

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

# Aquabis(2-amino-1,3-thiazole-4-acetato- $\kappa^2O,N^3$ )nickel(II)

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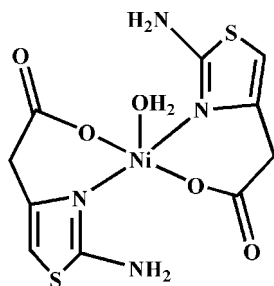
Received 27 April 2009; accepted 13 May 2009

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(C-C) = 0.003$  Å;  $R$  factor = 0.024;  $wR$  factor = 0.065; data-to-parameter ratio = 12.1.

In the crystal structure of the title compound,  $[Ni(C_5H_5N_2O_2S)_2(H_2O)]$ , the  $Ni^{II}$  cation is located on a twofold rotation axis and chelated by two 2-amino-1,3-thiazole-4-acetate (ata) anions in the basal coordination plane; a water molecule located on the same twofold rotation axis completes the distorted square-pyramidal coordination geometry. Intermolecular  $O-H\cdots O$  and  $N-H\cdots O$  hydrogen bonding, as well as  $\pi-\pi$  stacking between parallel thiazole rings [centroid-centroid distance 3.531 (8) Å], helps to stabilize the crystal structure.

## Related literature

For general background to the potential use of discrete and polymeric metal-organic complexes as functional materials in catalysis, molecular recognition, separation and non-linear optics, see: Batten & Robson (1998); Fujita *et al.* (1994); Han *et al.* (2008); Wu *et al.* (2001).



## Experimental

### Crystal data

$[Ni(C_5H_5N_2O_2S)_2(H_2O)]$   
 $M_r = 391.07$   
 Monoclinic,  $C2/c$   
 $a = 12.0875$  (12) Å  
 $b = 9.1278$  (9) Å  
 $c = 12.7715$  (12) Å  
 $\beta = 95.1190$  (10)°  
 $V = 1403.5$  (2) Å<sup>3</sup>

$Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.71$  mm<sup>-1</sup>

$T = 293$  K  
 $0.12 \times 0.10 \times 0.06$  mm

### Data collection

Bruker SMART CCD diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{min} = 0.821$ ,  $T_{max} = 0.904$

3487 measured reflections  
 1231 independent reflections  
 1119 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.014$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$   
 $wR(F^2) = 0.065$   
 $S = 1.01$   
 1231 reflections

102 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{max} = 0.31$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.29$  e Å<sup>-3</sup>

**Table 1**

Selected bond lengths (Å).

Ni1—O1	2.0243 (15)	Ni1—N2	2.0465 (18)
Ni1—O3	1.999 (2)		

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A $\cdots$ O1 <sup>i</sup>	0.86	2.10	2.816 (3)	140
N1—H1B $\cdots$ O2 <sup>ii</sup>	0.86	1.99	2.839 (3)	170
O3—H3 $\cdots$ O2 <sup>iii</sup>	0.82	1.94	2.7211 (19)	158

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

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); 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.

This work was supported financially by the National Natural Science Foundation of China (grant No. 20773104), the Program for New Century Excellent Talents in Universities (NCET-06-0891), the Natural Science Foundation of Hubei Province of China (2008CDB030) and the Important Project of Hubei Provincial Education Office (Z20091301).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2518).

## References

- Batten, S. R. & Robson, R. (1998). *Angew. Chem. Int. Ed.* **37**, 1460–1494.  
 Bruker (1997). SMART and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Fujita, M., Kwon, Y. J., Washizu, S. & Ogura, K. (1994). *J. Am. Chem. Soc.* **116**, 1151–1152.  
 Han, S. S., Furukawa, H., Yaghi, O. M. & Goddard, W. A. III (2008). *J. Am. Chem. Soc.* **130**, 11580–11581.  
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Wu, Z.-Y., Xu, D.-J. & Feng, Z.-X. (2001). *Polyhedron*, **20**, 281–284.

## supporting information

*Acta Cryst.* (2009). E65, m666 [doi:10.1107/S1600536809017978]

**Aquabis(2-amino-1,3-thiazole-4-acetato- $\kappa^2O,N^3$ )nickel(II)****Qiu-Fen He, Dong-Sheng Li, Jun Zhao, Xi-Jun Ke and Cai Li****S1. Comment**

The rational design and synthesis of novel discrete and polymeric metal-organic complexes have attracted intense interest owing to the realisation of their potential for use as functional materials in catalysis, molecular recognition, separation, and nonlinear optics (Batten & Robson, 1998; Fujita *et al.*, 1994). As for the construction of these inorganic/organic hybrid materials, carboxylate ligands have proven to be an efficacious choice (Wu *et al.*, 2001). The employment of multifunctional ligands bearing both anionic and neutral donor atoms, such as nicotinate, isonicotinate, and various pyridinedicarboxylates, has resulted in the preparation of many functional coordination polymers, some with intriguing optical or gas sorption properties (Han *et al.*, 2008). Herein we report the hydrothermal synthesis, structural characterization of the title complex.

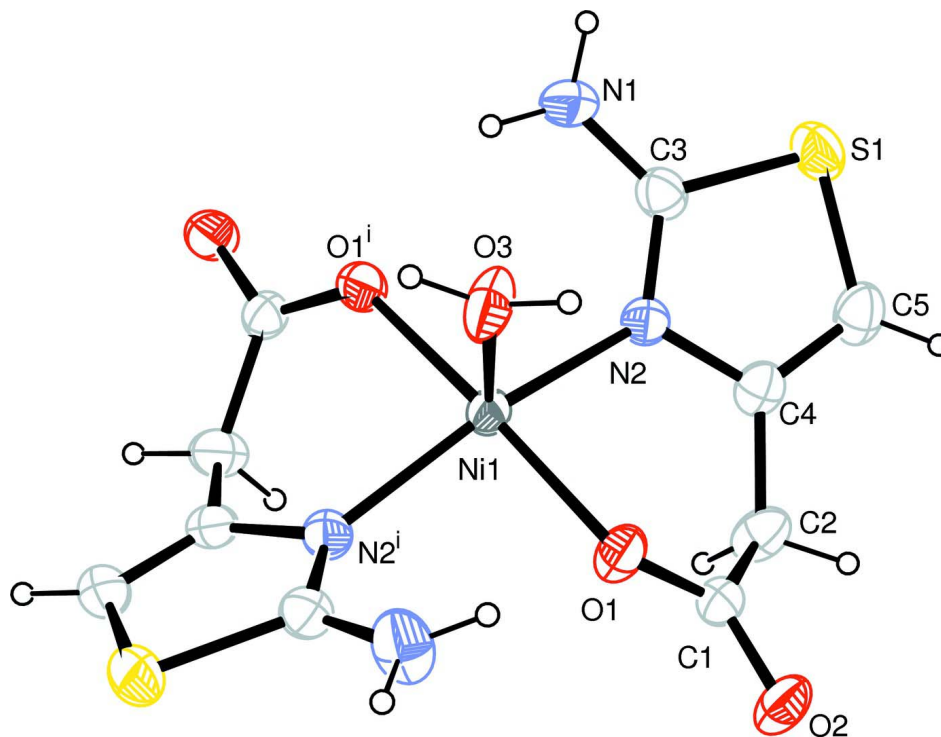
The molecular structure of the title complex is shown in Fig. 1. The Ni<sup>II</sup> ion is located on a twofold rotation axis and has a slightly distorted square-pyramidal geometry formed by two oxygen atoms, two nitrogen atoms from two ligands and one coordinated water molecules (Table 1). The amido N atoms forms N—H $\cdots$ O hydrogen bonds with carboxylate O atoms, linking the molecules into one dimensional chains, which are then linked into a two-dimensional sheet by aromatic  $\pi$ - $\pi$  stacking between S1-thiazole and S1<sup>i</sup>-thiazole [symmetry code: (i) -x, 1 - y, 1 - z] rings [centroid-centroid distance 3.531 (8) Å]. Furthermore, the two-dimensional layers are extended to a three-dimensional supramolecular structure by O—H $\cdots$ O hydrogen bonds (Table 2).

**S2. Experimental**

A mixture of Ni(CH<sub>3</sub>COOH)<sub>2</sub>·4H<sub>2</sub>O (0.025 g, 0.1 mmol), 2-amino-4-thiazoleacetic acid (0.0316 g, 0.2 mmol) and distilled water (10 ml) was sealed in a 25 ml Teflon-lined stainless autoclave. The pH value of the mixture was adjusted to 6 by a aqueous solution of NaOH (0.1 mol/L), and then heated at 393 K for 3 d. Green crystals were obtained on cooling to room temperature.

**S3. Refinement**

H atoms were placed in calculated positions and treated using a riding-model approximation with C—H = 0.93, with  $U_{iso}(H) = 1.2U_{eq}(C)$ ; O—H = 0.82 and N—H = 0.86 Å,  $U_{iso}(H) = 1.5U_{eq}(O,N)$ .



**Figure 1**

The molecular structure of the title compound with thermal ellipsoids plotted at 50% probability [symmetry code: (i)  $-x, y, -z + 1/2$ ].

### Aquabis(2-amino-1,3-thiazole-4-acetato- $\kappa^2O, N^3$ )nickel(II)

#### Crystal data

$[\text{Ni}(\text{C}_5\text{H}_5\text{N}_2\text{O}_2\text{S})_2(\text{H}_2\text{O})]$

$M_r = 391.07$

Monoclinic,  $C2/c$

Hall symbol:  $-C\ 2yc$

$a = 12.0875\ (12)\ \text{\AA}$

$b = 9.1278\ (9)\ \text{\AA}$

$c = 12.7715\ (12)\ \text{\AA}$

$\beta = 95.119\ (1)^\circ$

$V = 1403.5\ (2)\ \text{\AA}^3$

$Z = 4$

$F(000) = 800$

$D_x = 1.851\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2106 reflections

$\theta = 2.8\text{--}25.0^\circ$

$\mu = 1.71\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Prism, green

$0.12 \times 0.10 \times 0.06\ \text{mm}$

#### Data collection

Bruker SMART CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

CCD Profile fitting scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.821, T_{\max} = 0.904$

3487 measured reflections

1231 independent reflections

1119 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.014$

$\theta_{\max} = 25.0^\circ, \theta_{\min} = 2.8^\circ$

$h = -14 \rightarrow 14$

$k = -5 \rightarrow 10$

$l = -15 \rightarrow 14$

Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.024$

$wR(F^2) = 0.065$

$S = 1.01$

1231 reflections

102 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.034P)^2 + 2.301P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.31 \text{ e } \text{Å}^{-3}$

$\Delta\rho_{\min} = -0.29 \text{ e } \text{Å}^{-3}$

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 ( $\text{Å}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.0000	0.69428 (4)	0.2500	0.02321 (14)
N1	0.10680 (18)	0.7919 (2)	0.49121 (17)	0.0423 (6)
H1A	0.1428	0.7976	0.4363	0.051*
H1B	0.1341	0.8297	0.5496	0.051*
N2	-0.04038 (14)	0.6630 (2)	0.40062 (14)	0.0264 (4)
O1	-0.16405 (12)	0.68137 (17)	0.20264 (12)	0.0314 (4)
O2	-0.33123 (12)	0.5835 (2)	0.19153 (12)	0.0369 (4)
O3	0.0000	0.9133 (2)	0.2500	0.0401 (6)
H3	0.0570	0.9433	0.2270	0.060*
C1	-0.23701 (16)	0.5998 (2)	0.23761 (16)	0.0254 (5)
C2	-0.20703 (19)	0.5149 (3)	0.33761 (18)	0.0336 (5)
H2A	-0.2751	0.4820	0.3650	0.040*
H2B	-0.1657	0.4283	0.3204	0.040*
C3	0.00918 (19)	0.7248 (3)	0.48595 (17)	0.0295 (5)
C4	-0.14006 (17)	0.5971 (2)	0.42235 (17)	0.0280 (5)
C5	-0.16604 (19)	0.6117 (3)	0.52138 (18)	0.0364 (6)
H5	-0.2299	0.5739	0.5468	0.044*
S1	-0.06560 (5)	0.71004 (8)	0.59589 (5)	0.03934 (19)

Atomic displacement parameters ( $\text{Å}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ni1	0.0186 (2)	0.0286 (2)	0.0224 (2)	0.000	0.00139 (15)	0.000
N1	0.0395 (12)	0.0586 (15)	0.0285 (11)	-0.0167 (11)	0.0017 (9)	-0.0117 (10)
N2	0.0241 (9)	0.0319 (10)	0.0229 (9)	-0.0007 (8)	0.0009 (7)	-0.0001 (8)

O1	0.0225 (8)	0.0422 (9)	0.0291 (9)	-0.0047 (7)	0.0005 (6)	0.0090 (7)
O2	0.0217 (8)	0.0551 (11)	0.0327 (9)	-0.0077 (7)	-0.0033 (6)	0.0127 (8)
O3	0.0262 (12)	0.0300 (12)	0.0666 (17)	0.000	0.0190 (12)	0.000
C1	0.0217 (11)	0.0292 (11)	0.0252 (11)	0.0004 (9)	0.0016 (9)	-0.0006 (9)
C2	0.0290 (11)	0.0352 (13)	0.0354 (13)	-0.0065 (10)	-0.0038 (10)	0.0099 (11)
C3	0.0294 (12)	0.0343 (13)	0.0246 (12)	0.0031 (10)	0.0014 (9)	-0.0006 (10)
C4	0.0239 (10)	0.0314 (12)	0.0281 (12)	0.0023 (9)	-0.0004 (9)	0.0071 (10)
C5	0.0278 (12)	0.0504 (15)	0.0311 (13)	0.0004 (11)	0.0039 (10)	0.0096 (12)
S1	0.0384 (4)	0.0570 (4)	0.0230 (3)	0.0039 (3)	0.0044 (3)	-0.0030 (3)

*Geometric parameters (Å, °)*

Ni1—O1	2.0243 (15)	O2—C1	1.243 (3)
Ni1—O1 <sup>i</sup>	2.0243 (15)	O3—H3	0.8200
Ni1—O3	1.999 (2)	C1—C2	1.510 (3)
Ni1—N2	2.0465 (18)	C2—C4	1.494 (3)
Ni1—N2 <sup>i</sup>	2.0465 (18)	C2—H2A	0.9700
N1—C3	1.326 (3)	C2—H2B	0.9700
N1—H1A	0.8600	C3—S1	1.742 (2)
N1—H1B	0.8600	C4—C5	1.337 (3)
N2—C3	1.322 (3)	C5—S1	1.726 (3)
N2—C4	1.397 (3)	C5—H5	0.9300
O1—C1	1.266 (3)		
O3—Ni1—O1	93.34 (5)	O2—C1—C2	118.64 (19)
O3—Ni1—O1 <sup>i</sup>	93.34 (5)	O1—C1—C2	118.57 (18)
O1—Ni1—O1 <sup>i</sup>	173.33 (9)	C4—C2—C1	115.36 (19)
O3—Ni1—N2	98.02 (5)	C4—C2—H2A	108.4
O1—Ni1—N2	87.90 (7)	C1—C2—H2A	108.4
O1 <sup>i</sup> —Ni1—N2	91.17 (7)	C4—C2—H2B	108.4
O3—Ni1—N2 <sup>i</sup>	98.02 (5)	C1—C2—H2B	108.4
O1—Ni1—N2 <sup>i</sup>	91.17 (7)	H2A—C2—H2B	107.5
O1 <sup>i</sup> —Ni1—N2 <sup>i</sup>	87.90 (7)	N2—C3—N1	125.1 (2)
N2—Ni1—N2 <sup>i</sup>	163.96 (11)	N2—C3—S1	113.70 (17)
C3—N1—H1A	120.0	N1—C3—S1	121.23 (17)
C3—N1—H1B	120.0	C5—C4—N2	115.1 (2)
H1A—N1—H1B	120.0	C5—C4—C2	125.3 (2)
C3—N2—C4	110.83 (19)	N2—C4—C2	119.58 (19)
C3—N2—Ni1	125.93 (16)	C4—C5—S1	111.14 (18)
C4—N2—Ni1	121.96 (14)	C4—C5—H5	124.4
C1—O1—Ni1	128.58 (14)	S1—C5—H5	124.4
Ni1—O3—H3	109.5	C5—S1—C3	89.19 (11)
O2—C1—O1	122.8 (2)		
O3—Ni1—N2—C3	-50.65 (19)	C4—N2—C3—N1	177.7 (2)
O1—Ni1—N2—C3	-143.73 (19)	Ni1—N2—C3—N1	-15.1 (3)
O1 <sup>i</sup> —Ni1—N2—C3	42.88 (19)	C4—N2—C3—S1	-1.8 (2)
N2 <sup>i</sup> —Ni1—N2—C3	129.35 (19)	Ni1—N2—C3—S1	165.31 (11)

O3—Ni1—N2—C4	115.15 (16)	C3—N2—C4—C5	1.4 (3)
O1—Ni1—N2—C4	22.08 (17)	Ni1—N2—C4—C5	-166.37 (17)
O1 <sup>i</sup> —Ni1—N2—C4	-151.32 (17)	C3—N2—C4—C2	-177.3 (2)
N2 <sup>i</sup> —Ni1—N2—C4	-64.85 (16)	Ni1—N2—C4—C2	15.0 (3)
O3—Ni1—O1—C1	-135.01 (18)	C1—C2—C4—C5	126.8 (3)
N2—Ni1—O1—C1	-37.09 (19)	C1—C2—C4—N2	-54.7 (3)
N2 <sup>i</sup> —Ni1—O1—C1	126.88 (19)	N2—C4—C5—S1	-0.3 (3)
Ni1—O1—C1—O2	-167.76 (16)	C2—C4—C5—S1	178.27 (18)
Ni1—O1—C1—C2	10.2 (3)	C4—C5—S1—C3	-0.6 (2)
O2—C1—C2—C4	-140.5 (2)	N2—C3—S1—C5	1.44 (19)
O1—C1—C2—C4	41.5 (3)	N1—C3—S1—C5	-178.2 (2)

Symmetry code: (i)  $-x, y, -z+1/2$ .

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N1—H1A $\cdots$ O1 <sup>i</sup>	0.86	2.10	2.816 (3)	140
N1—H1B $\cdots$ O2 <sup>ii</sup>	0.86	1.99	2.839 (3)	170
O3—H3 $\cdots$ O2 <sup>iii</sup>	0.82	1.94	2.7211 (19)	158

Symmetry codes: (i)  $-x, y, -z+1/2$ ; (ii)  $x+1/2, -y+3/2, z+1/2$ ; (iii)  $x+1/2, y+1/2, z$ .