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N-(1,3-Benzothiazol-2-yl)-4-(dimethylamino)-benzylamine

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.035
wR factor = 0.076
Data-to-parameter ratio = 12.8

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

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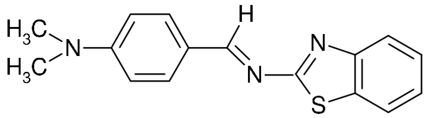
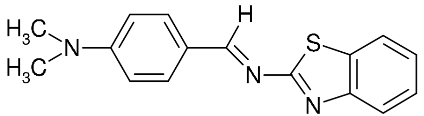
The title compound, $C_{16}H_{15}N_3S$, crystallizes with Z = 8 in space group $P2_1/c$. The two crystallographically independent molecules, *A* and *B*, are rotational isomers around the C—N bond joining the benzothiazole and dimethylaminoaryl moieties. Molecules *A* and *B* have different intramolecular hydrogen bonds: C—H···N for molecule *A* and C—H···S for molecule *B*. For both molecules, intermolecular C—H···π interactions are found between molecular pairs related by a centre of symmetry. The molecular packing is stabilized by C—H···π and π–π intermolecular interactions.

Comment

Most Schiff bases have antibacterial, anticancer, *anti*-inflammatory and antitoxic activities (Williams, 1972), and the sulfur-containing Schiff bases are particularly effective. Benzothiazolium groups have been used in organic dyes as either electron-withdrawing or electron-donating substituents, depending on whether the N atom is cationic or not (Zollinger, 1991). A number of thiazolyl- and benzothiazolylguanidines have been reported to exhibit antitubercular, antimalarial, central-nervous-system depressant, analgesic and antimicrobial activity against both Gram-positive and Gram-negative bacteria (Lakhan *et al.*, 2000).



Molecule A



Molecule B

(I)

Molecules *A* and *B* have the *E* configuration at the central C═N bond (Fig. 1). Rotational isomers *A* and *B* occur in the crystal structure as a result of a rotation around the C—N bond joining the benzothiazole and dimethylaminoaryl moieties. Selected geometric parameters are listed in Table 1. An intramolecular hydrogen bond is formed in each isomer: C—H···N type in isomer *A* and C—H···S type in isomer *B* (Table 2). For isomer *A*, the dihedral angle between the mean planes formed by the benzothiazole ring (C1–C6/S1/C7/N1) and the aryl group (C9–C14/N3/C15/C16) is 19.05 (9)°. The corresponding dihedral angle in isomer *B* is 13.84 (9)°.

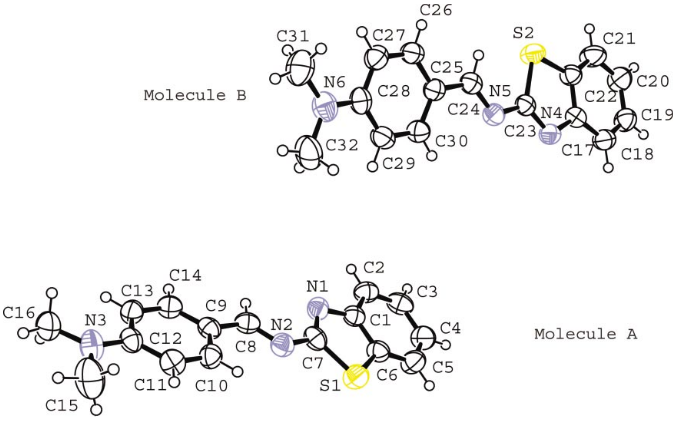


Figure 1
A view of the asymmetric unit of (I), showing the atom-numbering scheme and 50% probability displacement ellipsoids.

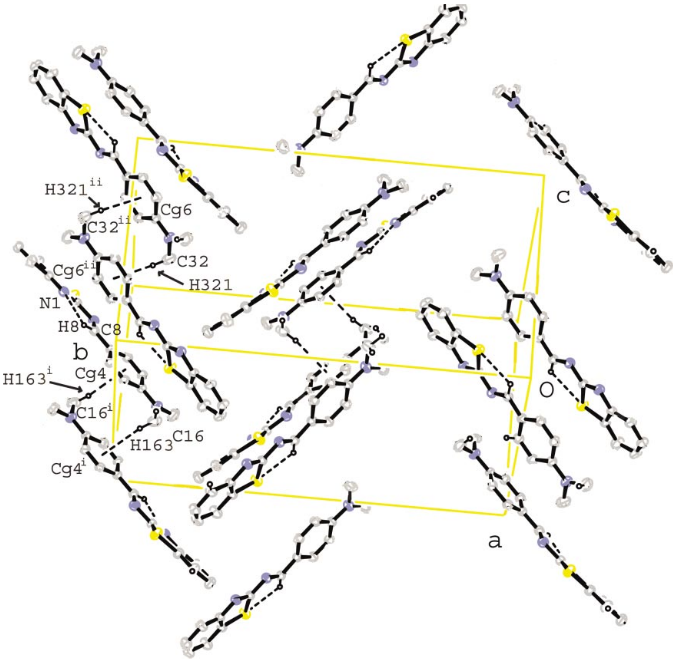


Figure 2
A diagram showing the intramolecular hydrogen bonds and C—H$\cdots\pi$-ring interactions as dashed lines. Displacement ellipsoids are drawn at the 30% probability level. *Cg*4 indicates the centre of gravity of the six-membered aryl ring of isomer *A* and *Cg*6 the corresponding centre of gravity for isomer *B*. [Symmetry codes: (i) $1 - x, -y, -z$; (ii) $-x, -y, 1 - z$.]

The dihedral angle is 42.70 (4)° between the mean molecular planes which are constituted by the non-H atoms of isomers *A* and *B*, respectively. In both isomers, intermolecular H$\cdots\pi$-ring interactions are observed between dimethylaminoaryl moieties related by a centre of symmetry (Fig. 2). Similar C—H$\cdots\pi$ interactions are found in a thiazole derivative having a short H$\cdots$*Cg* distance of 2.93 Å (Barbarín *et al.*, 2003). Although the title compound has been described (Guo *et al.*, 2002), no previous crystal structure determination is available.

There are many weak intermolecular π–π interactions between the aryl and benzothiazole rings. Dipole–dipole and van der Waals interactions are also effective in the molecular packing in the crystal structure.

Experimental

A solution of 2-aminobenzothiazole (5 mmol) in *n*-butanol (20 ml) was added dropwise to a hot solution of 4-(*N*,*N*-dimethylamino)-benzaldehyde (5 mmol) in *n*-butanol (30 ml). The mixture was refluxed for 2 h. Then solution was reduced to half-volume (25 ml) by evaporation and allowed to cool. The precipitated product was filtered off and recrystallized from absolute ethanol. UV/vis (DMSO): λ_{max} (log ε) = 341 nm. IR (KBr, cm^{-1}): ν(C═N, azomethine) 1610 (s), ν(C═N, thiazole) 1577 (*s*), ν(C—S—C) 671 (*m*). ^{1}H NMR (d_6–DMSO, 200 MHz, p.p.m.): 8.99 (*s*, C—H), 7.99–6.80 (*m*, 8H), 3.06 (*s*, 6H). Analysis found: C 68.44, H 5.09, N 14.53%; calculated for $C_{16}H_{15}N_3S$: C 68.33, H 5.34, N 14.95%.

Crystal data

$C_{16}H_{15}N_3S$
M_r = 281.37
Monoclinic, $P2_1/c$
a = 11.7771 (8) Å
b = 22.6876 (12) Å
c = 11.7725 (9) Å
β = 116.822 (5)°
V = 2807.1 (3) Å^3
Z = 8

D_x = 1.332 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 14170 reflections
θ = 1.8–27.1°
μ = 0.22 mm^{-1}
T = 293 (2) K
Plate, orange
0.66 × 0.37 × 0.11 mm

Data collection

Stoe IPDS-2 diffractometer
φ and ω scans
Absorption correction: by integration (*X-RED*32; Stoe & Cie, 2002)
T_{min} = 0.899, T_{max} = 0.979
17 481 measured reflections

4662 independent reflections
2653 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 25.0°
$h = -14 \rightarrow 13$
$k = -26 \rightarrow 26$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.076
S = 0.81
4662 reflections
365 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0358P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.010
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.400 (3)	C17—N4	1.391 (3)
C6—S1	1.729 (2)	C22—S2	1.733 (2)
C7—N1	1.305 (3)	C23—N4	1.299 (2)
C7—N2	1.399 (3)	C23—N5	1.376 (3)
C7—S1	1.726 (2)	C23—S2	1.771 (2)
C8—N2	1.269 (2)	C24—N5	1.291 (2)
C8—C9	1.452 (3)	C24—C25	1.432 (3)
N1—C7—N2	128.7 (2)	C8—N2—C7	117.8 (2)
N2—C7—S1	114.13 (17)	C24—N5—C23	119.38 (19)
N4—C23—N5	121.8 (2)	C7—S1—C6	89.02 (11)
N5—C23—S2	122.99 (16)	C22—S2—C23	88.76 (11)
C9—C8—N2—C7	178.4 (2)	C25—C24—N5—C23	175.93 (18)
N1—C7—N2—C8	11.5 (4)	N4—C23—N5—C24	175.59 (19)
S1—C7—N2—C8	−167.18 (16)	S2—C23—N5—C24	−7.5 (3)

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

$D-\mathrm{H}\cdots A$	$D-\mathrm{H}$	$\mathrm{H}\cdots A$	$D\cdots A$	$D-\mathrm{H}\cdots A$
C8—H8···N1	0.93	2.48	2.818 (3)	102
C24—H24···S2	0.93	2.53	3.000 (2)	112

All H atoms were placed in calculated positions (C—H = 0.93–0.96 Å) and refined using a riding model. Their U_{iso} values were constrained to be 1.2 (1.5 for methyl groups) times U_{eq} of the carrier atom.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); 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* publication routines (Farrugia, 1999).

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