

(2,2'-Diamino-4,4'-bi-1,3-thiazole- κ^2N,N')-bis(glycinato- κ^2N,O)zinc(II) dihydrate**Bing-Xin Liu,^a Jian-Yong Yu^a and Duan-Jun Xu^{b*}**^aDepartment of Chemistry, Shanghai University, People's Republic of China, and ^bDepartment of Chemistry, Zhejiang University, People's Republic of China

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Key indicators

Single-crystal X-ray study

T = 295 K

Mean $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$

R factor = 0.021

wR factor = 0.054

Data-to-parameter ratio = 16.7

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

In the title Zn^{II} complex, $[\text{Zn}(\text{C}_2\text{H}_4\text{NO}_2)_2(\text{C}_6\text{H}_6\text{N}_4\text{S}_2)] \cdot 2\text{H}_2\text{O}$, the Zn^{II} ion is coordinated by two glycinate anions and a diaminobithiazole (DABT) molecule in a distorted octahedral geometry. Two thiazole rings of the same DABT are twisted with respect to each other with a dihedral angle of $10.56(6)^\circ$. The glycinate chelates to the Zn^{II} ion by the amino N and carboxylate O atoms; the chelating five-membered ring displays an envelope configuration. A twofold rotation axis passes through the Zn atom and the mid-point of the C—C bond linking the two thiazole rings.

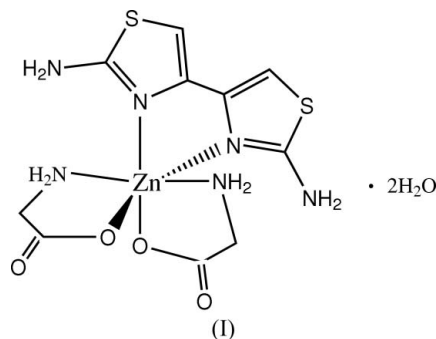
Received 21 November 2005

Accepted 6 December 2005

Online 10 December 2005

Comment

We are interested in metal complexes with diaminobithiazole (DABT) because of their potential magnetic properties (Sun *et al.*, 1997). As part of an ongoing investigation of DABT complexes (Liu *et al.*, 2001), we present here the crystal structure of the title Zn^{II} complex, (I).



The molecular structure of (I) is shown in Fig. 1. A twofold rotation axis passes through the Zn atom and the mid-point of the C—C bond linking the two thiazole rings. Two glycinate anions and one DABT molecule chelate to the Zn^{II} ion in a distorted octahedral geometry (Table 1). Thiazole rings of the same DABT are twisted with respect to the each other with a dihedral angle of $10.56(6)^\circ$, comparable to the Co^{II} analog [$9.68(6)^\circ$; Yu *et al.*, 2005]. The chelating five-membered ring of the glycinate anion displays an envelope conformation, atom N3 being displaced $0.390(2) \text{ \AA}$ from the mean plane formed by the other four atoms.

The classical O—H...O and N—H...O hydrogen-bonding network stabilizes the crystal structure (Table 2).

Experimental

An aqueous solution (20 ml) containing DABT (1 mmol) and ZnCl_2 (1 mmol) was mixed with another aqueous solution (10 ml) of glycine (2 mmol) and NaOH (1 mmol). The mixture was refluxed for 4 h. The

solution was filtered after cooling to room temperature. Single crystals of (I) were obtained from the filtrate after one week.

Crystal data

[Zn(C₂H₄NO₂)₂(C₆H₆N₄S₂)]·2H₂O
M_r = 447.79
 Monoclinic, *C*2/*c*
a = 13.121 (2) Å
b = 9.0063 (16) Å
c = 14.124 (2) Å
 β = 92.365 (6)°
V = 1667.7 (5) Å³
Z = 4
D_x = 1.783 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 5886 reflections
 θ = 2.8–25.0°
 μ = 1.77 mm⁻¹
T = 295 (2) K
 Prism, colorless
 0.25 × 0.20 × 0.16 mm

Data collection

Rigaku R-Axis RAPID diffractometer
 ω scans
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
T_{min} = 0.628, *T_{max}* = 0.750
 7912 measured reflections
 1918 independent reflections
 1808 reflections with *I* > 2σ(*I*)
R_{int} = 0.018
 θ_{max} = 27.5°
h = -16 → 16
k = -10 → 11
l = -18 → 18

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.021
wR (*F*²) = 0.054
S = 1.08
 1918 reflections
 115 parameters
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0209P)^2 + 2.0364P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 (Δ/σ)_{max} = 0.001
 Δρ_{max} = 0.30 e Å⁻³
 Δρ_{min} = -0.22 e Å⁻³
 Extinction correction: SHELXL97
 Extinction coefficient: 0.0134 (5)

Table 1

Selected bond lengths (Å).

Zn—O1	2.1714 (11)	N1—C1	1.3901 (19)
Zn—N1	2.1823 (13)	N1—C3	1.3212 (19)
Zn—N3	2.1185 (13)	N2—C3	1.333 (2)
S1—C2	1.7219 (19)	C1—C2	1.344 (2)
S1—C3	1.7417 (17)	C1—C1 ⁱ	1.469 (3)

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

Table 2

Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
O1W—H1A...O1 ⁱⁱ	0.88	2.18	2.976 (2)	151
O1W—H1B...O2	0.90	2.00	2.878 (2)	167
N2—H2A...O1 ⁱ	0.87	2.37	3.098 (2)	141
N2—H2B...O2 ⁱⁱⁱ	0.86	2.09	2.9059 (19)	159
N3—H3A...O2 ^{iv}	0.88	2.47	3.3209 (19)	165
N3—H3B...O1W ^v	0.90	2.22	3.051 (2)	154

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

H atoms bonded to C atoms were placed in calculated positions, with C—H = 0.93 Å (aromatic) or 0.97 Å (methylene), and included in the final cycles of refinement as riding, with *U*_{iso}(H) = 1.2*U*_{eq}(C).

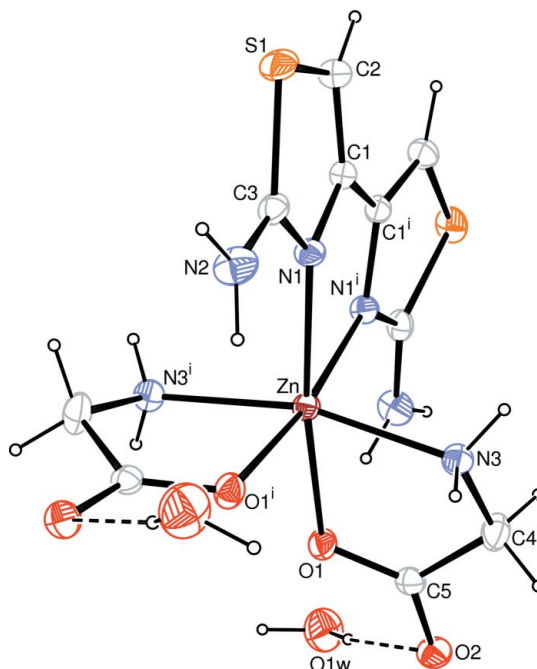


Figure 1

The molecular structure of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). Dashed lines indicate hydrogen bonds [symmetry code: (i) -x + 1, y, -z + 1/2].

Other H atoms were located in a difference Fourier map and refined as riding in their as-found relative positions with *U*_{iso}(H) = 1.5*U*_{eq}(carrier).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The project was supported by the Educational Development Foundation of Shanghai Educational Committee, China (No. AB0448).

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