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Key indicators

Single-crystal X-ray study
T = 293 K
Mean $\sigma(C-C)$ = 0.006 Å
R factor = 0.054
wR factor = 0.121
Data-to-parameter ratio = 15.3

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

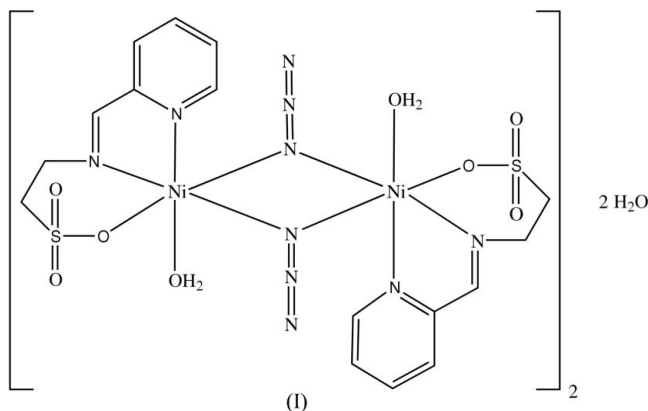
Di- μ -azido- $\kappa^4N:N$ -bis{aqua[2-(2-pyridylmethylidene-amino)ethanesulfonato- κ^3N,N',O]nickel(II)} dihydrate

The title complex, $[Ni_2(C_8H_9N_2O_3S)_2(N_3)_2(H_2O)_2] \cdot 2H_2O$, was synthesized in a methanol–water solution. The asymmetric unit consists of two half-molecules of the complex and two water molecules. Four N and two O atoms form the coordination environment of each Ni atom, resulting in a distorted octahedral configuration. The two halves of each independent dimer are related by a crystallographic inversion centre, which lies at the centre of the ring formed by the two Ni atoms and the coordinating atoms of the two azide anions. The molecules are linked by O–H...O hydrogen bonds, generating an interesting double zigzag infinite chain structure in the *ac* plane.

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Comment

The investigation of Schiff base complexes containing sulfur, and of complexes of amino acid Schiff bases (Casella & Gullotti, 1981, 1986; Wang *et al.*, 1994), has recently aroused considerable interest, due to the antiviral, anticancer and antibacterial activities of these compounds. Taurine, also known as 2-aminosulfonic acid, is indispensable to human beings and plays an important role in physiological functions. In this contribution, we present the synthesis and crystal structure of a new binuclear Ni^{II} dimer, (I), with a tridentate Schiff base ligand containing taurine.



The coordination environment of each Ni atom (shown in Figs. 1 and 2) contains two N atoms and one O atom (from the tridentate Schiff base ligand), two N-atom donors from bridging azides, and one O atom from a coordinated water molecule, resulting in a slightly distorted octahedral geometry. The two halves of each independent dimer are related by a crystallographic inversion centre, which lies at the centre of the ring formed by the two Ni atoms and the coordinating atoms of the two azide anions. The Ni1...Ni1ⁱ and Ni2...Ni2ⁱ

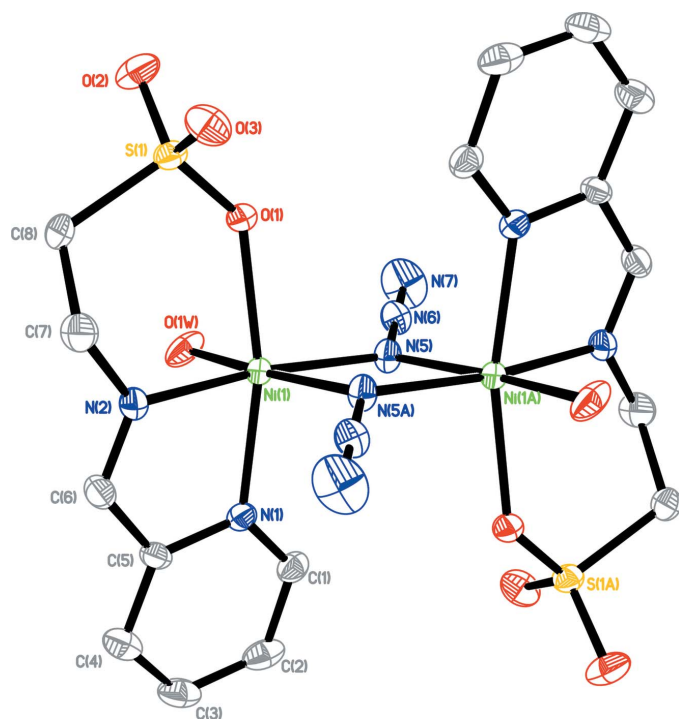


Figure 1

The molecular structure of (I), showing one of the two independent complex molecules, with displacement ellipsoids drawn at the 30% probability level. H atoms and solvent molecules have been omitted for clarity. Unlabelled atoms and those with the suffix A are related to labelled atoms by $(-x + 1, -y + 1, -z)$.

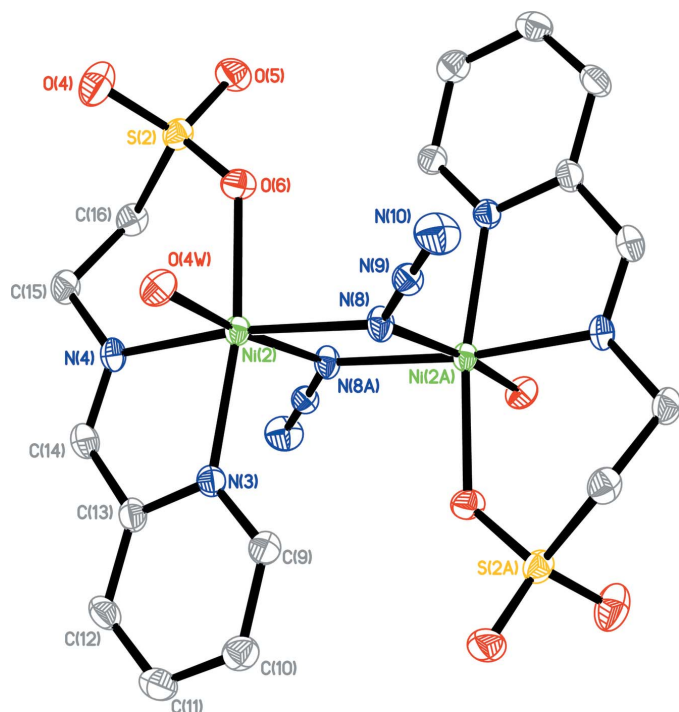


Figure 2

The molecular structure of (I), showing the other independent complex molecule, with displacement ellipsoids drawn at the 30% probability level. H atoms and solvent molecules have been omitted for clarity. Unlabelled atoms and those with the suffix A are related to labelled atoms by $(-x + 1, -y + 1, -z)$.

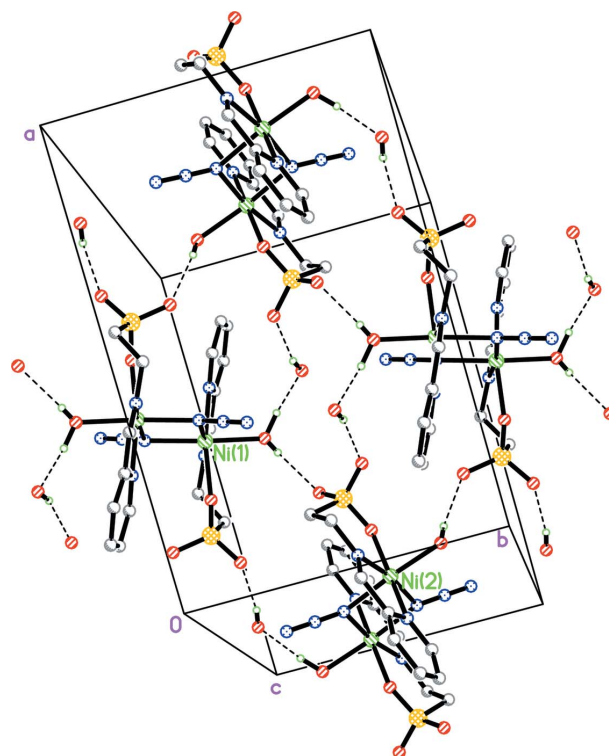


Figure 3

The double zigzag infinite chain structure of (I), linked *via* hydrogen bonds (dashed lines) lying in the *ab* plane. H atoms have been omitted for clarity, except for those involved in hydrogen-bonded interactions.

separations are 3.216 (3) and 3.259 (3) Å, respectively, distances that are too long for a metal–metal bond (Vahrenkamp, 1978). The Ni1–N5–Ni1ⁱ and Ni2–N8–Ni2ⁱ angles are 100.48 (13) and 101.25 (12)°, respectively, both in the range 100–107° corresponding to a normal *M*–*N*–*M* bond angle (*M* = Cu, Ni, and Mn^{II}) (Chaudhuri *et al.*, 1996). The two independent complex molecules in the asymmetric unit (shown in Figs. 1 and 2) possess identical coordination environments. While there are significant differences between the bond lengths and angles of the two crystallographically independent molecules, they are all small and can probably be accounted for by differences in the packing. There is a 16-membered ring $(-S-O-H-O-H-O-H-O-)_2$ between two neighbouring units, formed by two intramolecular hydrogen bonds (O1W–H1D···O3W and O3W–H3C···O4ⁱⁱ; see Tables for all symmetry codes) and an intermolecular hydrogen bond (O1W–H1C···O5ⁱ) in each unit. The solvent and coordinated water involve neighbouring units *via* O3W–H3C···O4ⁱⁱ and O4W–H4···O3, respectively, leading to an interesting double zigzag infinite chain structure in the *ac* plane.

Experimental

The potassium salt of the Schiff base ligand *N*-(2-pyridylmethylidene)taurine, *L*, was synthesized according to the method of Zeng *et al.* (2003). *L* (1.0 mmol) in methanol (10 ml) was added dropwise to a stirred solution of Ni(ClO₄)₂·6H₂O (1.0 mmol) in methanol and water (1:1 *v/v*, 10 ml). To this mixed solution, a solution of sodium azide

(2.0 mmol) in water and methanol (1:1 v/v, 4 ml) was added slowly. The resulting deep-green solution was filtered and left to stand for two weeks to evaporate slowly at room temperature, giving green prism-shaped single crystals in a yield of 65%. Analysis found (%): C 27.49, H 3.65, N 20.02, S 9.16; required (%): C 27.43, H 3.71, N 20.00, S 9.14. IR (KBr, ν , cm^{-1}): 1041.9, 1152.8, 1187.7 (SO_3); 1600, 1646.3 ($\text{C}=\text{N} + \text{C}=\text{C}$); 2065.5 (N_3^-); 3508.8 (OH).

Crystal data

$[\text{Ni}_2(\text{C}_8\text{H}_9\text{N}_2\text{O}_3\text{S})_2(\text{N}_3)_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$	$D_x = 1.768 \text{ Mg m}^{-3}$
$M_r = 700.01$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 5504 reflections
$a = 15.6693 (17) \text{ \AA}$	$\theta = 3.0\text{--}27.5^\circ$
$b = 10.4272 (8) \text{ \AA}$	$\mu = 1.66 \text{ mm}^{-1}$
$c = 17.1803 (15) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 110.503 (3)^\circ$	Prism, green
$V = 2629.2 (4) \text{ \AA}^3$	$0.30 \times 0.14 \times 0.08 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	6040 independent reflections
ω scans	5108 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan SADABS (Sheldrick, 1996)	$R_{\text{int}} = 0.045$
$T_{\text{min}} = 0.756, T_{\text{max}} = 0.876$	$\theta_{\text{max}} = 27.5^\circ$
19894 measured reflections	$h = -20 \rightarrow 19$
	$k = -10 \rightarrow 13$
	$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2 + 1.9453P]$
$R[F^2 > 2\sigma(F^2)] = 0.054$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.121$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.15$	$\Delta\rho_{\text{max}} = 0.54 \text{ e \AA}^{-3}$
6040 reflections	$\Delta\rho_{\text{min}} = -0.49 \text{ e \AA}^{-3}$
393 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1 Selected geometric parameters (\AA , $^\circ$).

Ni1—N2	2.042 (3)	Ni2—O6	2.078 (2)
Ni1—O1W	2.063 (3)	Ni2—N3	2.080 (3)
Ni1—N1	2.077 (3)	Ni2—O4W	2.079 (3)
Ni1—N5	2.089 (3)	Ni2—N4	2.083 (3)
Ni1—N5 ⁱ	2.094 (3)	Ni2—N8	2.103 (3)
Ni1—O1	2.122 (2)	Ni2—N8 ⁱⁱ	2.113 (3)
O1W—Ni1—N5 ⁱ	171.16 (13)	O4W—Ni2—N8 ⁱⁱ	171.40 (11)

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

Table 2 Hydrogen-bond geometry (\AA , $^\circ$).

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
O1W—H1C \cdots O5 ⁱⁱ	0.69 (4)	2.04 (5)	2.723 (4)	173 (5)
O1W—H1D \cdots O3W	0.97 (6)	1.71 (6)	2.684 (5)	174 (5)
O2W—H2D \cdots O2	0.74 (7)	2.06 (7)	2.788 (4)	168 (7)
O3W—H3C \cdots O4 ⁱⁱⁱ	0.79 (7)	2.03 (7)	2.765 (5)	156 (6)
O4W—H4C \cdots O3 ^{iv}	0.72 (5)	2.14 (5)	2.843 (4)	165 (6)
O4W—H4D \cdots O2W	0.90 (5)	1.85 (5)	2.743 (5)	175 (4)

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

H atoms bonded to C atoms were positioned geometrically with C—H distances 0.93–0.97 \AA , and treated as riding atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. H atoms bonded to O atoms were located in difference maps and refined isotropically.

Data collection: *CrystalClear* (Rigaku Corp., 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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