

**catena-Poly[[chloro(2,2'-diamino-4,4'-bi-1,3-thiazole- $\kappa^2N,N'$ )cadmium(II)]- $\mu$ -glycinato- $\kappa^2N,O'$ ]****Bing-Xin Liu,<sup>a</sup> Jian-Yong Yu<sup>a</sup> and Duan-Jun Xu<sup>b\*</sup>**<sup>a</sup>Department of Chemistry, Shanghai University, People's Republic of China, and <sup>b</sup>Department of Chemistry, Zhejiang University, People's Republic of China

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In the polymeric title complex,  $[\text{Cd}(\text{C}_2\text{H}_4\text{NO}_2)\text{Cl}(\text{C}_6\text{H}_6\text{N}_4\text{S}_2)]_n$ , the glycinate anions bridge neighbouring  $\text{Cd}^{\text{II}}$  ions to form zigzag chains along the  $b$  axis direction. The  $\text{Cd}^{\text{II}}$  ion is coordinated by two glycinate ions (one  $O$ -monodentate and one  $N,O$ -bidentate), a  $\text{Cl}^-$  ion and a bidentate diamino-bithiazole ligand in a distorted octahedral geometry. Various  $\text{N}-\text{H}\cdots\text{O}$  and  $\text{N}-\text{H}\cdots\text{Cl}$  hydrogen bonds between adjacent complex chains help to consolidate the crystal packing.

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**Key indicators**

Single-crystal X-ray study

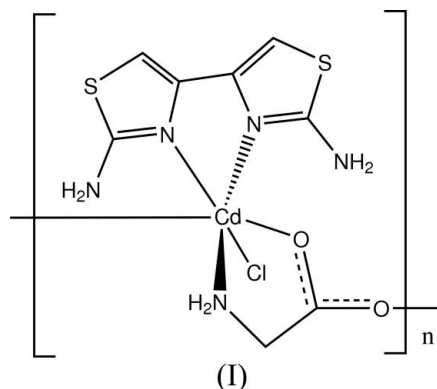
 $T = 295 \text{ K}$ Mean  $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$  $R$  factor = 0.014 $wR$  factor = 0.034

Data-to-parameter ratio = 17.3

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

**Comment**

Transition metal complexes containing the diamino-bithiazole ( $\text{C}_6\text{H}_6\text{N}_4\text{S}_2$ ; DABT) molecule have attracted our attention because of their interesting magnetic properties (Sun *et al.*, 1997), and a series of metal complexes incorporating DABT has been prepared in our laboratory (Liu *et al.*, 2001; Liu & Xu, 2004). As part of our ongoing investigations of DABT complexes, the title  $\text{Cd}^{\text{II}}$  complex, (I), has been prepared and its crystal structure is presented here.



A segment of the polymeric structure of (I) is shown in Fig. 1. The  $\text{Cd}^{\text{II}}$  ion has a distorted octahedral coordination geometry, formed by a bidentate DABT molecule, a  $\text{Cl}^-$  ion and two glycinate anions (one  $O$ -monodentate and one  $N,O$ -bidentate).

The DABT molecule chelating the  $\text{Cd}^{\text{II}}$  atom in (I) is close to planar, with a dihedral angle of  $2.35 (12)^\circ$  between the two thiazole mean planes. This is comparable with the dihedral angle of  $4.30 (12)^\circ$  found in another  $\text{Cd}^{\text{II}}$  complex of DABT with oxydiacetate (Liu *et al.*, 2004), but differs appreciably from the value of  $20.02 (8)^\circ$  found in an  $\text{Ni}^{\text{II}}$  complex of DABT with iminodiacetate (Liu & Xu, 2005).

Each glycinate anion plays a dual role of chelating and bridging ligand. The amino N atom and one carboxyl O atom chelate to a  $\text{Cd}^{\text{II}}$  ion to form a five-membered  $\text{Cd}$ -glycinate

ring. This ring displays an envelope conformation, with atom C8 lying at the flap position and displaced from the mean plane formed by the other four atoms by 0.443 (3) Å. The carboxyl atom O2 bridges to a neighbouring Cd<sup>II</sup> ion to form a zigzag polymeric chain propagating along the *b* axis direction. The carboxylate atoms O1 and O2 coordinate to the Cd<sup>II</sup> ions with *anti* and *syn* configurations, respectively. It is notable that the Cd–O1 bond involving the *anti* configuration is much longer than the Cd–O2 bond (Table 1).

Adjacent polymeric chains in (I) are linked to each other via N–H···O and N–H···Cl hydrogen bonds (Table 2).

**Experimental**

An aqueous solution (20 ml) containing DABT (0.20 g, 1 mmol) and CdCl<sub>2</sub>·2H<sub>2</sub>O (0.22 g, 1 mmol) was mixed with another aqueous solution (10 ml) of glycine (0.15 g, 2 mmol) and NaOH (0.04 g, 1 mmol). The mixture was refluxed for 6 h, and the solution was then cooled to room temperature and filtered. Yellow single crystals of (I) were obtained from the filtrate after 10 d.

*Crystal data*

[Cd(C <sub>2</sub> H <sub>4</sub> NO <sub>2</sub> )Cl(C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> S <sub>2</sub> )]	<i>D<sub>x</sub></i> = 2.133 Mg m <sup>-3</sup>
<i>M<sub>r</sub></i> = 420.18	Mo Kα radiation
Monoclinic, <i>P</i> 2 <sub>1</sub>	Cell parameters from 2650 reflections
<i>a</i> = 7.0335 (7) Å	<i>θ</i> = 2.5–26.0°
<i>b</i> = 10.2471 (8) Å	<i>μ</i> = 2.20 mm <sup>-1</sup>
<i>c</i> = 9.4840 (8) Å	<i>T</i> = 295 (2) K
<i>β</i> = 106.830 (6)°	Prism, yellow
<i>V</i> = 654.26 (10) Å <sup>3</sup>	0.25 × 0.20 × 0.15 mm
<i>Z</i> = 2	

*Data collection*

Rigaku R-AXIS RAPID diffractometer	2976 independent reflections
<i>ω</i> scans	2950 reflections with <i>I</i> > 2σ( <i>I</i> )
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	<i>R<sub>int</sub></i> = 0.022
<i>T<sub>min</sub></i> = 0.582, <i>T<sub>max</sub></i> = 0.710	<i>θ<sub>max</sub></i> = 27.5°
12962 measured reflections	<i>h</i> = -9 → 9
	<i>k</i> = -13 → 13
	<i>l</i> = -12 → 12

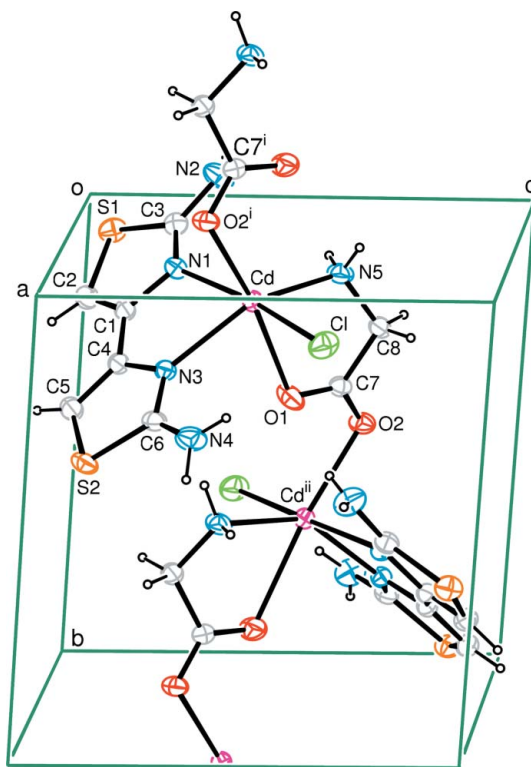
*Refinement*

Refinement on <i>F</i> <sup>2</sup>	<i>w</i> = 1/[σ <sup>2</sup> ( <i>F<sub>o</sub></i> <sup>2</sup> ) + (0.0182 <i>P</i> ) <sup>2</sup> + 0.0651 <i>P</i> ]
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )] = 0.014	where <i>P</i> = ( <i>F<sub>o</sub></i> <sup>2</sup> + 2 <i>F<sub>c</sub></i> <sup>2</sup> )/3
<i>wR</i> ( <i>F</i> <sup>2</sup> ) = 0.034	(Δ/σ) <sub>max</sub> = 0.002
<i>S</i> = 1.09	Δρ <sub>max</sub> = 0.22 e Å <sup>-3</sup>
2976 reflections	Δρ <sub>min</sub> = -0.38 e Å <sup>-3</sup>
172 parameters	Absolute structure: Flack (1983), with 1393 Friedel pairs
H-atom parameters constrained	Flack parameter: 0.010 (12)

**Table 1**  
Selected geometric parameters (Å, °).

Cd–Cl	2.5556 (5)	Cd–N5	2.2951 (17)
Cd–N1	2.3764 (12)	Cd–O1	2.5598 (16)
Cd–N3	2.3137 (15)	Cd–O2 <sup>i</sup>	2.3418 (13)
N1–Cd–N3	72.40 (6)	C2–S1–C3	89.67 (9)
N5–Cd–O1	69.55 (5)	C5–S2–C6	89.63 (9)

Symmetry code: (i) -*x* + 1, *y* - ½, -*z* + 1.



**Figure 1**  
A fragment of the polymeric chain in (I), showing 40% probability displacement ellipsoids (arbitrary spheres for H atoms). [Symmetry codes: (i) -*x* + 1, *y* - ½, -*z* + 1; (ii) -*x*, *y* + ½, -*z* + 1.]

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

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
N2–H2A···O1 <sup>i</sup>	0.88	2.49	3.340 (3)	164
N2–H2B···O2 <sup>ii</sup>	0.82	2.18	2.993 (3)	171
N4–H4A···Cl <sup>iii</sup>	0.88	2.47	3.288 (2)	155
N4–H4B···Cl	0.84	2.50	3.334 (2)	171
N5–H5A···Cl <sup>iv</sup>	0.91	2.81	3.579 (2)	142

Symmetry codes: (i) -*x* + 1, *y* - ½, -*z* + 1; (ii) -*x*, *y* - ½, -*z* + 1; (iii) -*x* + 2, *y* + ½, -*z* + 1; (iv) *x* - 1, *y*, *z*.

H atoms bonded to C atoms were placed in calculated positions, with C–H = 0.93 Å (aromatic) or 0.97 Å (methylene), and refined in riding mode, with *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C). Other H atoms were located in a difference map and refined as riding in their as-found relative positions, with *U*<sub>iso</sub>(H) = 1.5*U*<sub>eq</sub>(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).

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