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## Key indicators

Single-crystal X-ray study

T = 295 K

Mean  $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$ 

R factor = 0.047

wR factor = 0.108

Data-to-parameter ratio = 18.6

For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Bis(2,2'-diamino-4,4'-bi-1,3-thiazole-  
N,N')(dichloro)cobalt(II) dihydrate

The crystal structure of the title compound,  $[\text{Co}(\text{C}_6\text{H}_6\text{N}_4\text{S}_2)_2\text{Cl}_2] \cdot 2\text{H}_2\text{O}$ , comprises an octahedral  $\text{Co}^{\text{II}}$  complex and water of crystallization. Two Cl atoms and two diaminobithiazole (DABT) ligands coordinate to the  $\text{Co}^{\text{II}}$  atom in a *cis* configuration. The overlapped arrangement and the short separation of 3.46 (2) Å between parallel DABT rings suggest the existence of  $\pi$ - $\pi$  stacking interactions. A short  $\text{S} \cdots \text{S}$  contact of 3.1822 (17) Å is observed between DABT ligands.

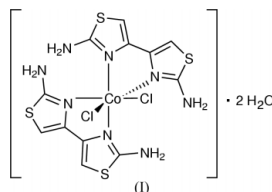
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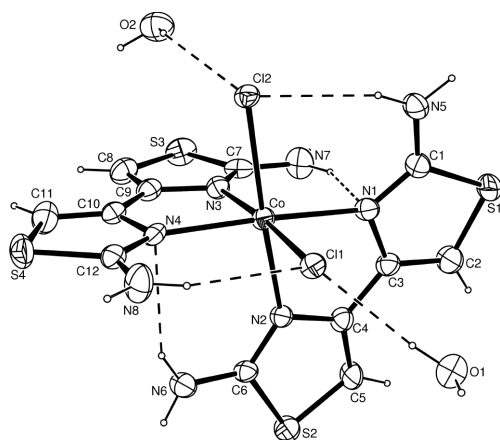
## Comment

Metal complexes with 2,2'-diamino-4,4'-bi-1,3-thiazole (DABT) have been shown to have potential applications in various fields. For example, a  $\text{Co}^{\text{II}}$  complex and a  $\text{Ni}^{\text{II}}$  complex with DABT have been found to be effective inhibitors of DNA synthesis of tumor cells (Waring, 1981; Fisher *et al.*, 1985). As part of a series of structural investigations of metal complexes with DABT, the title  $\text{Co}^{\text{II}}$  complex, (I), was prepared in our laboratory.

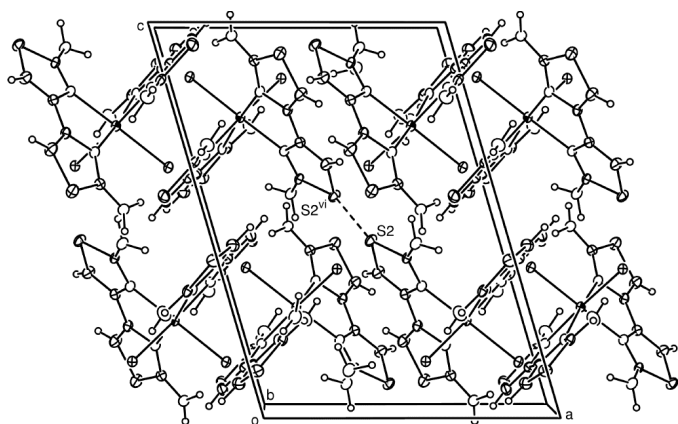


The molecular structure of (I) is shown in Fig. 1. While two Cl atoms are *cis* coordinated to the  $\text{Co}^{\text{II}}$  atom, two DABT ligands chelate to the  $\text{Co}^{\text{II}}$  atom to form a distorted octahedral coordination geometry (Table 1). The  $\text{Co}-\text{Cl1}$  distance of 2.4994 (11) and the  $\text{Co}-\text{Cl2}$  distance of 2.4998 (11) Å are similar to those [2.469 (3) and 2.499 (3) Å] found in  $\text{Co}(\text{DABT})_2\text{Cl}_2$  methanol solvate (Tian *et al.*, 1996). The distances between the amino-N and thiazole-C atoms, ranging from 1.327 (5) to 1.343 (5) Å, suggest electron delocalization between the thiazole rings and the amino groups, whereas the bond distances of 1.455 (5) and 1.457 (5) Å imply that both C3-C4 and C9-C10 are single bonds formed by  $sp^2$ -hybridized C atoms.

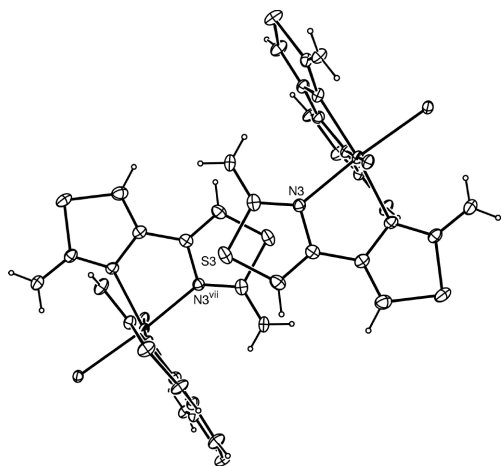
A hydrogen-bonding network occurs in the crystal. The amino groups are involved in intramolecular hydrogen bonds, both with coordinated thiazole-N atoms and with coordinated Cl atoms, as shown in Fig. 1. The amino groups are also hydrogen-bonded to water or to Cl atoms of neighboring molecules. Solvent water molecules play the roles of both donor and acceptor in the hydrogen-bonding network (Table 2).



**Figure 1**  
The molecular structure of (I), with 30% probability displacement ellipsoids. Dashed lines indicate hydrogen bonds.



**Figure 2**  
A molecular packing diagram. The dashed line indicates the short contact between S atoms [symmetry code: (vi)  $1 - x, 1 - y, 1 - z$ ].



**Figure 3**  
A view of the  $\pi$ - $\pi$  stacking between BADT rings [symmetry code: (vii)  $2 - x, 1 - y, 1 - z$ ].

A  $\pi$ - $\pi$  stacking interaction occurs in the crystal. The parallel arrangement of DABT rings is illustrated in Fig. 2. Bithiazole rings related by an inversion center overlap each other, as shown in Fig. 3. The separation between neighboring parallel thiazole rings is 3.46 (2) Å. A short contact of

3.1822 (17) Å is observed between atoms S2 and S2<sup>vi</sup> [symmetry code (vi):  $1 - x, 1 - y, 1 - z$ ] (Fig. 2).

## Experimental

Good quality crystals of DABT were obtained using the method of Erlenmeyer (1948). Crystals of the title complex were obtained by a solution diffusion method, using an H-shaped glass tube. Solutions of  $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$  and DABT were introduced into the two branches of the H tube. Pink single crystals of the title compound were obtained after 3 weeks.

### Crystal data

[ $\text{Co}(\text{C}_6\text{H}_6\text{N}_4\text{S}_2)_2\text{Cl}_2$ ] $\cdot 2\text{H}_2\text{O}$   
 $M_r = 562.44$   
 Monoclinic,  $P2_1/c$   
 $a = 10.8616$  (12) Å  
 $b = 13.6096$  (15) Å  
 $c = 15.0657$  (17) Å  
 $\beta = 106.282$  (12)°  
 $V = 2137.7$  (4) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.748$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 10880 reflections  
 $\theta = 2.5$ – $24.0^\circ$   
 $\mu = 1.47$  mm<sup>-1</sup>  
 $T = 295$  (2) K  
 Prism, pink  
 $0.28 \times 0.22 \times 0.18$  mm

### Data collection

Bruker SMART CCD diffractometer  
 $\omega$  and  $\varphi$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 1999)  
 $T_{\text{min}} = 0.660, T_{\text{max}} = 0.765$   
 13046 measured reflections

4872 independent reflections  
 2794 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.067$   
 $\theta_{\text{max}} = 27.5^\circ$   
 $h = -13 \rightarrow 14$   
 $k = -17 \rightarrow 10$   
 $l = -18 \rightarrow 19$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.047$   
 $wR(F^2) = 0.108$   
 $S = 0.86$   
 4872 reflections  
 262 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0453P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.88$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.78$  e Å<sup>-3</sup>

**Table 1**

Selected interatomic distances (Å).

Co–N4	2.128 (3)	Co–Cl2	2.4998 (11)
Co–N1	2.137 (3)	N5–C1	1.340 (5)
Co–N2	2.155 (3)	N6–C6	1.338 (5)
Co–N3	2.188 (3)	N7–C7	1.343 (5)
Co–Cl1	2.4994 (11)	N8–Cl2	1.327 (5)

**Table 2**

Hydrogen-bonding geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1–H1A $\cdots$ C11	0.96	2.27	3.228 (3)	172
O1–H1B $\cdots$ O2 <sup>i</sup>	0.95	1.96	2.823 (4)	150
O2–H2A $\cdots$ Cl2	0.86	2.43	3.153 (3)	142
N5–H5A $\cdots$ O1 <sup>ii</sup>	0.87	2.12	2.905 (4)	149
N5–H5B $\cdots$ Cl2	0.96	2.36	3.275 (3)	160
N6–H6A $\cdots$ Cl1 <sup>iii</sup>	0.94	2.52	3.364 (3)	150
N6–H6A $\cdots$ Cl2 <sup>iii</sup>	0.94	2.78	3.419 (3)	126
N6–H6B $\cdots$ N4	0.90	2.30	3.137 (5)	155
N7–H7A $\cdots$ Cl2 <sup>iv</sup>	0.97	2.45	3.386 (4)	164
N7–H7B $\cdots$ N1	0.96	2.41	3.217 (5)	141
N8–H8A $\cdots$ O2 <sup>v</sup>	0.90	2.09	2.972 (5)	169
N8–H8B $\cdots$ Cl1	0.90	2.29	3.142 (4)	157

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

H atoms on water and amino groups were located in a difference Fourier map and were included in the structure-factors calculation with fixed positional parameters and  $U_{\text{iso}}$  of  $0.05 \text{ \AA}^2$ . Other H atoms were placed in calculated positions, with C—H =  $0.93 \text{ \AA}$  and N—H =  $0.86 \text{ \AA}$ , and included in the final cycles of refinement using a riding model, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$  of the parent atoms.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; 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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