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2,2′-Diamino-4,4′-bi-1,3-thiazole

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The centrosymmetric molecule of the title compound, $C_6H_6N_4S_2$ (DABT), displays a *trans* planar configuration, except that the amino groups are inclined slightly to the bithiazole plane. The N—C bond distance of 1.309 (2) Å within the thiazole ring is shorter than in DABT chloride [1.335 (6) Å] and in a DABT–metal complex [1.322 (3) Å]. The separation of 3.717 (3) Å between parallel bithiazole rings of neighboring molecules indicates a normal van der Waals contact.

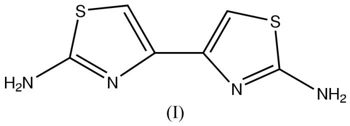
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.002 Å
R factor = 0.033
wR factor = 0.084
Data-to-parameter ratio = 16.0

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

Comment

Transition metal complexes with 2,2′-diamino-4,4′-bithiazole (DABT) or its derivatives have shown interesting properties and potential application in many fields (Waring, 1981; Fisher *et al.*, 1985). The structures of several complexes have been determined in order to understand the relationship between their properties and structures (Tian *et al.*, 1996; Liu *et al.*, 2001). The crystal structure of the title compound, (I), is reported here, to enable comparison of the structures of DABT in metal complexes and the uncomplexed state.



(I)

The structure of (I) is shown in Fig. 1. The centrosymmetric molecule displays a *trans* configuration, but the amino groups are inclined slightly to the bithiazole plane, with a dihedral angle of 14.8 (3)°. The *trans* configuration is different from the *cis* configuration found in DABT–metal complexes (Tian *et al.*, 1996; Liu *et al.*, 2001), but agrees with that found in 2,2′-diamino-4,4′-1,3-thiazolium dichloride (Liu *et al.*, 2002). The N3—C2 distance of 1.309 (2) Å within the thiazole ring is shorter than in the dichloride [1.335 (6) Å] and in the DABT–Cu^{II} complex [1.322 (3) Å]. The N6—C2 bond distance of 1.354 (2) Å suggests there is electron delocalization between the thiazole ring and the amino group.

Bithiazole rings of neighboring molecules, related by an inversion center, overlap each other with a normal van der Waals contact of 3.717 (3) Å. Intermolecular hydrogen bonding is observed between the amino group and the N3 atom of a neighboring molecule, the N···N separation and N—H···N angle being 3.187 (3) Å and 156°, respectively.

Experimental

Fine crystals of DABT were obtained by the method of Erlenmeyer (1948). Single crystals of (I) were obtained as a by-product from an aqueous solution during the preparation of a DABT–Mn(II) complex.

Crystal data

$C_6H_6N_4S_2$
$M_r = 198.27$
Monoclinic, $P2_1/n$
$a = 5.151$ (2) Å
$b = 11.468$ (3) Å
$c = 6.555$ (3) Å
$\beta = 92.71$ (1)°
$V = 386.8$ (3) Å^3
$Z = 2$

$D_x = 1.702$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2358 reflections
$\theta = 4.3$–27.2°
$\mu = 0.63$ mm^{-1}
$T = 150$ (1) K
Prism, colorless
0.25 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
$T_{\min} = 0.855$, $T_{\max} = 0.904$
2404 measured reflections

881 independent reflections
792 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.036$
$\theta_{\max} = 27.5°$
$h = -6 \rightarrow 6$
$k = -14 \rightarrow 14$
$l = -8 \rightarrow 7$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.084$
$S = 1.10$
881 reflections
55 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0471P)^2 + 0.1354P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.003$
$\Delta\rho_{\max} = 0.40$ e Å^{-3}
$\Delta\rho_{\min} = -0.31$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C5	1.7255 (17)	N6—C2	1.354 (2)
S1—C2	1.7461 (17)	C4—C5	1.358 (2)
N3—C2	1.309 (2)	C4—C4$^{\rm i}$	1.462 (3)
N3—C4	1.3988 (19)		

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

H atoms were located in a difference Fourier map and were included in the final cycles of refinement, with fixed positional parameters and $U_{\rm iso} = 0.08$ Å^2.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SIR*-92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

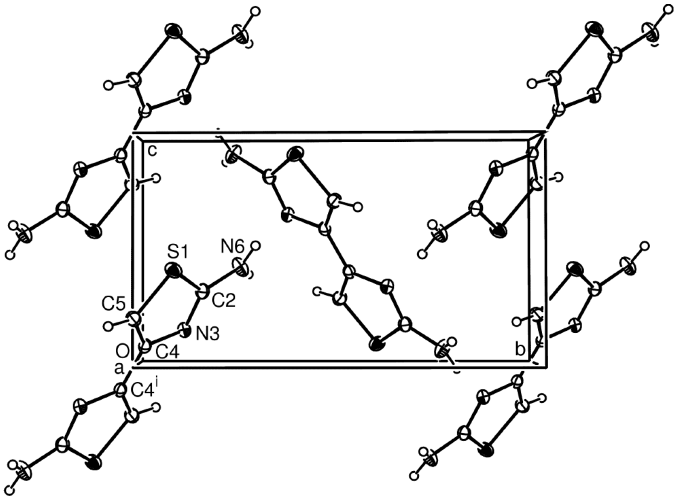


Figure 1
A packing diagram of (I), with 50% probability displacement ellipsoids.

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