WA	0.79 (3)	C2—C7	1.374 (3)
O2—C8	1.259 (2)	C7—H7A	0.9300
N4—C1	1.323 (2)	C3—H3A	0.9300
O2W^{i}—Ni1—O2W	180.00 (8)	N3—N4—C2	121.12 (15)
O2W^{i}—Ni1—O1W	90.81 (7)	N3—N2—N1	110.27 (15)
O2W—Ni1—O1W	89.19 (7)	N1—C1—N4	108.89 (17)
O2W^{i}—Ni1—O1W^{i}	89.19 (7)	N1—C1—H1A	125.6
O2W—Ni1—O1W^{i}	90.81 (7)	N4—C1—H1A	125.6
O1W—Ni1—O1W^{i}	180.0	N2—N3—N4	106.69 (16)

O2W^{i}—Ni1—N1^{i}	92.56 (7)	O1—C8—O2	124.76 (17)
O2W—Ni1—N1^{i}	87.44 (7)	O1—C8—C5	118.33 (17)
O1W—Ni1—N1^{i}	88.07 (7)	O2—C8—C5	116.91 (17)
O1W^{i}—Ni1—N1^{i}	91.93 (7)	C5—C6—C7	120.97 (18)
O2W^{i}—Ni1—N1	87.44 (7)	C5—C6—H6A	119.5
O2W—Ni1—N1	92.56 (7)	C7—C6—H6A	119.5
O1W—Ni1—N1	91.93 (7)	C3—C4—C5	120.80 (18)
O1W^{i}—Ni1—N1	88.07 (7)	C3—C4—H4A	119.6
N1^{i}—Ni1—N1	180.0	C5—C4—H4A	119.6
Ni1—O2W—H2WB	120 (2)	C3—C2—C7	121.79 (17)
Ni1—O2W—H2WA	115 (2)	C3—C2—N4	119.42 (16)
H2WB—O2W—H2WA	106 (3)	C7—C2—N4	118.79 (16)
H3WB—O3W—H3WA	106 (3)	C6—C5—C4	119.21 (17)
C1—N1—N2	106.30 (15)	C6—C5—C8	119.98 (17)
C1—N1—Ni1	128.19 (13)	C4—C5—C8	120.81 (17)
N2—N1—Ni1	124.50 (12)	C2—C7—C6	118.51 (18)
Ni1—O1W—H1WB	122.5 (18)	C2—C7—H7A	120.7
Ni1—O1W—H1WA	125 (2)	C6—C7—H7A	120.7
H1WB—O1W—H1WA	106 (3)	C2—C3—C4	118.70 (17)
C1—N4—N3	107.85 (15)	C2—C3—H3A	120.6
C1—N4—C2	131.03 (16)	C4—C3—H3A	120.6
O2W^{i}—Ni1—N1—C1	19.06 (17)	C1—N4—C2—C3	−3.8 (3)
O2W—Ni1—N1—C1	−160.94 (17)	N3—N4—C2—C3	176.84 (18)
O1W—Ni1—N1—C1	109.78 (17)	C1—N4—C2—C7	176.2 (2)
O1W^{i}—Ni1—N1—C1	−70.22 (17)	N3—N4—C2—C7	−3.1 (3)
N1^{i}—Ni1—N1—C1	−106 (100)	C7—C6—C5—C4	−1.7 (3)
O2W^{i}—Ni1—N1—N2	−174.01 (16)	C7—C6—C5—C8	177.90 (18)
O2W—Ni1—N1—N2	5.99 (16)	C3—C4—C5—C6	1.5 (3)
O1W—Ni1—N1—N2	−83.29 (16)	C3—C4—C5—C8	−178.04 (18)
O1W^{i}—Ni1—N1—N2	96.71 (16)	O1—C8—C5—C6	178.18 (18)
N1^{i}—Ni1—N1—N2	61 (100)	O2—C8—C5—C6	−1.9 (3)
C1—N1—N2—N3	0.2 (2)	O1—C8—C5—C4	−2.3 (3)
Ni1—N1—N2—N3	−169.14 (14)	O2—C8—C5—C4	177.66 (18)
N2—N1—C1—N4	−0.5 (2)	C3—C2—C7—C6	1.2 (3)
Ni1—N1—C1—N4	168.30 (12)	N4—C2—C7—C6	−178.79 (17)
N3—N4—C1—N1	0.6 (2)	C5—C6—C7—C2	0.3 (3)
C2—N4—C1—N1	−178.81 (17)	C7—C2—C3—C4	−1.4 (3)
N1—N2—N3—N4	0.2 (2)	N4—C2—C3—C4	178.65 (18)
C1—N4—N3—N2	−0.5 (2)	C5—C4—C3—C2	0.0 (3)
C2—N4—N3—N2	179.00 (17)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WA···O1^{ii}	0.79 (3)	1.92 (3)	2.704 (2)	171 (3)

O1W—H1WB···O2^{iii}	0.80 (3)	1.93 (3)	2.724 (2)	172 (3)
O2W—H2WB···O2^{iv}	0.77 (3)	2.04 (3)	2.771 (2)	160 (3)
O2W—H2WA···O3W^{v}	0.80 (3)	1.91 (3)	2.697 (3)	168 (3)
O3W—H3WB···O1^{vi}	0.74 (3)	2.21 (3)	2.917 (2)	162 (3)
O3W—H3WA···O2^{vii}	0.84 (3)	1.96 (3)	2.793 (2)	173 (3)

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

Fig. 1

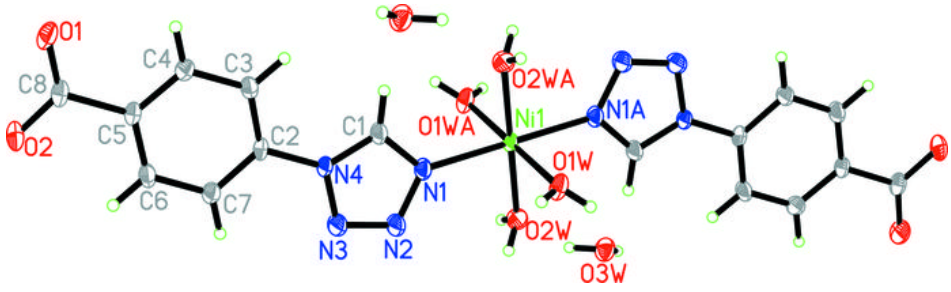

O1
C8
O2
C4
C3
C5
C2
C6
C7
C1
N4
N3
N2
N1
O1WA
O2WA
Ni1
N1A
O1W
O2W
O3W

Fig. 2