Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Amino-4-methylbenzothiazole

Robin S. Tanke[a]* and Bruce M. Foxman[b]

[a]Department of Chemistry, University of Wisconsin–Stevens Point, Stevens Point, WI 54481, USA, and [b]Department of Chemistry, Brandeis University, Waltham, MA 02454, USA
Correspondence e-mail: rtanke@uwsp.edu

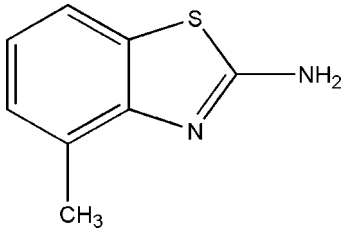
Received 1 November 2007; accepted 8 November 2007

Key indicators: single-crystal X-ray study; T = 208 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.133; data-to-parameter ratio = 16.0.

The title compound, $C_8H_8N_2S$, was crystallized from heptane with a minimal amount of toluene. The crystal structure is stabilized by intermolecular N—H···N and N—H···S hydrogen bonds. The crystal structure viewed down the b axis shows the molecules packed in a bilayer fashion, with alternating hydrophilic and hydrophobic regions.

Related literature

For the crystal structures of similar 2-aminobenzothiazole compounds, see: Jai-nhuknan *et al.* (1997); Goubitz *et al.* (2001).



Experimental

Crystal data

$C_8H_8N_2S$
M_r = 164.22
Monoclinic, $P2_1/c$
a = 12.860 (4) Å
b = 3.931 (1) Å
c = 15.208 (5) Å
β = 92.968 (5)°
V = 767.8 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.35 mm^{-1}
T = 208 K
0.20 × 0.20 × 0.05 mm

Data collection

Bruker SMART diffractometer
Absorption correction: multi-scan (*APEX2*; Bruker, 2006)
T_{min} = 0.93, T_{max} = 0.98
4667 measured reflections
1620 independent reflections
1214 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.133
S = 1.06
1620 reflections
101 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N1^{i}	0.86	2.10	2.949 (3)	168
N2—H2B···S^{ii}	0.86	2.86	3.672 (2)	158

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+2, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *APEX2* (Bruker, 2006); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *CRYSTALS*; software used to prepare material for publication: *CAMERON* (Watkin *et al.*, 1996).

The authors acknowledge the Small Molecule X-ray Crystallography Summer School hosted by Professor Arnold Rheingold at the University of California–San Diego, and the University of Wisconsin–Stevens Point Letters and Science Foundation and Chemistry Department.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2029).

References

Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487.
Bruker (2006). *APEX2*. Version 2. Bruker AXS Inc., Madison, Wisconsin, USA.
Goubitz, K., Sonneveld, E. J. & Schenk, H. (2001). *Z. Kristallogr.* **216**, 176–181.
Jai-nhuknan, J., Karipides, A. G., Hughes, J. M. & Cantrell, J. S. (1997). *Acta Cryst.* C**53**, 381–383.
Sheldrick, G. M. (1997). *SHELXS97*. University of Göttingen, Germany.
Watkin, D. J., Prout, C. K. & Pearce, L. J. (1996). *CAMERON*. Chemical Crystallography Laboratory, University of Oxford, England.

  doi:10.1107/S1600536807056978

supplementary materials

Acta Cryst. (2007). E**63**, o4718 [**doi:10.1107/S1600536807056978**]

2-Amino-4-methylbenzothiazole

R. S. Tanke and B. M. Foxman

Comment

The crystal structures of 2-amino-6-fluorobenzothiazole (Jai-nhuknan *et al.*, 1997) and 2-aminobenzothiazole (Goubitz *et al.*, 2001) have been described in the literature. Herein we report the molecular and crystal structure of the title compound (Fig. 1).

The benzothiazole unit is essentially planar, with the a mean deviation of 0.0095 Å from the least-squares plane defined by the nine constituent atoms. The molecular packing is stabilized by N—H···N hydrogen bonds between a H atom of amino group and the N atom of thiazole ring, *i.e.* N2—H2A···N1^{i} (Table 1 and Fig. 2). The molecular packing is further stabilized by N—H···S interactions between a H atom of amino group and the S atom of thiazole ring, *i.e.* N2—H2B···S^{ii} (Table 1 and Fig. 2). The crystal structure viewed down the *b* axis shows the molecules packed in a bilayer fashion, with alternating hydrophilic and hydrophobic regions (Fig. 2). The geometry of the benzothiazole ring is consistent with other 2-aminobenzothiazoles included in the Cambridge Crystallographic Data Base. The C1—S and C7—S bond distances of 1.773 (3) Å and 1.739 (3) Å respectively, are in between the 1.81 Å average distance for a carbon-sulfur single bond and the 1.61 Å average distance for a carbon-sulfur double bond; this is typical for benzothiazoles.

Experimental

A commercial sample of 2-amino-4-methylbenzothiazole was used. Single crystals were obtained by slow evaporation of a heptane solution of a minimal amount of toluene over 24 h.

Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å for aromatic H atoms, 0.96 Å for methyl H atoms and 0.86 Å for amino H atoms, respectively, and with U_{iso}(H) = 1.2Ueq(C) for aromatic, U_{iso}(H) = 1.5Ueq(C) for methyl and 1.2Ueq(N) for amino H atoms.

Figures

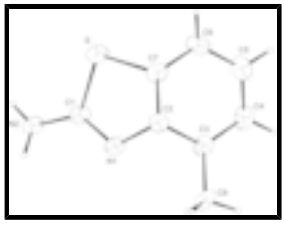


Fig. 1. The molecular structure of the title compound, showing displacement ellipsoids drawn at the 30% probability level.

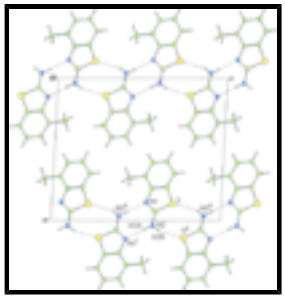


Fig. 2. N—H···H and N—H···S hydrogen bonds (dotted lines) in the title compound. [Symmetry codes: (i) −*x* + 2, −*y* + 1, −*z* + 1; (ii) −*x* + 2, *y* − 1/2, −*z* + 3/2.]

2-Amino-4-methylbenzothiazole

Crystal data

$C_8H_8N_2S$	F_{000} = 344
M_r = 164.22	D_x = 1.421 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 410 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 12.860 (4) Å	Cell parameters from 1578 reflections
b = 3.931 (1) Å	θ = 3.0–26.7º
c = 15.208 (5) Å	μ = 0.35 mm^{-1}
β = 92.968 (5)º	T = 208 K
V = 767.8 (4) Å^3	Plate, colorless
Z = 4	0.20 × 0.20 × 0.05 mm

Data collection

Bruker SMART diffractometer	1620 independent reflections
Radiation source: fine-focus sealed tube	1214 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.044
Detector resolution: 10.0 pixels mm^{-1}	θ_{max} = 27.0º
T = 208 K	θ_{min} = 1.6º
ω/2θ scans	h = −15→16
Absorption correction: multi-scan (APEX2; Bruker, 2006)	k = −2→4
T_{min} = 0.93, T_{max} = 0.98	l = −15→19
4667 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H-atom parameters constrained
$wR(F^2)$ = 0.133	$w = 1/[\sigma^2(F_o^2) + (0.067P)^2 + 0.1789P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.06	$(\Delta/\sigma)_{max}$ = <0.001
1620 reflections	$\Delta\rho_{max}$ = 0.38 e Å^{-3}
101 parameters	$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S	0.88006 (5)	0.19348 (17)	0.71306 (4)	0.0340 (2)
N1	0.87146 (16)	0.4635 (5)	0.55501 (12)	0.0304 (5)
N2	1.03526 (18)	0.2365 (6)	0.60024 (14)	0.0404 (6)
H2A	1.0624	0.2938	0.5519	0.048*
H2B	1.0724	0.1338	0.6407	0.048*
C1	0.9346 (2)	0.3079 (7)	0.61254 (16)	0.0320 (6)
C2	0.77322 (19)	0.4973 (6)	0.58816 (15)	0.0283 (6)
C3	0.6867 (2)	0.6432 (6)	0.54202 (16)	0.0311 (6)
C4	0.5937 (2)	0.6539 (7)	0.58380 (18)	0.0375 (7)
H4	0.5356	0.7498	0.5545	0.045*
C7	0.7623 (2)	0.3662 (6)	0.67334 (16)	0.0297 (6)
C8	0.6993 (2)	0.7835 (7)	0.45000 (17)	0.0356 (6)
H8A	0.6332	0.8621	0.4259	0.053*
H8B	0.7250	0.6075	0.4131	0.053*
H8C	0.7478	0.9693	0.4529	0.053*
C6	0.6684 (2)	0.3798 (7)	0.71419 (17)	0.0369 (7)
H6	0.6623	0.2935	0.7706	0.044*
C5	0.5843 (2)	0.5256 (7)	0.66839 (19)	0.0398 (7)
H5	0.5205	0.5384	0.6944	0.048*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S	0.0405 (4)	0.0345 (4)	0.0267 (4)	−0.0020 (3)	−0.0010 (3)	0.0031 (3)
N1	0.0348 (12)	0.0320 (11)	0.0240 (11)	0.0005 (10)	−0.0015 (9)	0.0003 (9)
N2	0.0396 (14)	0.0531 (15)	0.0281 (12)	0.0104 (11)	−0.0015 (10)	0.0077 (10)
C1	0.0389 (15)	0.0308 (13)	0.0262 (13)	0.0003 (11)	0.0001 (11)	−0.0018 (10)

C2	0.0326 (14)	0.0256 (13)	0.0266 (13)	−0.0011 (11)	0.0004 (10)	−0.0044 (10)
C3	0.0357 (14)	0.0270 (13)	0.0301 (13)	0.0036 (11)	−0.0031 (11)	−0.0029 (11)
C4	0.0358 (16)	0.0334 (14)	0.0426 (16)	0.0038 (12)	−0.0041 (13)	−0.0064 (12)
C7	0.0355 (15)	0.0252 (13)	0.0279 (13)	−0.0037 (11)	−0.0019 (11)	−0.0031 (10)
C8	0.0419 (16)	0.0318 (14)	0.0318 (14)	0.0081 (12)	−0.0109 (12)	0.0032 (11)
C6	0.0449 (17)	0.0351 (15)	0.0312 (14)	−0.0062 (13)	0.0073 (12)	−0.0039 (11)
C5	0.0332 (15)	0.0392 (15)	0.0476 (17)	−0.0015 (13)	0.0077 (13)	−0.0081 (13)

Geometric parameters (Å, °)

S—C7	1.739 (3)	C3—C8	1.521 (4)
S—C1	1.773 (3)	C4—C5	1.393 (4)
N1—C1	1.314 (3)	C4—H4	0.9300
N1—C2	1.391 (3)	C7—C6	1.388 (4)
N2—C1	1.347 (3)	C8—H8A	0.9600
N2—H2A	0.8600	C8—H8B	0.9600
N2—H2B	0.8600	C8—H8C	0.9600
C2—C3	1.406 (3)	C6—C5	1.380 (4)
C2—C7	1.408 (3)	C6—H6	0.9300
C3—C4	1.384 (4)	C5—H5	0.9300
C7—S—C1	88.74 (12)	C5—C4—H4	118.9
C1—N1—C2	110.2 (2)	C6—C7—C2	121.9 (2)
C1—N2—H2A	120.0	C6—C7—S	128.5 (2)
C1—N2—H2B	120.0	C2—C7—S	109.61 (19)
H2A—N2—H2B	120.0	C3—C8—H8A	109.5
N1—C1—N2	124.7 (2)	C3—C8—H8B	109.5
N1—C1—S	115.7 (2)	H8A—C8—H8B	109.5
N2—C1—S	119.55 (19)	C3—C8—H8C	109.5
N1—C2—C3	124.6 (2)	H8A—C8—H8C	109.5
N1—C2—C7	115.8 (2)	H8B—C8—H8C	109.5
C3—C2—C7	119.6 (2)	C5—C6—C7	117.9 (3)
C4—C3—C2	117.6 (2)	C5—C6—H6	121.1
C4—C3—C8	123.2 (2)	C7—C6—H6	121.1
C2—C3—C8	119.2 (2)	C6—C5—C4	120.9 (3)
C3—C4—C5	122.1 (3)	C6—C5—H5	119.6
C3—C4—H4	118.9	C4—C5—H5	119.6
C2—N1—C1—N2	−180.0 (2)	C8—C3—C4—C5	−179.6 (2)
C2—N1—C1—S	−0.8 (3)	N1—C2—C7—C6	−179.4 (2)
C7—S—C1—N1	0.6 (2)	C3—C2—C7—C6	−0.8 (4)
C7—S—C1—N2	179.9 (2)	N1—C2—C7—S	−0.1 (3)
C1—N1—C2—C3	−178.0 (2)	C3—C2—C7—S	178.53 (18)
C1—N1—C2—C7	0.6 (3)	C1—S—C7—C6	179.0 (3)
N1—C2—C3—C4	179.1 (2)	C1—S—C7—C2	−0.28 (19)
C7—C2—C3—C4	0.6 (4)	C2—C7—C6—C5	0.4 (4)
N1—C2—C3—C8	−1.4 (4)	S—C7—C6—C5	−178.8 (2)
C7—C2—C3—C8	−179.9 (2)	C7—C6—C5—C4	0.1 (4)
C2—C3—C4—C5	−0.1 (4)	C3—C4—C5—C6	−0.3 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···N1^{i}	0.86	2.10	2.949 (3)	168
N2—H2B···S^{ii}	0.86	2.86	3.672 (2)	158

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) −*x*+2, *y*−1/2, −*z*+3/2.

Fig. 1

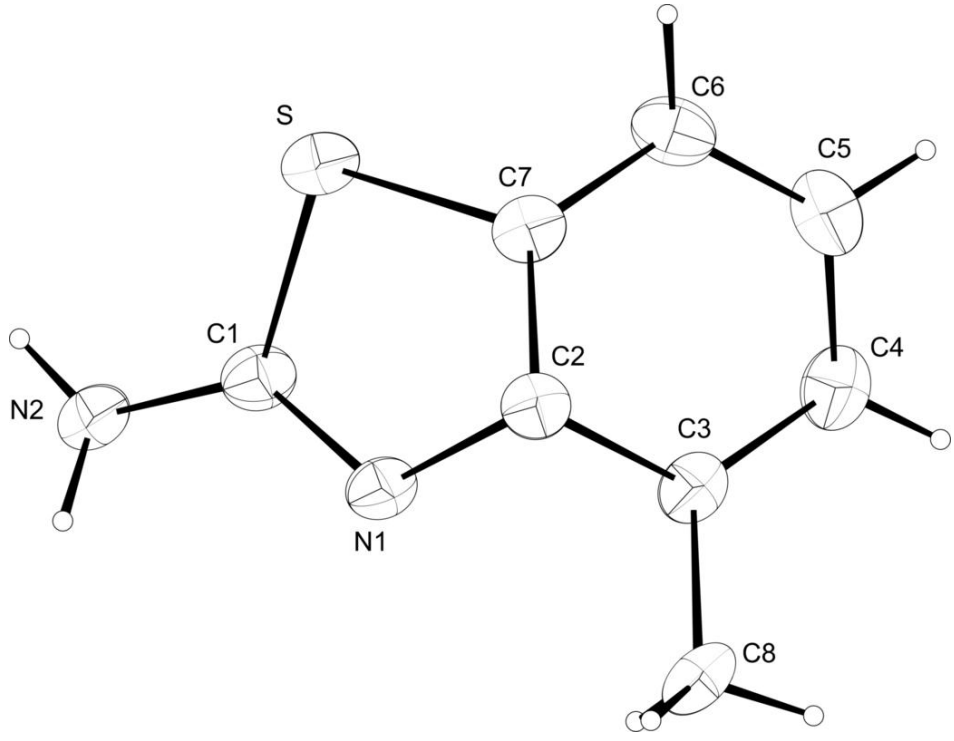


Fig. 2