

Aqua(2,2'-diamino-4,4'-bi-1,3-thiazole- $\kappa^2N,N'$ )-(thiodiacetato- $\kappa^3O,S,O'$ )cobalt(II) dihydrateBing-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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## Key indicators

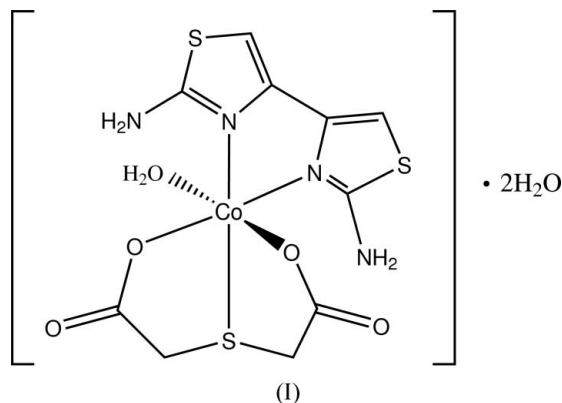
Single-crystal X-ray study  
 $T = 295$  K  
Mean  $\sigma(C-C) = 0.005$  Å  
 $R$  factor = 0.042  
 $wR$  factor = 0.102  
Data-to-parameter ratio = 13.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title  $\text{Co}^{\text{II}}$  complex,  $[\text{Co}(\text{C}_6\text{H}_6\text{N}_4\text{S}_2)(\text{C}_4\text{H}_4\text{O}_4\text{S})(\text{H}_2\text{O})] \cdot 2\text{H}_2\text{O}$ , assumes a distorted octahedral coordination geometry formed by a diaminobithiazole (DABT) ligand, a thiodiacetate dianion (TDA) and a water molecule. The TDA dianion chelates to the  $\text{Co}^{\text{II}}$  atom with a facial configuration. Within the chelating DABT ligand, the two thiazole rings are twisted with respect to each other [dihedral angle =  $12.04$  ( $9^\circ$ )].

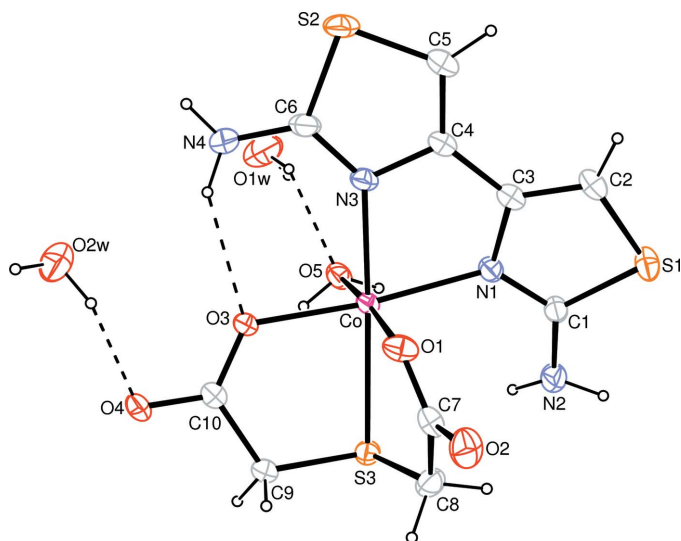
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## Comment

Transition metal complexes of diaminobithiazole (DABT) have shown potential application in some fields, such as the effective inhibitors of DNA synthesis of the tumor cells (Waring, 1981; Fisher *et al.*, 1985). As part of our ongoing investigation of metal complexes incorporating the DABT ligand (Liu *et al.*, 2001), the title  $\text{Co}^{\text{II}}$  compound, (I), was prepared and its X-ray crystal structure is reported here.



The molecular structure of (I) is shown in Fig. 1. The  $\text{Co}^{\text{II}}$  complex assumes a distorted octahedral coordination geometry formed by a DABT ligand, a thiodiacetate dianion (TDA) and a coordinated water molecule. The tridentate TDA dianion chelates to the  $\text{Co}^{\text{II}}$  atom with a facial configuration. Both chelating five-membered rings display envelope conformations, which is consistent with that found in an  $\text{Ni}^{\text{II}}$  complex with a chelating TDA ligand (Pan *et al.*, 2005). The DABT ligand chelates to the  $\text{Co}^{\text{II}}$  atom with an average  $\text{Co}-\text{N}$  bond distance of  $2.110$  (3) Å (Table 1), which is comparable to the value of  $2.097$  (3) Å found in a corresponding compound,  $[\text{Co}(\text{DABT})(\text{ODA})(\text{H}_2\text{O})]$  (ODA is oxydiacetate; Shen *et al.*, 2004). The two thiazole rings of the DABT ligand are twisted with respect to each other around the  $\text{C}3-\text{C}4$  bond, with a dihedral angle of  $12.04$  ( $9^\circ$ ). This conformation is also found in  $[\text{Cd}(\text{DABT})_2\text{Cl}_2]$  (Liu *et al.*, 2003), but it differs



**Figure 1**  
The molecular structure of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). Dashed lines indicate hydrogen bonding.

from the planar configuration of DABT found in [Cu(DABT)Cl<sub>2</sub>] (Liu *et al.*, 2001).

A partially overlapping arrangement of parallel thiazole rings related by an inversion centre is observed (Fig. 2). The face-to-face separation between the mean planes of the S1-thiazole and S1<sup>vi</sup>-thiazole rings is 3.558 (18) Å [symmetry code (vi):  $-x, 1 - y, 1 - z$ ], which is significantly shorter than the thickness of the aromatic ring (3.7 Å) and suggests the existence of  $\pi$ - $\pi$  stacking. There is extensive hydrogen bonding in the crystal structure of (I) (Table 2).

## Experimental

An aqueous solution (20 ml) containing DABT (0.20 g, 1 mmol) and CoCl<sub>2</sub>·6H<sub>2</sub>O (0.24 g, 1 mmol) was mixed with an aqueous solution (10 ml) of H<sub>2</sub>TDA (0.15 g, 1 mmol) and NaOH (0.08 g, 2 mmol). The mixture was refluxed for 5 h. The solution was cooled to room temperature and then filtered. Single crystals of (I) were obtained from the filtrate after 3 d.

### Crystal data

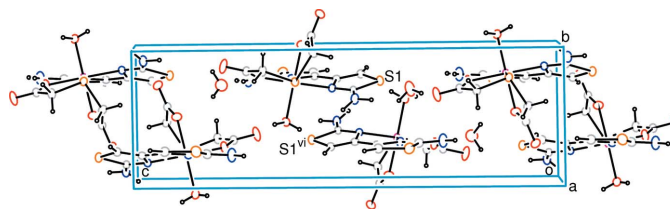
[Co(C<sub>6</sub>H<sub>6</sub>N<sub>4</sub>S<sub>2</sub>)(C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>S)·  
(H<sub>2</sub>O)]·2H<sub>2</sub>O  
*M<sub>r</sub>* = 459.38  
Monoclinic, *P*2<sub>1</sub>/*c*  
*a* = 10.6918 (11) Å  
*b* = 7.1329 (7) Å  
*c* = 22.794 (2) Å  
 $\beta$  = 102.538 (2)°  
*V* = 1696.9 (3) Å<sup>3</sup>  
*Z* = 4

*D<sub>x</sub>* = 1.798 Mg m<sup>-3</sup>  
Mo *K*α radiation  
Cell parameters from 6855  
reflections  
 $\theta$  = 3.0–24.0°  
 $\mu$  = 1.42 mm<sup>-1</sup>  
*T* = 295 (2) K  
Prism, pink  
0.30 × 0.20 × 0.15 mm

### Data collection

Rigaku R-Axis RAPID  
diffractometer  
 $\omega$  scans  
Absorption correction: multi-scan  
(*ABSCOR*; Higashi, 1995)  
*T<sub>min</sub>* = 0.665, *T<sub>max</sub>* = 0.802  
8649 measured reflections

3003 independent reflections  
2513 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.031  
 $\theta_{\max}$  = 25.0°  
*h* = -9 → 12  
*k* = -8 → 8  
*l* = -27 → 19



**Figure 2**  
A packing diagram for (I), showing  $\pi$ - $\pi$  stacking between the S1-thiazole and S1<sup>vi</sup>-thiazole rings [symmetry code: (vi)  $-x, 1 - y, 1 - z$ ]. H atoms have been omitted for clarity.

### Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.042  
*wR* (*F*<sup>2</sup>) = 0.102  
*S* = 1.04  
3003 reflections  
226 parameters  
H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0449P)^2 + 1.2046P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

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

$$\Delta\rho_{\max} = 0.32 \text{ e } \text{Å}^{-3}$$

$$\Delta\rho_{\min} = -0.38 \text{ e } \text{Å}^{-3}$$

**Table 1**

Selected bond lengths (Å).

Co—S3	2.5143 (10)	Co—O5	2.102 (2)
Co—O1	2.078 (2)	Co—N1	2.121 (3)
Co—O3	2.044 (2)	Co—N3	2.100 (3)

**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...O2W <sup>i</sup>	0.92	2.09	2.943 (4)	154
N2—H2B...O2 <sup>ii</sup>	0.92	2.41	3.168 (4)	140
N4—H4A...O3	0.89	2.23	3.003 (4)	144
N4—H4B...O1W <sup>iii</sup>	0.85	2.15	2.950 (5)	156
O5—H5A...O4 <sup>iv</sup>	0.83	1.85	2.656 (3)	165
O5—H5B...O2 <sup>ii</sup>	0.86	1.90	2.727 (3)	162
O1W—H1C...O5	0.88	2.15	2.879 (4)	141
O1W—H1D...O1 <sup>ii</sup>	0.94	2.46	3.330 (4)	154
O2W—H2C...S1 <sup>v</sup>	0.92	2.27	2.994 (3)	135
O2W—H2D...O3	0.89	2.48	3.249 (4)	145
O2W—H2D...O4	0.89	1.92	2.678 (4)	142

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

H atoms bonded to O and N atoms were located in a difference Fourier map and refined as riding on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O}, \text{N})$ . H atoms bonded to C atoms were placed in calculated positions with C—H = 0.97 (methylene) or 0.93 Å (aromatic), and were included in the final cycles of refinement in a riding mode, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSK, 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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