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2,2′-Diamino-4,4′-bi-1,3-thiazolium dichloride

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Key indicators

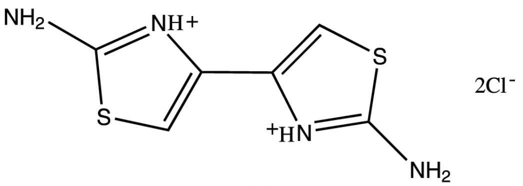
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.058
wR factor = 0.180
Data-to-parameter ratio = 13.6

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

The title compound, $C_6H_8N_4S_2^{2+}\cdot 2Cl^-$, includes a *trans,* planar bithiazole moiety occupying a special position on a crystallographic inversion centre. Both symmetry-independent N atoms participate in hydrogen-bonded links with the chloride anion [N···Cl 3.094 (5), 3.222 (5) and 3.362 (5) Å]. A short contact of 3.3201 (18) Å is also observed between the S atom of the thiazolium cation and the chloride anion.

Comment

Transition-metal complexes with 2,2′-diamino-4,4′-bithiazole (DABT) or its derivatives have shown interesting properties and promise potential applications in a number of fields (Waring, 1981; Fisher *et al.*, 1985; Sun *et al.*, 1997). A series of metal complexes, with DABT chelating to the metal atom, have recently been prepared in this laboratory and crystal structure determinations have been reported for several of them (Liu *et al.*, 2001). We present here the structure of DABT chloride, (I), thereby allowing comparison of the DABT structures in metal complexes and in the free state.



(I)

The molecular structure of (I) and a fragment of the crystal packing are shown in Fig. 1. The centrosymmetric molecule displays a *trans* structure, which differs from the *cis* configuration found in metal complexes. The two thiazole rings are coplanar, the maximum atomic deviation being 0.016 (3) Å (N3). The structure is also different from the twisted structure found in the metal complexes (Liu *et al.*, 2001).

The N—H groups of the heterocyclic protonated atom N3, as well as the N6 amino atom, are engaged in hydrogen bonds with the chloride anion (Table 1). The rather short Cl···S1^{ii} [symmetry code: (ii) $1+x$, $\frac{1}{2}-y$, $-\frac{1}{2}+z$] contact of 3.3201 (18) Å is also noteworthy. This contact is significantly shorter than the sum of the van der Waals radii (3.55 Å; Rodgers, 1994); it is comparable, however, with the S···Cl contact of 3.3175 (15) Å found in bis(2-amino-4-methylthiazolium) tetrachlorocopper (Fernández *et al.*, 1996).

Experimental

DABT was prepared according to the literature procedure of Erlenmeyer (1948). The title compound was obtained from an aqueous solution as a by-product in the course of the synthesis of an Ni^{II} complex with DABT, using $NiCl_2$ as a starting reagent.

Crystal data

$C_6H_8N_4S_2^{2+}\cdot 2Cl^-$
$M_r = 271.18$
Monoclinic, $P2_1/c$
$a = 4.8211$ (8) Å
$b = 9.2441$ (14) Å
$c = 12.0228$ (10) Å
$\beta = 98.224$ (12)°
$V = 530.31$ (13) Å^3
$Z = 2$

$D_x = 1.698$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 22 reflections
$\theta = 7.6$–$12.6°$
$\mu = 0.97$ mm^{-1}
$T = 298$ (2) K
Prism, orange
0.50 × 0.26 × 0.18 mm

Data collection

Rigaku AFC-7*S* diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.616$, $T_{max} = 0.840$
1163 measured reflections
1037 independent reflections
886 reflections with $I > 2\sigma(I)$

$R_{int} = 0.049$
$\theta_{max} = 26.0°$
$h = 0 \rightarrow 5$
$k = 0 \rightarrow 11$
$l = -14 \rightarrow 14$
3 standard reflections every 150 reflections intensity decay: 0.3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.180$
$S = 1.12$
1037 reflections
76 parameters
Only coordinates of H atoms refined

$w = 1/[\sigma^2(F_o^2) + (0.0944P)^2 + 1.6P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.86$ e Å^{-3}
$\Delta\rho_{min} = -0.83$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C2	1.718 (5)	N3—C4	1.393 (6)
S1—C5	1.733 (5)	C4—C5	1.347 (7)
C2—N3	1.337 (6)	C4—C4^i	1.446 (10)
C2—N6	1.317 (7)		
C2—S1—C5	90.1 (2)	C5—C4—N3	112.3 (5)
N6—C2—N3	122.5 (5)	C5—C4—C4^i	128.7 (6)
N6—C2—S1	125.5 (4)	N3—C4—C4^i	119.1 (5)
N3—C2—S1	111.9 (4)	C4—C5—S1	111.9 (4)
C2—N3—C4	113.8 (4)		

Symmetry code: (i) $1 - x, -y, 1 - z$.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···Cl	1.03 (8)	2.10 (8)	3.094 (5)	159 (6)
N6—H6*A*···Cl^i	0.94 (8)	2.40 (8)	3.222 (5)	146 (7)
N6—H6*B*···Cl	0.97 (8)	2.50 (8)	3.362 (5)	148 (7)

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

H atoms were located in a difference Fourier map and refined isotropically with a fixed displacement parameter of 0.08 Å^2, N—H = 0.95–1.03 Å and C5—H5 = 1.10 (8) Å.

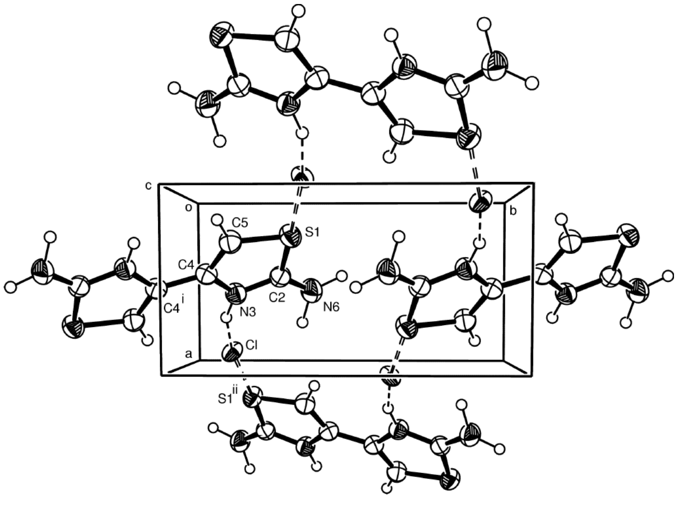


Figure 1
The molecular packing of (I) in the unit cell, shown with 30% probability displacement ellipsoids for non-H atoms. The dashed lines show the hydrogen bonds while the double dashed lines show the short contact between Cl and S atoms. [Symmetry codes: (i) $1 - x, -y, 1 - z$; (ii) $1 + x, \frac{1}{2} - y, -\frac{1}{2} + z$.]

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1985); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994).

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