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4-(Benzo[*d*]thiazol-2-yl)-*N*,*N*-dimethylaniline

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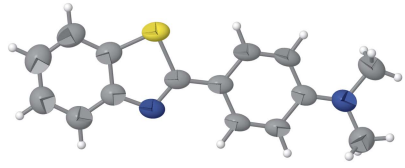
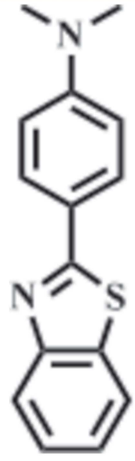
Structural data: full structural data are available from iucrdata.iucr.org

The whole molecule of the title compound, $C_{15}H_{14}N_2S$, is approximately planar, with an r.m.s. deviation of 0.0382 Å from the best-fit mean plane through all 18 non-H atoms. In the crystal, dimers form through π–π stacking interactions between the benzene rings of adjacent benzothiazole ring systems, with a centroid–centroid separation of 3.6834 (16) Å.

3D view



Chemical scheme



Structure description

Benzothiazole is an important bicyclic ring system that is present in a variety of materials with biological applications (Prajapati *et al.*, 2014). Water solubility and biocompatibility can be tuned in such systems by introducing different substituent groups on the benzothiazole ring system (Li *et al.*, 2015). Also, because of their unique photophysical properties, solid-state emitters based on benzothiazole have been attracting considerable interest over the past few years in the field of optoelectronic devices (Padalkar *et al.*, 2016). A series of benzothiazole derivatives have also been used recently recently both as fluorescent probes for anions and as bioactive molecules in living cells (Li *et al.*, 2015; Zhang *et al.*, 2015; Qian *et al.*, 2016). In order to better understand the structure-property relationships of benzothiazole derivatives, we have synthesized the title compound and its structure is reported here.

As shown in Fig. 1, the whole molecule is approximately planar, with an r.m.s. deviation of 0.0382 Å from the best-fit mean plane through all 18 non-H atoms. The benzothiazole ring system is inclined to the benzene ring by 4.59 (4)°. This planarity is reinforced by a weak intramolecular C13—H13···S1 contact (Table 1) that encloses an *S*(5) ring. The bond lengths in the structure are similar to those found in a closely related compound (Lynn *et al.*, 2012). In the crystal, dimers are formed through an offset π–π stacking interaction between two adjacent C1–C6 rings (Fig. 2) [$Cg2\cdots Cg2^{i}$ = 3.6834 (16) Å;

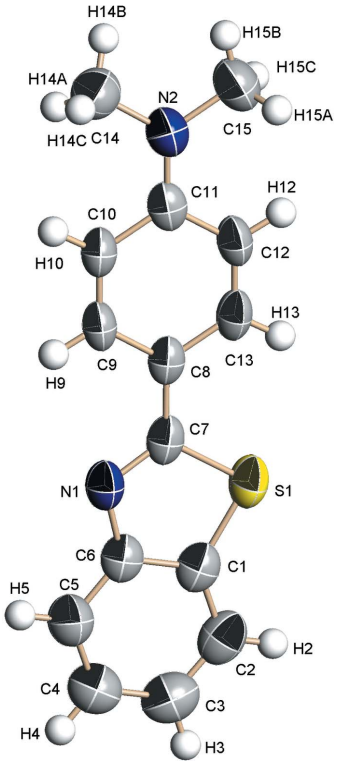


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

symmetry code: (i) $-x + 2, -y, -z + 1$]. No other significant contacts are found between the dimers.

Synthesis and crystallization

4-(Dimethylamino)benzaldehyde (2.98 g, 20 mmol) and 4-aminothiophenol (2.50 g, 20 mmol) were dissolved in 50 ml of ethyl alcohol and heated to reflux for 6 h. The reaction mixture was cooled to room temperature and filtered to obtain 4.69 g of yellow crystals (yield = 92.3%). ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.04 (d, J = 7.8 Hz, 1H), 7.93 (d, J = 8.1 Hz, 1H), 7.89 (d, J = 8.9 Hz, 2H), 7.47 (t, J = 7.6 Hz, 1H), 7.36 (t, J = 7.6 Hz, 1H), 6.82 (d, J = 8.9 Hz, 2H), 3.02 (s, 6H).

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···S1	0.93	2.71	3.127 (3)	108

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{14}N_2S$
M_r	254.34
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	296
a, b, c (Å)	11.0177 (15), 7.8508 (11), 29.691 (4)
V (Å^3)	2568.2 (6)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.23
Crystal size (mm)	0.30 × 0.20 × 0.20
Data collection	
Diffractometer	Bruker SMART2 CCD area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2000)
T_{min}, T_{max}	0.933, 0.955
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16833, 2256, 1606
R_{int}	0.043
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.154, 1.05
No. of reflections	2256
No. of parameters	165
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.14, −0.23

Computer programs: *SMART2* and *SAINT* (Bruker, 2000), *SHELXS97*, *SHELXL97* and *SHELXTL* (Sheldrick, 2008).

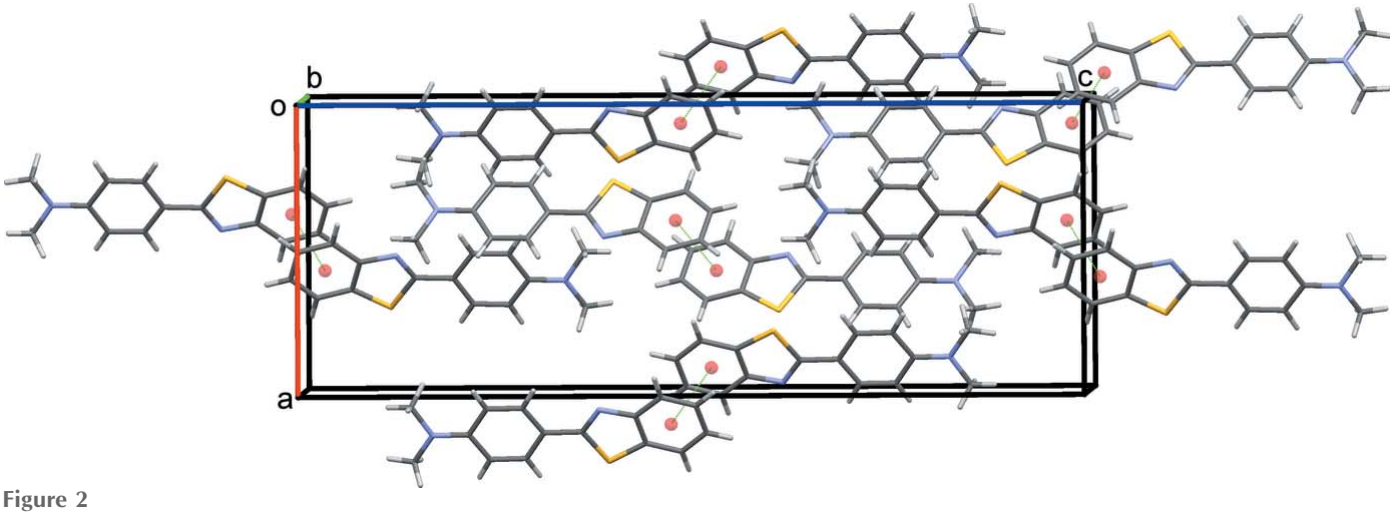


Figure 2
Stacking interactions between adjacent C1–C6 rings forming dimeric molecular pairs. Centroids are shown as red spheres linked by green dotted lines.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

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4-(Benzo[*d*]thiazol-2-yl)-*N*,*N*-dimethylaniline

Crystal data

$C_{15}H_{14}N_2S$
M_r = 254.34
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 11.0177 (15) Å
b = 7.8508 (11) Å
c = 29.691 (4) Å
V = 2568.2 (6) Å^3
Z = 8
F(000) = 1072
D_x = 1.316 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 3029 reflections
θ = 2.3–23.8°
μ = 0.23 mm^{-1}
T = 296 K
Rod-like, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART2 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2000)
T_{min} = 0.933, T_{max} = 0.955
16833 measured reflections
2256 independent reflections
1606 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 25.0°, θ_{min} = 2.3°
h = −13→13
k = −9→9
l = −34→35

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.154
S = 1.05
2256 reflections
165 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.77770 (6)	0.01253 (8)	0.60466 (2)	0.0696 (3)
N1	0.96074 (15)	0.2173 (2)	0.61401 (7)	0.0612 (5)
C9	0.96654 (17)	0.2058 (3)	0.71182 (9)	0.0568 (6)
H9	1.0276	0.2661	0.6972	0.068*
C6	0.93875 (18)	0.2027 (3)	0.56823 (8)	0.0593 (6)
C8	0.87971 (17)	0.1203 (2)	0.68596 (7)	0.0529 (5)
C11	0.87395 (17)	0.1146 (2)	0.78151 (8)	0.0562 (6)
C10	0.96477 (17)	0.2037 (3)	0.75759 (8)	0.0585 (6)
H10	1.0245	0.2620	0.7735	0.070*
C1	0.8422 (2)	0.0953 (3)	0.55647 (8)	0.0632 (6)
C7	0.88269 (17)	0.1277 (2)	0.63709 (8)	0.0551 (6)
C13	0.78936 (17)	0.0326 (3)	0.70975 (9)	0.0598 (6)
H13	0.7297	−0.0254	0.6937	0.072*
N2	0.87142 (17)	0.1140 (3)	0.82771 (7)	0.0711 (6)
C12	0.78625 (18)	0.0298 (3)	0.75562 (9)	0.0607 (6)
H12	0.7246	−0.0297	0.7701	0.073*
C5	1.0048 (2)	0.2827 (3)	0.53448 (10)	0.0757 (7)
H5	1.0690	0.3546	0.5418	0.091*
C2	0.8123 (2)	0.0686 (3)	0.51142 (10)	0.0779 (7)
H2	0.7482	−0.0025	0.5036	0.093*
C15	0.7785 (2)	0.0236 (4)	0.85263 (10)	0.0843 (8)
H15A	0.7000	0.0662	0.8443	0.126*
H15B	0.7909	0.0404	0.8843	0.126*
H15C	0.7832	−0.0958	0.8458	0.126*
C4	0.9750 (3)	0.2551 (3)	0.49059 (10)	0.0834 (8)
H4	1.0195	0.3084	0.4680	0.100*
C3	0.8790 (3)	0.1487 (4)	0.47891 (9)	0.0867 (8)
H3	0.8601	0.1319	0.4487	0.104*
C14	0.9704 (2)	0.1817 (4)	0.85393 (9)	0.0875 (8)
H14A	1.0460	0.1539	0.8396	0.131*
H14B	0.9686	0.1331	0.8836	0.131*
H14C	0.9626	0.3032	0.8560	0.131*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0590 (4)	0.0574 (4)	0.0923 (6)	−0.0116 (3)	−0.0100 (3)	−0.0052 (3)
N1	0.0511 (10)	0.0507 (11)	0.0818 (14)	−0.0054 (9)	−0.0010 (9)	−0.0012 (9)
C9	0.0404 (10)	0.0462 (11)	0.0840 (17)	−0.0056 (9)	0.0036 (10)	0.0009 (10)
C6	0.0549 (11)	0.0485 (12)	0.0745 (16)	0.0051 (10)	−0.0017 (11)	−0.0053 (10)

C8	0.0413 (10)	0.0371 (10)	0.0802 (15)	0.0027 (8)	−0.0037 (9)	−0.0019 (10)
C11	0.0469 (11)	0.0385 (11)	0.0833 (16)	0.0057 (9)	0.0043 (10)	0.0030 (10)
C10	0.0428 (11)	0.0533 (12)	0.0795 (17)	−0.0059 (9)	−0.0013 (10)	−0.0042 (11)
C1	0.0592 (12)	0.0496 (13)	0.0807 (16)	0.0071 (10)	−0.0074 (11)	−0.0070 (11)
C7	0.0429 (11)	0.0384 (11)	0.0838 (16)	0.0047 (9)	−0.0070 (10)	−0.0029 (10)
C13	0.0458 (12)	0.0431 (12)	0.0906 (19)	−0.0058 (9)	−0.0089 (11)	0.0002 (11)
N2	0.0649 (13)	0.0693 (13)	0.0791 (14)	−0.0098 (10)	0.0046 (10)	0.0022 (10)
C12	0.0458 (12)	0.0472 (13)	0.0890 (18)	−0.0075 (9)	0.0031 (10)	0.0068 (11)
C5	0.0708 (15)	0.0705 (16)	0.086 (2)	−0.0048 (13)	0.0014 (13)	−0.0022 (13)
C2	0.0772 (16)	0.0642 (16)	0.092 (2)	0.0036 (13)	−0.0166 (15)	−0.0115 (15)
C15	0.0753 (17)	0.0795 (19)	0.098 (2)	−0.0083 (14)	0.0139 (14)	0.0124 (15)
C4	0.0898 (18)	0.0784 (19)	0.082 (2)	0.0054 (15)	0.0059 (15)	0.0010 (14)
C3	0.099 (2)	0.0790 (18)	0.0820 (18)	0.0163 (16)	−0.0088 (16)	−0.0074 (16)
C14	0.0789 (17)	0.102 (2)	0.0818 (19)	−0.0037 (16)	−0.0025 (14)	−0.0044 (15)

Geometric parameters (Å, º)

S1—C1	1.725 (2)	C13—H13	0.9300
S1—C7	1.756 (2)	N2—C14	1.442 (3)
N1—C7	1.305 (3)	N2—C15	1.449 (3)
N1—C6	1.385 (3)	C12—H12	0.9300
C9—C10	1.359 (3)	C5—C4	1.361 (4)
C9—C8	1.398 (3)	C5—H5	0.9300
C9—H9	0.9300	C2—C3	1.366 (4)
C6—C5	1.389 (3)	C2—H2	0.9300
C6—C1	1.402 (3)	C15—H15A	0.9600
C8—C13	1.401 (3)	C15—H15B	0.9600
C8—C7	1.452 (3)	C15—H15C	0.9600
C11—N2	1.372 (3)	C4—C3	1.392 (4)
C11—C12	1.403 (3)	C4—H4	0.9300
C11—C10	1.413 (3)	C3—H3	0.9300
C10—H10	0.9300	C14—H14A	0.9600
C1—C2	1.393 (3)	C14—H14B	0.9600
C13—C12	1.363 (4)	C14—H14C	0.9600
C1—S1—C7	89.41 (11)	C14—N2—C15	116.0 (2)
C7—N1—C6	110.82 (18)	C13—C12—C11	121.5 (2)
C10—C9—C8	122.2 (2)	C13—C12—H12	119.2
C10—C9—H9	118.9	C11—C12—H12	119.2
C8—C9—H9	118.9	C4—C5—C6	119.5 (2)
N1—C6—C5	125.4 (2)	C4—C5—H5	120.3
N1—C6—C1	115.3 (2)	C6—C5—H5	120.3
C5—C6—C1	119.4 (2)	C3—C2—C1	118.8 (3)
C9—C8—C13	116.4 (2)	C3—C2—H2	120.6
C9—C8—C7	120.94 (19)	C1—C2—H2	120.6
C13—C8—C7	122.62 (19)	N2—C15—H15A	109.5
N2—C11—C12	122.2 (2)	N2—C15—H15B	109.5
N2—C11—C10	121.2 (2)	H15A—C15—H15B	109.5

C12—C11—C10	116.6 (2)	N2—C15—H15C	109.5
C9—C10—C11	121.3 (2)	H15A—C15—H15C	109.5
C9—C10—H10	119.4	H15B—C15—H15C	109.5
C11—C10—H10	119.4	C5—C4—C3	121.2 (3)
C2—C1—C6	120.6 (2)	C5—C4—H4	119.4
C2—C1—S1	130.0 (2)	C3—C4—H4	119.4
C6—C1—S1	109.43 (17)	C2—C3—C4	120.6 (3)
N1—C7—C8	124.11 (18)	C2—C3—H3	119.7
N1—C7—S1	115.06 (17)	C4—C3—H3	119.7
C8—C7—S1	120.83 (15)	N2—C14—H14A	109.5
C12—C13—C8	122.0 (2)	N2—C14—H14B	109.5
C12—C13—H13	119.0	H14A—C14—H14B	109.5
C8—C13—H13	119.0	N2—C14—H14C	109.5
C11—N2—C14	121.6 (2)	H14A—C14—H14C	109.5
C11—N2—C15	121.8 (2)	H14B—C14—H14C	109.5

C7—N1—C6—C5	179.6 (2)	C1—S1—C7—N1	−1.29 (16)
C7—N1—C6—C1	−1.3 (3)	C1—S1—C7—C8	178.67 (17)
C10—C9—C8—C13	0.5 (3)	C9—C8—C13—C12	−0.3 (3)
C10—C9—C8—C7	178.81 (19)	C7—C8—C13—C12	−178.59 (19)
C8—C9—C10—C11	−0.2 (3)	C12—C11—N2—C14	171.5 (2)
N2—C11—C10—C9	−179.3 (2)	C10—C11—N2—C14	−9.5 (3)
C12—C11—C10—C9	−0.3 (3)	C12—C11—N2—C15	0.8 (3)
N1—C6—C1—C2	−179.1 (2)	C10—C11—N2—C15	179.80 (19)
C5—C6—C1—C2	0.0 (3)	C8—C13—C12—C11	−0.2 (3)
N1—C6—C1—S1	0.4 (2)	N2—C11—C12—C13	179.4 (2)
C5—C6—C1—S1	179.49 (17)	C10—C11—C12—C13	0.4 (3)
C7—S1—C1—C2	179.9 (2)	N1—C6—C5—C4	178.8 (2)
C7—S1—C1—C6	0.47 (16)	C1—C6—C5—C4	−0.2 (3)
C6—N1—C7—C8	−178.27 (18)	C6—C1—C2—C3	0.1 (4)
C6—N1—C7—S1	1.7 (2)	S1—C1—C2—C3	−179.2 (2)
C9—C8—C7—N1	−2.9 (3)	C6—C5—C4—C3	0.3 (4)
C13—C8—C7—N1	175.30 (18)	C1—C2—C3—C4	−0.1 (4)
C9—C8—C7—S1	177.11 (14)	C5—C4—C3—C2	−0.2 (4)
C13—C8—C7—S1	−4.7 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···S1	0.93	2.71	3.127 (3)	108