

Aquabis(2-amino-1,3-thiazole-4-acetato- κ^2O,N^3)nickel(II)

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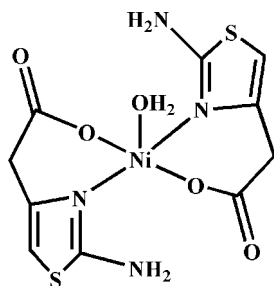
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(C-C) = 0.003$ Å; R factor = 0.024; wR factor = 0.065; data-to-parameter ratio = 12.1.

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. Inter-molecular $O-H \cdots O$ 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) Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.71$ mm⁻¹

$T = 293$ 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⁻³
 $\Delta\rho_{min} = -0.29$ e Å⁻³

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 ⁱ	0.86	2.10	2.816 (3)	140
N1—H1B \cdots O2 ⁱⁱ	0.86	1.99	2.839 (3)	170
O3—H3 \cdots O2 ⁱⁱⁱ	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.

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

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supplementary materials

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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^{II} 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 π - π stacking between S1-thiazole and S1ⁱ-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).

Experimental

A mixture of Ni(CH₃COOH)₂·4H₂O (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.

Refinement

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

Figures

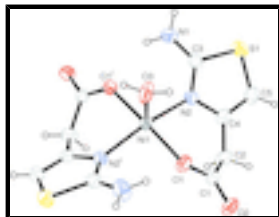


Fig. 1. The molecular structure of the title compound with thermal ellipsoids plotted at 50% probability [symmetry code: (i) $-x, y, -z + 1/2$].

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Crystal data

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Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 12.0875$ (12) Å

$b = 9.1278$ (9) Å

$c = 12.7715$ (12) Å

$\beta = 95.1190$ (10)°

$V = 1403.5$ (2) Å³

$Z = 4$

$F_{000} = 800$

$D_x = 1.851$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 2106 reflections

$\theta = 2.8$ – 25.0 °

$\mu = 1.71$ mm⁻¹

$T = 293$ K

Prism, green

$0.12 \times 0.10 \times 0.06$ mm

Data collection

Bruker SMART CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$ K

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 $I > 2\sigma(I)$

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

$\theta_{\max} = 25.0$ °

$\theta_{\min} = 2.8$ °

$h = -14 \rightarrow 14$

$k = -5 \rightarrow 10$

$l = -15 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

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

$wR(F^2) = 0.065$

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

$S = 1.01$	$(\Delta/\sigma)_{\max} < 0.001$
1231 reflections	$\Delta\rho_{\max} = 0.31 \text{ e } \text{\AA}^{-3}$
102 parameters	$\Delta\rho_{\min} = -0.29 \text{ e } \text{\AA}^{-3}$
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 (\AA^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 (\AA^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)

supplementary materials

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 (\AA , $^\circ$)

Ni1—O1	2.0243 (15)	O2—C1	1.243 (3)
Ni1—O1 ⁱ	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 ⁱ	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 ⁱ	93.34 (5)	O1—C1—C2	118.57 (18)
O1—Ni1—O1 ⁱ	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 ⁱ —Ni1—N2	91.17 (7)	C4—C2—H2B	108.4
O3—Ni1—N2 ⁱ	98.02 (5)	C1—C2—H2B	108.4
O1—Ni1—N2 ⁱ	91.17 (7)	H2A—C2—H2B	107.5
O1 ⁱ —Ni1—N2 ⁱ	87.90 (7)	N2—C3—N1	125.1 (2)
N2—Ni1—N2 ⁱ	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 ⁱ —Ni1—N2—C3	42.88 (19)	C4—N2—C3—S1	-1.8 (2)
N2 ⁱ —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 ⁱ —Ni1—N2—C4	-151.32 (17)	C3—N2—C4—C2	-177.3 (2)
N2 ⁱ —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 ⁱ —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 codes: (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 ⁱ	0.86	2.10	2.816 (3)	140
N1—H1B \cdots O2 ⁱⁱ	0.86	1.99	2.839 (3)	170
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Symmetry codes: (i) $-x, y, -z+1/2$; (ii) $x+1/2, -y+3/2, z+1/2$; (iii) $x+1/2, y+1/2, z$.

