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## Key indicators

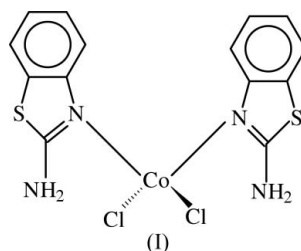
Single-crystal X-ray study  
 $T = 296$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.028  
 $wR$  factor = 0.073  
Data-to-parameter ratio = 16.2For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Bis(2-aminobenzothiazole- $\kappa N$ )dichlorocobalt(II)

In the title compound,  $[\text{CoCl}_2(\text{C}_7\text{H}_6\text{N}_2\text{S})_2]$ , the Co atom has a slightly distorted tetrahedral coordination geometry, involving two Cl atoms and two N atoms from the thiazole unit [ $\text{Co}-\text{Cl} = 2.2435$  (8) and  $2.2476$  (8) Å, and  $\text{Co}-\text{N} = 2.0252$  (18) and  $2.0308$  (17) Å]. The interplanar angle between the two benzothiazole groups is  $76.44$  (4)°. The amino groups, acting as donor, participate in intra- and intermolecular  $\text{N}-\text{H}\cdots\text{Cl}$  hydrogen bonds, with  $\text{N}\cdots\text{Cl}$  distances in the range  $3.244$  (2)– $3.302$  (2) Å. There are also intermolecular  $\pi-\pi$ ,  $\text{N}-\text{H}\cdots\pi$  and  $\text{C}-\text{H}\cdots\pi$  interactions in the crystal structure.

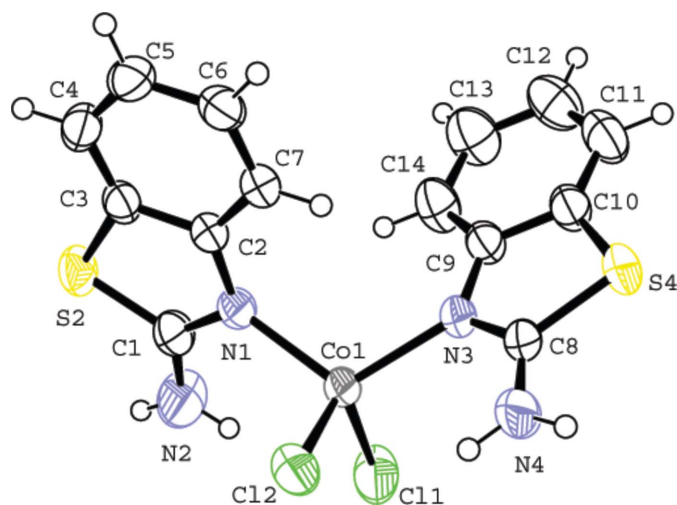
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## Comment

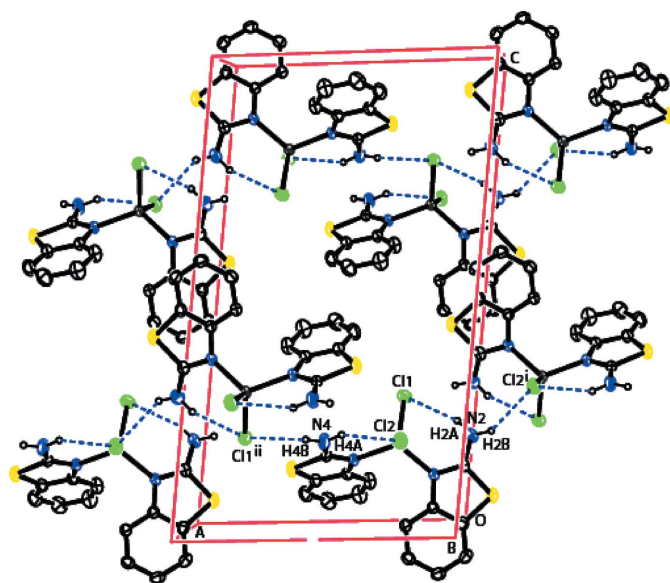
Small and simple heterocyclic structures often exhibit complex biological properties. Substituted benzothiazoles show anti-tumour (Goldfarb *et al.*, 1999), anti-infective and antifungal (Sener *et al.*, 2000), and antihelmintic activities (Nadkarn *et al.*, 2000). Bis(benzothiazole) compounds have been studied as potential mimics for metalloproteins (Thompson *et al.*, 1982), and it is well known that N and S atoms play a key role in the coordination of metals at the active sites of numerous metallobiomolecules (Karlin & Zubieta, 1983). The structures of many metal complexes of 2-amino-1,3-thiazole derivatives, in which the metal is directly bound to the ligand, are known; these complexes include most of the first-row transition metals (*i.e.* Mn–Zn). In all but a few cases, the thiazole units bind to the metal *via* endocyclic N atoms (Lynch & Duckhouse, 2001; Usman *et al.*, 2003). We report here the X-ray crystal structure of the title compound, (I).



In the structure of (I), the tetrahedral Co coordination environment is built up of two  $\text{Cl}^-$  ligands and the amino N atoms of two neutral monodentate 2- $\text{NH}_2$ -bta ligands (Fig. 1). This  $\text{CoCl}_2\text{N}_2$  coordination forms a slightly distorted tetrahedral geometry, the angles around the Co atom ranging from  $104.70$  (6) to  $113.90$  (7)°; the two benzothiazole ligands form a dihedral angle of  $76.44$  (4)°. This compares well with the value of  $77.86$  (3)° reported for other benzothiazole units (Batı *et al.*, 2005). It is noteworthy that the two amino groups are not both located on the same side because of steric hindrance. Each

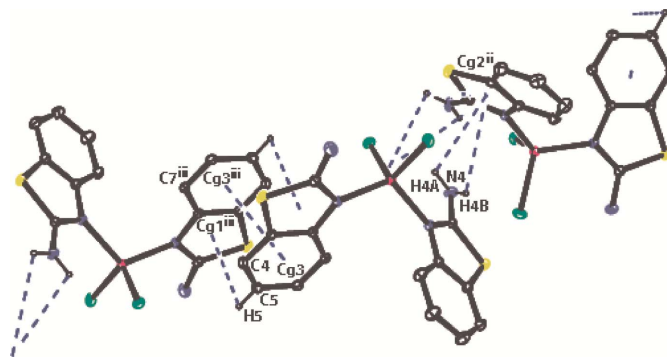


**Figure 1**  
The asymmetric unit of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.



**Figure 2**  
The crystal structure of (I). H atoms have been omitted unless involved in hydrogen bonds (dashed lines). [Symmetry codes: (i)  $-x, -\frac{1}{2} + y, \frac{1}{2} - z$ ; (ii)  $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$ ]

benzothiazole ligand is planar; the angles between the mean planes through the five- and six-membered rings of each ligand being  $1.14 (9)^\circ$  and  $0.21 (14)^\circ$ . The  $\text{CoCl}_2$  unit is preserved within the complex [ $\text{Co}-\text{Cl1} = 2.2435 (8)$  and  $\text{Co}-\text{Cl2} = 2.2476 (8) \text{ \AA}$ ], accompanied by a  $\text{Cl1}-\text{Co1}-\text{Cl2}$  angle of  $112.23 (3)^\circ$ . In the paper of Prabakaran *et al.*, 2001, the corresponding  $\text{Co}-\text{Cl}$  bond distances are slightly longer [ $2.2917 (14)$  and  $2.2760 (13) \text{ \AA}$ ] and the  $\text{Cl}-\text{Co}-\text{Cl}$  bond angle is larger [ $117.15 (5)^\circ$ ]. The bond lengths and angles in (I) are shown in Table 1. The  $\text{C1}-\text{N1}$ ,  $\text{C1}-\text{N2}$ ,  $\text{C8}-\text{N3}$  and  $\text{C8}-\text{N4}$  bonds are somewhat shorter than the  $\text{C2}-\text{N1}$  and  $\text{C9}-\text{N3}$  bonds, as a result of pronounced delocalization in the  $-\text{N}=\text{C}=\text{N}-$  fragment of the 2-aminobenzothiazole ring.



**Figure 3**  
The crystal structure of (I). H atoms have been omitted unless involved in  $\pi-\pi$ ,  $\text{N}-\text{H}\cdots\pi$  and  $\text{C}-\text{H}\cdots\pi$  interactions. (dashed lines). [Symmetry codes: (ii)  $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$ ; (iii)  $-x, 2 - y, -z$ ]

As shown in Table 2 and Fig. 2, the crystal structure of (I) is stabilized by  $\text{N}-\text{H}\cdots\text{Cl}$  hydrogen bonds. The amino groups of both thiazole ligands are hydrogen-bonded to the Cl atom by intramolecular  $\text{N2}-\text{H2A}\cdots\text{Cl1}$  and  $\text{N4}-\text{H4A}\cdots\text{Cl2}$  hydrogen bonds. In the crystal structure, the amino groups also act as donors, forming  $\text{N2}-\text{H2B}\cdots\text{Cl2}^{\text{i}}$  and  $\text{N4}-\text{H4B}\cdots\text{Cl1}^{\text{ii}}$  hydrogen bonds to atoms Cl2 and Cl1, respectively (Table 2).  $\text{N4}-\text{H4B}\cdots\text{Cl1}$  hydrogen bonds interconnect the molecules into chains along the  $a$ -axis direction; these are further interconnected into a three dimensional network by  $\text{N2}-\text{H2B}\cdots\text{Cl2}$  hydrogen bonds (Fig. 2).

In the crystal structure of complex (I), there is an intermolecular  $\pi-\pi$  interaction between the phenyl rings of the benzothiazole ligands. The phenyl rings are oriented in such a way that the perpendicular distance from the (C2-C7) ring (centroid  $\text{Cg3}$ ) to the  $\text{Cg3}^{\text{iii}}$  ring is  $3.403 \text{ \AA}$ , the closest distance being  $\text{C4}\cdots\text{C7}^{\text{iii}} = 3.578 \text{ \AA}$ . The distance between the ring centroids is  $3.5849 (13) \text{ \AA}$  (symmetry code:  $-x, 2 - y, -z$ ) (Fig. 3). There are also  $\text{N}-\text{H}\cdots\pi$  and  $\text{C}-\text{H}\cdots\pi$  interactions between rings (S4/C8/N3/C9/C10) (centroid  $\text{Cg2}$ ) and (S2/C1/N1/C2/C3) (centroid  $\text{Cg1}$ ) and atoms H4A/H4B(N4) of the amino group and atom H5(C5) of the phenyl ring of benzothiazole ligand have the following geometric parameters: (i) the distance between atoms H4A and H4B bonded to atom N4 and the ring centroid  $\text{Cg2}^{\text{ii}}$  are  $3.194$  and  $3.346 \text{ \AA}$ , respectively, [symmetry code: (ii)  $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$ ] and the  $\text{N4}-\text{H4A}/\text{H4B}\cdots\text{Cg2}^{\text{ii}}$  angles are  $105.7$  and  $94.9^\circ$ , respectively; the distance between atom H5 bonded to atom C5 and the ring centroid  $\text{Cg1}^{\text{iii}}$  is  $3.389 \text{ \AA}$  [symmetry code: (iii)  $-x, 2 - y, -z$ ] and the  $\text{C5}-\text{H5}\cdots\text{Cg1}^{\text{iii}}$  angle is  $90.2^\circ$  (Fig. 3).

## Experimental

An ethanol solution of 2-aminobenzothiazole (4 mmol in 10 ml of ethanol) was added dropwise to  $\text{CoCl}_2\cdot 6\text{H}_2\text{O}$  (2 mmol in 5 ml of ethanol) with stirring. The colour of the solution immediately changed to blue. The mixture was then refluxed for 2 h and the resulting solution was left to stand at room temperature. After several days, blue crystals were obtained and dried under vacuum.

## Crystal data

[CoCl<sub>2</sub>(C<sub>7</sub>H<sub>6</sub>N<sub>2</sub>S)<sub>2</sub>] $M_r = 430.23$ Monoclinic,  $P2_1/c$  $a = 11.7144$  (9) Å $b = 7.3595$  (4) Å $c = 20.0240$  (15) Å $\beta = 96.454$  (6)° $V = 1715.4$  (2) Å<sup>3</sup> $Z = 4$  $D_x = 1.666$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation $\mu = 1.56$  mm<sup>-1</sup> $T = 296$  K

Prism, blue

 $0.56 \times 0.52 \times 0.47$  mm

## Data collection

STOE IPDS 2 diffractometer

 $\omega$  scans

Absorption correction: integration

 $(X-RED32; \text{Stoe \& Cie, 2002})$  $T_{\min} = 0.474, T_{\max} = 0.561$ 

21789 measured reflections

3361 independent reflections

2700 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.052$  $\theta_{\text{max}} = 26.0^\circ$ 

## Refinement

Refinement on  $F^2$  $R[F^2 > 2\sigma(F^2)] = 0.028$  $wR(F^2) = 0.073$  $S = 1.01$ 

3361 reflections

208 parameters

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0395P)^2 + 0.3849P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\text{max}} = 0.004$  $\Delta\rho_{\text{max}} = 0.45$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.31$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

Co1—N1	2.0252 (18)	N1—C1	1.323 (3)
Co1—N3	2.0308 (17)	N1—C2	1.397 (3)
Co1—Cl1	2.2435 (8)	N2—C1	1.322 (3)
Co1—Cl2	2.2476 (8)	N3—C8	1.325 (3)
S2—C1	1.737 (2)	N3—C9	1.398 (3)
S4—C8	1.743 (2)	N4—C8	1.315 (3)
N1—Co1—N3	113.90 (7)	C1—N1—Co1	124.43 (16)
N1—Co1—Cl1	110.36 (6)	C2—N1—Co1	122.23 (13)
N3—Co1—Cl1	106.25 (6)	C8—N3—Co1	124.69 (16)
N1—Co1—Cl2	104.70 (6)	C9—N3—Co1	123.90 (14)
N3—Co1—Cl2	109.53 (6)	N2—C1—N1	124.0 (2)
Cl1—Co1—Cl2	112.23 (3)	N4—C8—N3	125.1 (2)
N3—Co1—N1—C1	151.45 (19)	Cl2—Co1—N3—C8	27.3 (2)
Cl1—Co1—N1—C1	32.0 (2)	Co1—N1—C1—N2	-18.6 (4)
Cl2—Co1—N1—C1	-88.9 (2)	Co1—N3—C8—N4	-3.6 (4)
Cl1—Co1—N3—C8	-94.10 (19)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2B $\cdots$ Cl2 <sup>i</sup>	0.86	2.58	3.301 (2)	142
N2—H2A $\cdots$ Cl1	0.86	2.43	3.247 (2)	158
N4—H4B $\cdots$ Cl1 <sup>ii</sup>	0.86	2.48	3.302 (2)	160
N4—H4A $\cdots$ Cl2	0.86	2.47	3.244 (2)	151

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

All H atoms were placed in idealized positions, with C—H = 0.93–0.98 Å, N—H = 0.86 Å, and then treated as riding atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$ .

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); 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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