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(2,2′-Diamino-4,4′-bi-1,3-thiazole-κ^2*N*,*N*′)-bis(glycinato-κ^2*N*,*O*)nickel(II) dihydrate

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In the crystal structure of the title compound, $[Ni(C_2H_4NO_2)_2(C_6H_6N_4S_2)]\cdot 2H_2O$, the Ni^{II} atom is located on a twofold axis and is coordinated by a diaminobithiazole ligand and two glycinate anions in a distorted octahedral geometry. The glycinate anions chelate to the Ni^{II} atom through the amino N and carboxyl O atoms, and display an envelope conformation. Hydrogen bonding consolidates the crystal structure.

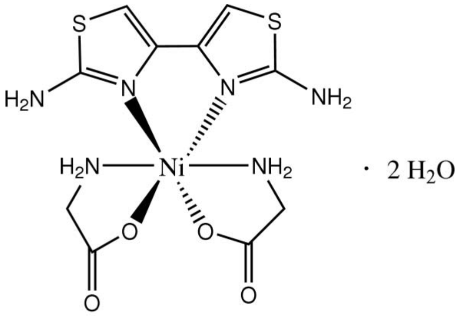
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.025
wR factor = 0.063
Data-to-parameter ratio = 16.6

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

Comment

As metal complexes containing the diaminobithiazole (DABT) ligand have shown interesting magnetic properties (Sun *et al.*, 1997), a series of transition metal complexes incorporating DABT has been prepared in our laboratory (Liu & Xu, 2004). As part of the ongoing investigation into the structures of the DABT complexes, we present here the structure of the title Ni^{II} complex, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The complex has a distorted octahedral coordination geometry, formed by one DABT and two glycinate ligands. The Ni atom and the mid-point of the C—C bond linking the two thiazole rings are located on a twofold axis. The Ni^{II} complex is isomorphous with the Co^{II} complex (Yu *et al.*, 2005). The Ni—O and Ni—N bond distances in (I) (Table 1) are about 0.04 Å shorter than the corresponding Co—O and Co—N bond distances found in the Co^{II} analogue.

A hydrogen-bonding network (Table 2) consolidates the crystal structure of (I).

Experimental

An aqueous solution (20 ml) containing DABT (0.20 g, 1 mmol) and $NiCl_2$ (0.13 g, 1 mmol) was mixed with an aqueous solution (10 ml) of glycine (0.15 g, 2 mmol) and NaOH (0.08 g, 2 mmol). The mixture was refluxed for 6 h. The solution was filtered after cooling to room temperature. Green single crystals of (I) were obtained from the filtrate after three days.

Crystal data

$[Ni(C_2H_4NO_2)_2(C_6H_6N_4S_2)]\cdot 2H_2O$
$M_r = 441.13$
Monoclinic, $C2/c$
$a = 13.0342\ (12)$ Å
$b = 8.9631\ (11)$ Å
$c = 14.0836\ (12)$ Å
$\beta = 92.811\ (8)^\circ$
$V = 1643.4\ (3)$ Å^3
$Z = 4$
$D_x = 1.783$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1802 reflections
$\theta = 2.8$–26.0°
$\mu = 1.48$ mm^{-1}
$T = 295\ (2)$ K
Prism, green
0.25 × 0.22 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.678$, $T_{max} = 0.795$
8498 measured reflections
1888 independent reflections
1749 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 27.5^\circ$
$h = -16 \rightarrow 16$
$k = -11 \rightarrow 11$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.063$
$S = 1.05$
1888 reflections
114 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.031P)^2 + 1.8149P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni—O1	2.0958 (11)	Ni—N3	2.0918 (13)
Ni—N1	2.1177 (13)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H1A···O1^{iii}	0.91	2.12	2.947 (2)	150
O1w—H1B···O2	0.89	2.02	2.884 (2)	164
N2—H2A···O2^{ii}	0.89	2.09	2.923 (2)	157
N2—H2B···O1^{i}	0.82	2.42	3.068 (2)	136
N3—H3A···O1w^{iv}	0.90	2.28	3.098 (2)	151
N3—H3B···O2^{v}	0.87	2.45	3.2814 (19)	160

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

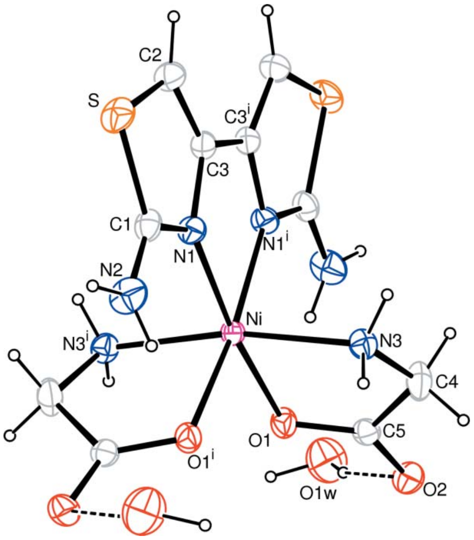


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms); dashed lines indicate the hydrogen bonding [symmetry code: (i) $-x+1, y, -z+\frac{1}{2}$].

The C-bound H atoms were placed in calculated positions with C—H distances of 0.93 Å (aromatic) or 0.97 Å (methylene), and included in the final cycles of refinement in riding mode with $U_{iso}(H) = 1.2U_{eq}(C)$. Other H atoms were located in a difference Fourier map and refined as riding in their as-found relative positions (Table 2) with $U_{iso}(H) = 1.5U_{eq}$(carrier atom).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Acta Cryst. (2006). E**62**, m222–m223 Liu *et al.* • $[Ni(C_2H_4NO_2)_2(C_6H_6N_4S_2)]\cdot 2H_2O$ **m223**