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[Bis(triazol-1-yl)acetato]nickel(II) monohydrate

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Key indicators

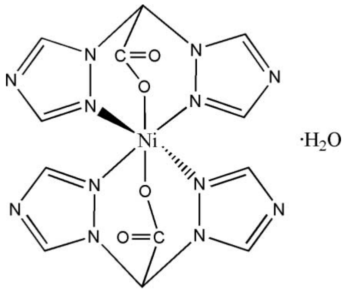
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
H-atom completeness 84%
Disorder in solvent or counterion
R factor = 0.050
wR factor = 0.160
Data-to-parameter ratio = 13.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

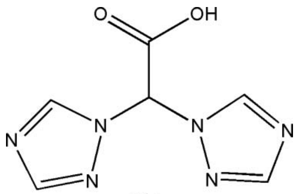
The title complex, $[\mathrm{Ni(C_6H_3N_6O_2)_2}]\cdot\mathrm{H_2O}$, contains an $\mathrm{Ni^{II}}$ ion on a twofold axis bound to two tridentate chelating bis(triazol-1-yl)acetate anions and one uncoordinated water molecule. In the complex, weak intermolecular C—H···O hydrogen bonds interconnect units to form a three-dimensional net with one-dimensional channels along the *c*-axis direction occupied by disordered water molecules.

Comment

Since Trofimenko (1967) first modified poly(pyrazol-1-yl)borate ligands using 1,2,4-triazole to form poly(triazol-1-yl)borate ligands which combine the coordination properties of both pyrazoles and imidazoles, considerable attention has been paid to their applications in coordination polymers (Lobbia *et al.*, 1991; Janiak, 1994; Shiu *et al.*, 1994; Macleod *et al.*, 1996). Compared with poly(triazolyl)borate ligands, similar substitutions of bis(1,2,4-triazol-1-yl)methanes (BTM) have been explored in coordination and metal–organic chemistry (Tang *et al.*, 2000; Tang *et al.*, 2002; Effendy *et al.*, 2003; Effendy *et al.*, 2004), acting as chelating ligands with endodentate N atoms (Tang *et al.*, 2002), as bridging ligands with exodentate N atoms (Tang *et al.*, 2000; Effendy *et al.*, 2004), or coordinated to the metal center in both coordination modes (Effendy *et al.*, 2003). A mononuclear nickel(II) complex (I) was synthesized with a new bis(1,2,4-triazol-1-yl)acetic acid (Hbta) ligand and its structure determined by single-crystal X-ray diffraction.



(I)



Hbta

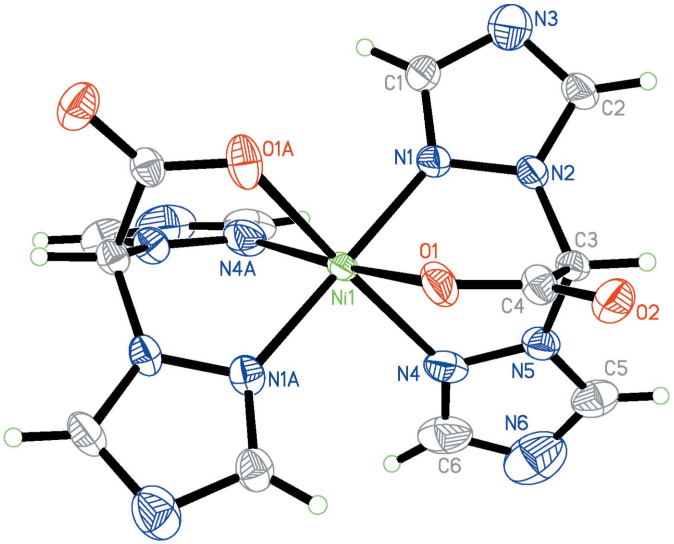


Figure 1
The molecular structure of the title complex, with displacement ellipsoids drawn at the 30% probability level. [Symmetry code: (A) $x - y$, $-y$, $-z + \frac{1}{3}$.]

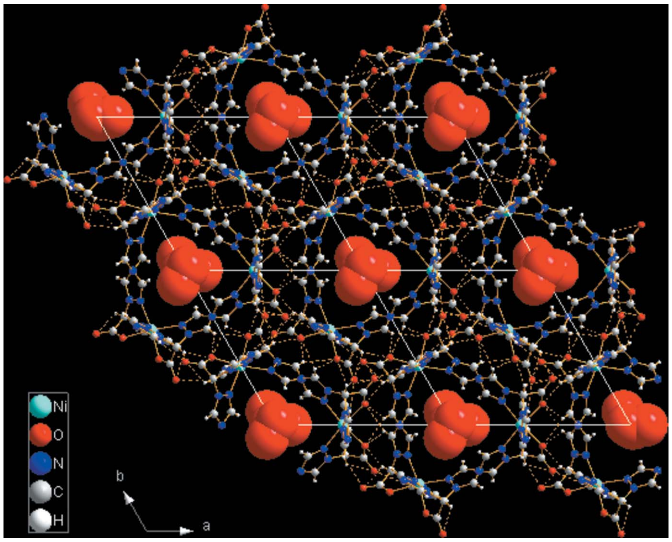


Figure 2
The title complex, viewed along the *c* axis, illustrating the one-dimensional channels occupied by disordered water molecules.

In the title complex, the Ni^{II} ion, situated on a twofold axis, has slightly distorted octahedral geometry (Table 1 and Fig. 1), in which the equatorial plane contains two endodentate triazole N atoms [N4 and N4^{i}, symmetry code: (i) $x - y$, $-y$, $-z + \frac{1}{3}$] and two carboxylate O atoms (O1 and O1^{i}) with the largest deviation of 0.0047 Å, at O1. The axial positions are occupied by the other endodentate N atoms of the bta ligand (N1 and N1^{i}). In this complex, the ligand bis(1,2,4-triazol-1-yl)acetic acid (Hbta) is tridentate and chelates to the Ni^{II} ion with two endodentate N atoms from the triazoles [Ni1—N1 = 1.993 (4) Å and Ni1—N4 = 2.185 (6) Å] and one carboxylate O atom [Ni1—O1 = 2.142 (5) Å], generating three six-membered metal-organic rings (Ni1—N1—N2—C3—N5—N4, Ni1—O1—C4—C3—N5—N4, Ni1—N1—N2—C3—C4—O1) which exist in half-chair conformations. The plane of the carboxylate group is almost perpendicular to the six-membered Ni1—N1—N2—C3—N5—N4 metal-organic ring [dihedral angle of 89.7 (3)°]. The two triazole rings in one bta ligand form a dihedral angle of 55.3 (4)°, larger than that of 45.4° found in [Ag_3(BTM)$_4$](CF_3SO_3)$_3$] (Effendy *et al.*, 2003).

In the crystal structure, C—H···O hydrogen bonds (Table 2) interconnect the mononuclear Ni^{II} units, generating one-dimensional channels, occupied by disordered water molecules, along the *c*-axis direction (Fig. 2). These interactions help to stabilize the packing arrangement in the crystal structure.

Experimental

Nickel(II) perchlorate hexahydrate (0.5 mmol, 183.3 mg) was dissolved in distilled water (5 ml), and added to a solution of bis(triazol-1-yl)acetic acid (0.5 mmol, 96.5 mg) in ethanol (5 ml). Sodium hydroxide (1 mol l^{-1}) was added to give pH = 7.0, and the mixture was then refluxed for 2 h. It was slowly cooled to room temperature, filtered, and the filtrate was slowly evaporated at room temperature. Dark-green single crystals of the title complex suitable for X-ray diffraction were obtained after about four weeks (yield: 17%). CHN analysis found: C 31.12, H 2.31, N 36.39%; calculated for $C_{12}H_{12}N_{12}NiO_5$: C 31.17, H 2.38, N 36.36%.

Crystal data

[Ni($C_6H_3N_6O_2$)$_2$]·H_2O
M_r = 463.05
Trigonal, $P3_221$
a = 12.406 (3) Å
c = 12.211 (7) Å
V = 1627.5 (11) Å^3
Z = 3
D_x = 1.417 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.94 mm^{-1}
T = 293 (2) K
Block, green
0.20 × 0.14 × 0.12 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.860, T_{max} = 1.000 (expected range = 0.768–0.893)
8800 measured reflections
1928 independent reflections
1792 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.160
S = 1.12
1928 reflections
147 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1281P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.05 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}
Absolute structure: Flack (1983), 821 Friedel pairs
Flack parameter: 0.01 (3)

Table 1
Selected geometric parameters (Å, °).

Ni1—N1	1.993 (4)	Ni1—N4	2.185 (6)
Ni1—O1	2.142 (5)		
N1—Ni1—N1^{i}	178.9 (3)	N1^{i}—Ni1—N4^{i}	86.90 (18)
N1—Ni1—O1	86.31 (15)	O1—Ni1—N4^{i}	172.44 (18)
N1^{i}—Ni1—O1	92.89 (15)	O1—Ni1—N4	82.90 (17)
O1—Ni1—O1^{i}	89.5 (2)	N4^{i}—Ni1—N4	104.7 (3)
N1—Ni1—N4^{i}	93.79 (18)		

Symmetry code: (i) $x - y$, $-y$, $-z + \frac{1}{3}$.

m194 Ling *et al.* • [Ni($C_6H_3N_6O_2$)$_2$]·H_2O *Acta Cryst.* (2007). E**63**, m193–m195

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

$D-\mathrm{H}\cdots A$	$D-\mathrm{H}$	$\mathrm{H}\cdots A$	$D\cdots A$	$D-\mathrm{H}\cdots A$
$C1-H1\cdots O2^{ii}$	0.93	2.53	3.29	139
$C2-H2\cdots O2^{iii}$	0.93	2.41	3.23	148
$C3-H3\cdots O1^{iii}$	0.98	2.43	3.35	157
$C5-H5\cdots O1^{iii}$	0.93	2.55	3.31	139
$C5-H5\cdots O1^{iv}$	0.93	2.65	3.48	148

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

H atoms were placed in calculated positions (C—H = 0.93–0.98Å) and refined using a riding model, with $U_{\mathrm{iso}}(\mathrm{H}) = 1.2\ U_{\mathrm{eq}}(\mathrm{C})$. The uncoordinated water molecule is disordered and their H atoms were not located. The water molecule was located in two positions with occupancies of 0.5.

Data collection: *SMART* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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, 2005); software used to prepare material for publication: *SHELXTL*.

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Acta Cryst. (2007). E**63**, m193–m195 Ling *et al.* • $[Ni(C_6H_3N_6O_2)_2]\cdot H_2O$ **m195**