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Triaqua[2-(2-pyridylmethyleneamino)ethanesulfonato-κ^3N,N',O]nickel(II) perchlorate monohydrate

Jia-Ming Li,[a,b] Yi-Min Jiang,[a]* Chao-Zhu Li[b] and Shu-Hua Zhang[c]

[a]College of Chemistry and Chemical Engineering, Guangxi Normal University, Guilin, Guangxi 541004, People's Republic of China, [b]Department of Chemistry and Biology, Qinzhou College, Qinzhou, Guangxi 535000, People's Republic of China, and [c]Department of Materials and Chemical Engineering, Guilin University of Technology, Guilin, Guangxi 541004, People's Republic of China

Correspondence e-mail: ljmmarise@163.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean *σ*(C–C) = 0.006 Å
R factor = 0.044
wR factor = 0.109
Data-to-parameter ratio = 13.2

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

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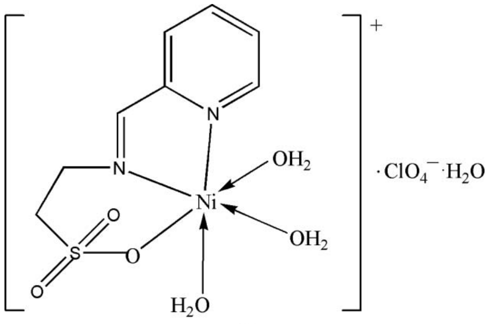
In the title compound, $[Ni(C_8H_9N_2O_3S)(H_2O)_3)]ClO_4\cdot H_2O$, the Ni^{II} atom is coordinated by the two N atoms [Ni—N = 2.054 (3) and 2.077 (3) Å] and one O atom [Ni—O = 2.070 (2) Å] from a tridentate 2-(2-pyridylmethylene)aminoethanesulfonate [or *N*-(2-pyridylmethylidene)taurine] ligand and three water molecules [Ni—O = 2.025 (3)–2.081 (3) Å] in a distorted octahedral geometry. An extensive three-dimensional network of O—H···O hydrogen bonds, involving perchlorate anions, and coordinating and non-coordinating water molecules, stabilizes the crystal packing.

Comment

In continuation of our structural study of Schiff base complexes (Li *et al.*, 2005; Jiang *et al.*, 2006), we present here the synthesis and crystal structure of the title Ni^{II} complex, (I), with a tridentate Schiff base ligand containing taurine.



(I)

In (I) (Fig. 1), the Ni^{II} atom is coordinated by the two N atoms and one O atom from the ligand *L* [H*L* = *N*-(2-pyridylmethylidene)taurine] and three water molecules in a slightly distorted octahedral geometry (Table 1). The equatorial plane O1/O4/N1/O6 is defined by two atoms (N1 and O1) from the tridentate ligand *L* and two atoms (O4 and O6) from the coordinating water molecules. The two axial positions are occupied by atoms N2 and O5 from *L* and a coordinating water molecule, respectively.

An extensive three-dimensional network of O—H···O hydrogen bonds (Table 2), involving perchlorate anions, and coordinating and non-coordinating water molecules, stabilizes the crystal packing (Fig. 2).

Experimental

The potassium salt of the Schiff base ligand *L* was synthesized according to the method of Li *et al.* (2005). *L* (1.0 mmol) in 10 ml of methanol was added dropwise to a stirred solution of

$Ni(ClO_4)_2 \cdot 6H_2O$ (1.0 mmol) in methanol (10 ml). The resulting deep-green solution was filtered and left to stand for two weeks to evaporate slowly at room temperature, giving green prismatic single crystals in a yield of 55%.

Crystal data

$[Ni(C_8H_9N_2O_3S)(H_2O)_3]ClO_4 \cdot H_2O$
$M_r = 443.46$
Orthorhombic, *Pbca*
$a = 7.818$ (2) Å
$b = 15.019$ (4) Å
$c = 28.156$ (7) Å
$V = 3305.7$ (15) Å^3
$Z = 8$
$D_x = 1.782$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.52$ mm^{-1}
$T = 293$ (2) K
Prism, green
0.25 × 0.10 × 0.10 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.703$, $T_{max} = 0.863$
14207 measured reflections
3253 independent reflections
2616 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 26.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.110$
$S = 1.06$
3253 reflections
246 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 3.2755P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.81$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O5	2.025 (3)	Ni1—O4	2.070 (3)
Ni1—N2	2.054 (3)	Ni1—N1	2.077 (3)
Ni1—O1	2.070 (2)	Ni1—O6	2.081 (3)
O5—Ni1—N2	179.26 (14)	O5—Ni1—O4	86.71 (13)
O5—Ni1—O1	88.35 (11)	N2—Ni1—O4	93.73 (12)
N2—Ni1—O1	92.26 (11)	O1—Ni1—O4	87.37 (12)

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4A···O7	0.84 (4)	2.12 (4)	2.927 (5)	160 (3)
O4—H4B···O11^{i}	0.84 (4)	2.03 (4)	2.840 (4)	161 (4)
O5—H5A···O11^{ii}	0.84 (4)	1.95 (4)	2.788 (4)	170 (5)
O5—H5B···O3^{iii}	0.85 (4)	2.01 (4)	2.779 (4)	150 (5)
O6—H6A···O7^{iv}	0.85 (4)	2.00 (4)	2.836 (5)	172 (4)
O6—H6B···O3^{v}	0.85 (4)	1.93 (4)	2.780 (4)	177 (5)
O11—H11A···O2^{iii}	0.85 (4)	2.09 (4)	2.882 (5)	159 (4)
O11—H11B···O2	0.85 (4)	2.12 (4)	2.939 (5)	164 (4)

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

The C-bound H atoms were geometrically positioned with C—H = 0.93–0.97 Å, and treated as riding with $U_{iso}(H) = 1.2U_{eq}(C)$. Water H atoms were located in a difference map and refined with O—H and H···H distance restraints of 0.85 (4) and 1.39 (4) Å, respectively, and $U_{iso}(H) = 1.2–1.5U_{eq}(O)$.

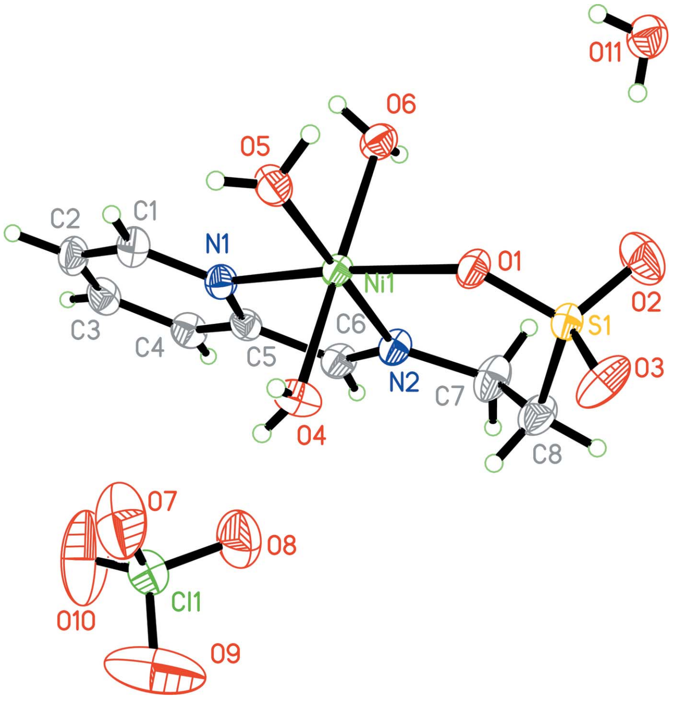


Figure 1
The asymmetric unit of (I), showing the atom-numbering scheme and displacement ellipsoids at the 30% probability level.

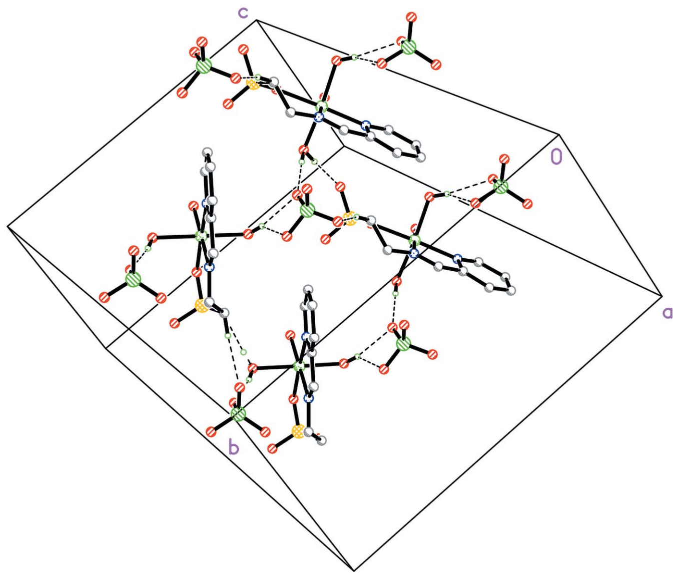


Figure 2
A portion of the crystal packing of (I), showing the hydrogen bonds as dashed lines. H atoms not involved in hydrogen bonds have been omitted for clarity.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SHELXTL* (Sheldrick, 1997*b*); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXL97*.

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