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3-Benzylsulfanyl-1*H*-1,2,4-triazol-5-amine

Shuai Zhang, Pei-Jiang Liu, Dong-Sheng Ma* and Guang-Feng Hou

College of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China
Correspondence e-mail: hgf1000@163.com

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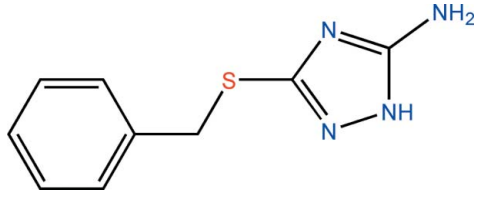
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.111; data-to-parameter ratio = 16.7.

In the title molecule, $C_9H_{10}N_4S$, the dihedral angle between the benzene and triazole rings is 81.05 (5)°. In the crystal, N—H···N hydrogen bonds link the molecules into infinite zigzag chains along [010].

Related literature

For the biological properties of 1,2,4-triazoles derivatives, see: Paulvannan *et al.* (2001); El-Sagheer & Brown (2011).



Experimental

Crystal data

$C_9H_{10}N_4S$
M_r = 206.27
Monoclinic, $P2_1/c$
a = 9.870 (2) Å
b = 9.6370 (19) Å
c = 10.398 (2) Å
β = 90.18 (3)°
V = 989.0 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 293 K
0.38 × 0.26 × 0.11 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.897, T_{max} = 0.970
9367 measured reflections
2267 independent reflections
1372 reflections with $I > 2\sigma(I)$
R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.111
S = 1.04
2267 reflections
136 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H41···N1^{i}	0.89 (1)	2.20 (2)	3.044 (3)	158 (3)
N2—H21···N3^{ii}	0.90 (1)	2.03 (2)	2.873 (2)	155 (2)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5211).

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supporting information

Acta Cryst. (2012). E**68**, o83 [doi:10.1107/S1600536811052159]

3-Benzylsulfanyl-1*H*-1,2,4-triazol-5-amine

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S1. Comment

We are paying attention to the synthesis and applications of substituted 1,2,4-triazoles due to their comprehensive biological activities such as antihypertensive, antifungal and antibacterial properties (Paulvannan *et al.*, 2001; El-Sagheer *et al.*, 2011). Herein, we report the synthesis and crystal structure of the title compound (I).

In (I) (Fig. 1), the benzene and triazole rings form a dihedral angle of 81.05 (5)°. In the crystal packing, the N—H···N hydrogen bonds (Table 1) link adjacent molecules into infinite zigzag chains along [010] (Fig. 2).

S2. Experimental

In aqueous (10 mL) solution of NaOH (0.40 g, 0.010 mol) and 5-amino-1*H*-1,2,4-triazole-3-thiol (1.16 g, 0.010 mol, commercial product) was added an ethanol (20 mL) solution of benzyl chloride (1.52 g, 0.012 mol) with stirring. After stirring for 10 min, the solution evaporated. Then the resulting precipitate was filtered off, diluted with water and purified to give the title compound. Colourless prismatic crystal suitable for X-ray analysis were obtained by recrystallization in chloroform solution.

S3. Refinement

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic); C—H = 0.97 Å (methylene), and with U_{iso}(H) = 1.2U_{eq}(C). N-bound H atom were found from Fourier map, and were refined with restraint N—H = 0.90 (1) Å and U_{iso}(H) = 1.5U_{eq}(N).

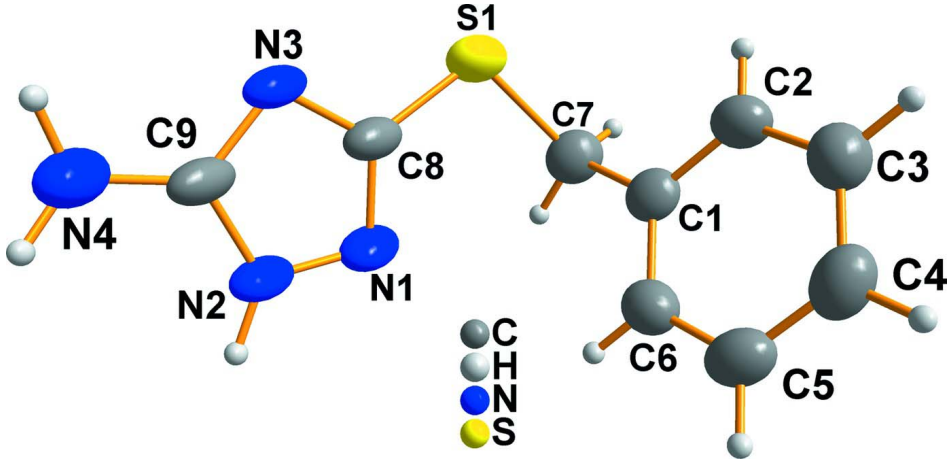

Figure 1

The molecular structure of (I) showing the atomic numbering and 30% probabilty displacement ellipsoids.

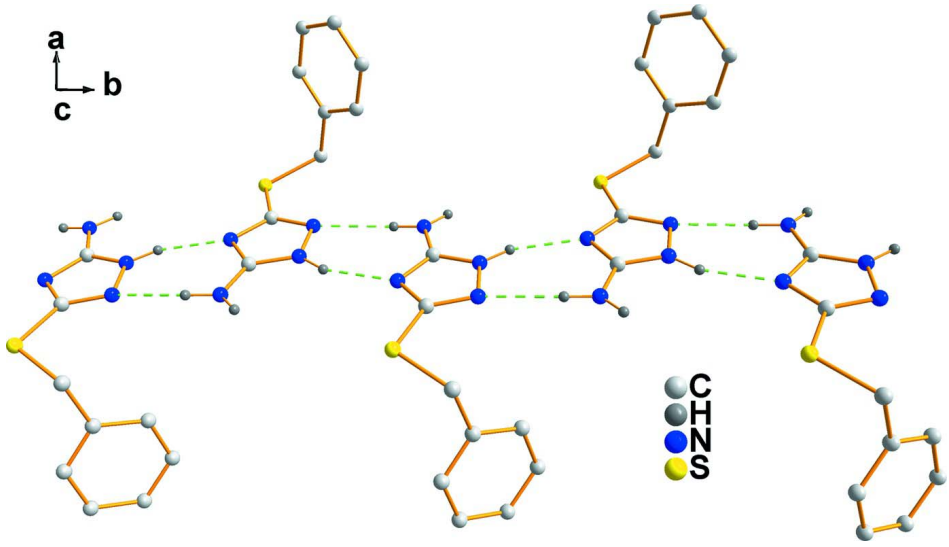

Figure 2

A portion of the crystal packing showing hydrogen-bonded (dashed lines) chains. C-bound H atoms omitted for clarity.

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Hall symbol: -P 2ybc
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$b = 9.6370$ (19) Å
$c = 10.398$ (2) Å
$\beta = 90.18$ (3)°
$V = 989.0$ (3) Å^3
$Z = 4$
$F(000) = 432$
$D_x = 1.385$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6282 reflections
$\theta = 3.5$–$27.5°$
$\mu = 0.29$ mm^{-1}
$T = 293$ K
Block, colorless
0.38 × 0.26 × 0.11 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.897$, $T_{max} = 0.970$
9367 measured reflections
2267 independent reflections
1372 reflections with $I > 2\sigma(I)$
$R_{int} = 0.059$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.5°$
$h = -12 \rightarrow 12$
$k = -12 \rightarrow 12$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.111$
$S = 1.04$
2267 reflections
136 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0455P)^2 + 0.1013P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ 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}
C1	0.9298 (2)	0.2955 (2)	0.45864 (19)	0.0424 (5)
C2	1.0473 (2)	0.2171 (2)	0.4593 (2)	0.0510 (6)
H2	1.0536	0.1402	0.5131	0.061*
C3	1.1549 (3)	0.2511 (3)	0.3816 (2)	0.0598 (7)
H3	1.2329	0.1969	0.3823	0.072*
C4	1.1468 (3)	0.3657 (3)	0.3029 (2)	0.0606 (7)
H4	1.2198	0.3896	0.2510	0.073*
C5	1.0312 (3)	0.4446 (3)	0.3008 (2)	0.0564 (6)
H5	1.0256	0.5214	0.2469	0.068*
C6	0.9232 (2)	0.4102 (2)	0.3784 (2)	0.0501 (6)
H6	0.8453	0.4644	0.3769	0.060*
C7	0.8148 (2)	0.2577 (3)	0.5473 (2)	0.0541 (6)
H7A	0.7510	0.3341	0.5495	0.065*
H7B	0.8506	0.2456	0.6335	0.065*
C8	0.6212 (2)	0.1615 (2)	0.3776 (2)	0.0442 (5)
C9	0.4869 (2)	0.1511 (2)	0.2191 (2)	0.0462 (6)
N1	0.5965 (2)	0.29303 (18)	0.3524 (2)	0.0541 (5)
N2	0.5088 (2)	0.28358 (17)	0.2498 (2)	0.0539 (5)
H21	0.473 (3)	0.3613 (18)	0.216 (2)	0.081*
N3	0.55663 (18)	0.06938 (16)	0.29881 (19)	0.0460 (5)
N4	0.4055 (2)	0.1079 (2)	0.1236 (2)	0.0665 (6)
H41	0.404 (3)	0.0173 (12)	0.107 (3)	0.100*
H42	0.368 (3)	0.167 (3)	0.068 (2)	0.100*
S1	0.72492 (7)	0.10082 (6)	0.50093 (7)	0.0582 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0478 (13)	0.0408 (11)	0.0385 (11)	−0.0047 (9)	−0.0002 (10)	−0.0064 (10)
C2	0.0548 (15)	0.0433 (13)	0.0548 (14)	0.0000 (10)	−0.0025 (12)	0.0058 (11)
C3	0.0481 (15)	0.0580 (15)	0.0735 (16)	0.0027 (12)	0.0074 (13)	0.0032 (13)
C4	0.0516 (16)	0.0676 (17)	0.0625 (15)	−0.0123 (13)	0.0078 (12)	0.0057 (14)

C5	0.0657 (18)	0.0511 (14)	0.0522 (14)	−0.0083 (12)	−0.0014 (13)	0.0119 (12)
C6	0.0508 (14)	0.0453 (12)	0.0543 (13)	0.0016 (10)	−0.0055 (11)	0.0007 (11)
C7	0.0587 (16)	0.0511 (13)	0.0525 (13)	−0.0024 (11)	0.0059 (12)	−0.0027 (11)
C8	0.0382 (12)	0.0273 (10)	0.0672 (14)	0.0003 (9)	0.0137 (11)	0.0022 (10)
C9	0.0393 (12)	0.0266 (10)	0.0728 (15)	−0.0016 (9)	0.0111 (11)	0.0016 (11)
N1	0.0525 (13)	0.0264 (9)	0.0834 (14)	0.0016 (8)	−0.0020 (11)	−0.0027 (9)
N2	0.0495 (12)	0.0245 (9)	0.0876 (15)	0.0002 (8)	−0.0015 (11)	0.0035 (9)
N3	0.0400 (10)	0.0226 (8)	0.0753 (13)	−0.0012 (7)	0.0092 (9)	0.0002 (9)
N4	0.0709 (16)	0.0374 (11)	0.0912 (17)	−0.0030 (10)	−0.0166 (13)	0.0004 (12)
S1	0.0576 (4)	0.0398 (3)	0.0774 (5)	−0.0023 (3)	0.0053 (3)	0.0130 (3)

Geometric parameters (Å, º)

C1—C2	1.384 (3)	C7—H7A	0.9700
C1—C6	1.386 (3)	C7—H7B	0.9700
C1—C7	1.509 (3)	C8—N1	1.317 (3)
C2—C3	1.377 (3)	C8—N3	1.365 (3)
C2—H2	0.9300	C8—S1	1.740 (2)
C3—C4	1.376 (3)	C9—N3	1.333 (3)
C3—H3	0.9300	C9—N2	1.334 (3)
C4—C5	1.371 (4)	C9—N4	1.342 (3)
C4—H4	0.9300	N1—N2	1.375 (3)
C5—C6	1.380 (3)	N2—H21	0.900 (10)
C5—H5	0.9300	N4—H42	0.892 (10)
C6—H6	0.9300	N4—H41	0.889 (10)
C7—S1	1.817 (2)	N4—H42	0.892 (10)
C2—C1—C6	118.5 (2)	C1—C7—H7B	108.8
C2—C1—C7	119.8 (2)	S1—C7—H7B	108.8
C6—C1—C7	121.7 (2)	H7A—C7—H7B	107.6
C3—C2—C1	121.0 (2)	N1—C8—N3	114.9 (2)
C3—C2—H2	119.5	N1—C8—S1	125.35 (18)
C1—C2—H2	119.5	N3—C8—S1	119.75 (15)
C4—C3—C2	119.8 (2)	N3—C9—N2	109.5 (2)
C4—C3—H3	120.1	N3—C9—N4	125.7 (2)
C2—C3—H3	120.1	N2—C9—N4	124.8 (2)
C5—C4—C3	120.0 (2)	C8—N1—N2	101.91 (18)
C5—C4—H4	120.0	C9—N2—N1	110.48 (19)
C3—C4—H4	120.0	C9—N2—H21	129.8 (18)
C4—C5—C6	120.1 (2)	N1—N2—H21	119.7 (17)
C4—C5—H5	119.9	C9—N3—C8	103.18 (17)
C6—C5—H5	119.9	H42—N4—C9	122 (2)
C5—C6—C1	120.6 (2)	H42—N4—H41	120 (3)
C5—C6—H6	119.7	C9—N4—H41	117 (2)
C1—C6—H6	119.7	H42—N4—H42	0 (2)
C1—C7—S1	113.99 (16)	C9—N4—H42	122 (2)
C1—C7—H7A	108.8	H41—N4—H42	120 (3)
S1—C7—H7A	108.8	C8—S1—C7	101.62 (11)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H41···N1^{i}	0.89 (1)	2.20 (2)	3.044 (3)	158 (3)
N2—H21···N3^{ii}	0.90 (1)	2.03 (2)	2.873 (2)	155 (2)

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