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2-Hydrazinyl-4-methyl-1,3-benzothiazole

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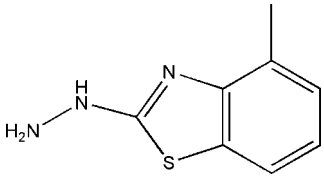
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.003 Å; R factor = 0.028; wR factor = 0.057; data-to-parameter ratio = 15.3.

The title compound, $C_8H_9N_3S$, is almost planar (r.m.s. deviation = 0.019 Å) apart from the terminal $-NH_2$ grouping [deviation of the N atom = 0.286 (2) Å]. In the crystal, molecules are linked by N—H···N hydrogen bonds, generating (001) sheets.

Related literature

For related structures and their biactivity, see Sun & Cui (2008); Liu & Liu (2011); Liu *et al.* (2011*a*,*b*). For the synthesis, see: Patel *et al.* (2010).



Experimental

Crystal data

$C_8H_9N_3S$
M_r = 179.24
Monoclinic, $P2_1$
a = 3.893 (2) Å
b = 7.312 (4) Å
c = 14.137 (8) Å
β = 93.416 (13)°
V = 401.7 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 113 K
0.28 × 0.18 × 0.10 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.910, T_{max} = 0.967
4186 measured reflections
1864 independent reflections
1614 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.057
S = 1.02
1864 reflections
122 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Absolute structure: Flack (1983), 836 Friedel pairs
Flack parameter: −0.09 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···N3^{i}	0.89 (1)	2.30 (2)	2.996 (3)	135 (2)
N3—H3A···N1^{ii}	0.92 (1)	2.21 (1)	3.077 (3)	156 (2)

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5894).

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supporting information

Acta Cryst. (2011). E**67**, o1641 [doi:10.1107/S1600536811020149]

2-Hydrazinyl-4-methyl-1,3-benzothiazole

Xu-Feng Liu, Xiao-Yong Yu and Shao-Liang Jiang

S1. Comment

Sulfur and nitrogen heterocyclic compounds have received considerable attention in recent years because of their medicinal and pesticidal importance, such as 1,3,4-thiadiazoles, pyrimidines, and 1,2,4-triazoles (Liu & Liu, 2011; Liu *et al.*, 2011a,b). For a related structure, see Sun & Cui (2008).

Single-crystal X-ray diffraction analysis reveals that the title compound crystallizes in the monoclinic space group P2(1). As shown in Fig. 1, the benzene and thiazole rings are almost in the same plane. As shown in Fig. 2, there are intermolecular N—H···N hydrogen bonds in the crystal.

S2. Experimental

The title compound was prepared according to the literature procedures (Patel *et al.*, (2010). Colourless prisms of (I) were grown by the slow evaporation of an ethanol solution at room temperature.

S3. Refinement

All the H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

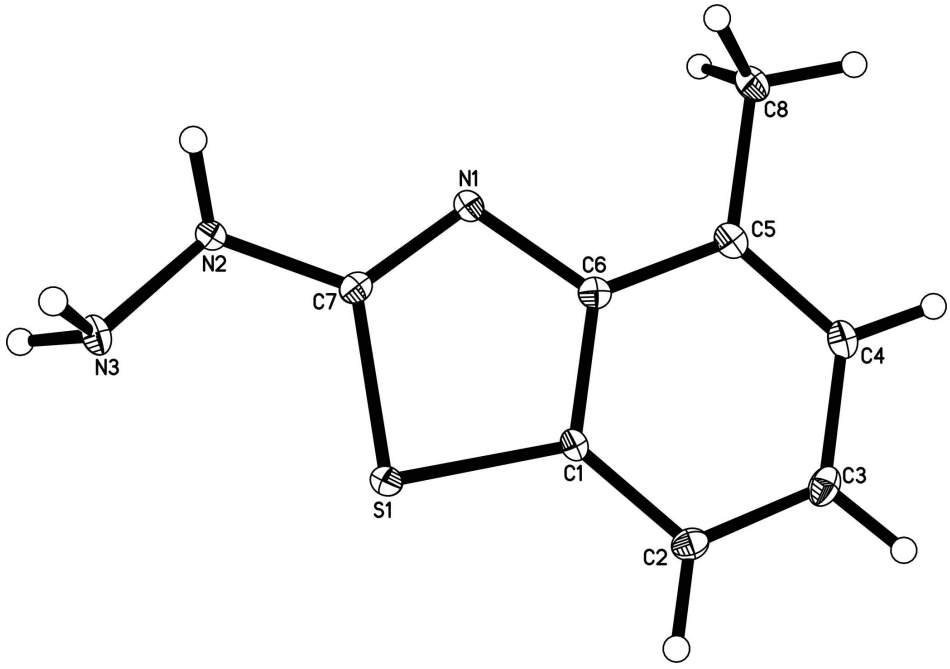

Figure 1

The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

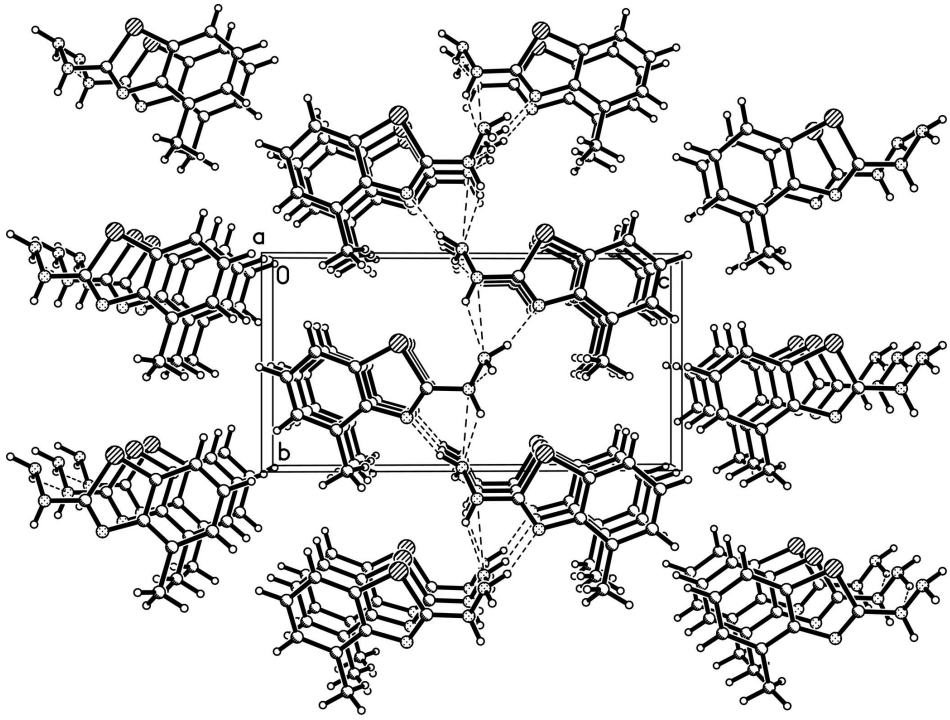

Figure 2

The crystal packing for (I).

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$C_8H_9N_3S$
$M_r = 179.24$
Monoclinic, $P2_1$
$a = 3.893$ (2) Å
$b = 7.312$ (4) Å
$c = 14.137$ (8) Å
$\beta = 93.416$ (13)°
$V = 401.7$ (4) Å^3
$Z = 2$
$F(000) = 188$
$D_x = 1.482$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1356 reflections
$\theta = 2.9$–$27.9°$
$\mu = 0.34$ mm^{-1}
$T = 113$ K
Prism, colorless
0.28 × 0.18 × 0.10 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Radiation source: rotating anode
Multilayer monochromator
Detector resolution: 14.63 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min} = 0.910$, $T_{max} = 0.967$
4186 measured reflections
1864 independent reflections
1614 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 27.9°$, $\theta_{min} = 1.4°$
$h = -5 \rightarrow 5$
$k = -9 \rightarrow 9$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.057$
$S = 1.02$
1864 reflections
122 parameters
5 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
$w = 1/[\sigma^2(F_o^2) + (0.006P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}
Absolute structure: Flack (1983), 836 Friedel pairs
Absolute structure parameter: −0.09 (6)

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 $F^2 > \sigma(F^2)$ 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}
S1	0.74281 (13)	0.41481 (6)	0.33097 (3)	0.01462 (12)
C5	0.2809 (5)	0.8047 (3)	0.18122 (14)	0.0144 (5)
N3	0.9465 (5)	0.4807 (2)	0.52579 (12)	0.0163 (4)

C2	0.5274 (5)	0.4513 (3)	0.13713 (13)	0.0163 (5)
H2A	0.6107	0.3333	0.1221	0.020*
N1	0.4899 (4)	0.7443 (2)	0.34709 (11)	0.0136 (4)
C4	0.2524 (5)	0.7352 (3)	0.08962 (14)	0.0158 (5)
H4	0.1480	0.8083	0.0403	0.019*
C6	0.4388 (5)	0.6942 (3)	0.25178 (13)	0.0127 (4)
C7	0.6412 (5)	0.6127 (3)	0.39382 (13)	0.0130 (4)
N2	0.7110 (4)	0.6159 (2)	0.49033 (12)	0.0150 (4)
C3	0.3711 (5)	0.5633 (3)	0.06809 (13)	0.0185 (5)
H3	0.3451	0.5208	0.0046	0.022*
C1	0.5572 (5)	0.5186 (3)	0.22906 (13)	0.0124 (4)
C8	0.1482 (5)	0.9932 (3)	0.20484 (14)	0.0182 (5)
H8A	0.3296	1.0618	0.2404	0.027*
H8B	−0.0518	0.9812	0.2433	0.027*
H8C	0.0810	1.0585	0.1461	0.027*
H2	0.761 (6)	0.7236 (19)	0.5172 (16)	0.060 (10)*
H3A	0.861 (4)	0.423 (3)	0.5774 (10)	0.043 (7)*
H3B	1.153 (3)	0.531 (3)	0.5428 (12)	0.038 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0167 (3)	0.0120 (2)	0.0151 (2)	0.0012 (3)	0.00115 (18)	0.0003 (2)
C5	0.0078 (11)	0.0166 (11)	0.0191 (11)	−0.0007 (10)	0.0026 (9)	0.0030 (9)
N3	0.0141 (11)	0.0180 (10)	0.0163 (9)	0.0006 (8)	−0.0015 (7)	0.0049 (8)
C2	0.0142 (11)	0.0169 (14)	0.0180 (10)	−0.0005 (9)	0.0029 (8)	−0.0029 (9)
N1	0.0139 (10)	0.0126 (9)	0.0142 (9)	0.0000 (7)	0.0007 (7)	0.0017 (7)
C4	0.0124 (12)	0.0188 (11)	0.0163 (11)	−0.0008 (9)	0.0004 (8)	0.0044 (9)
C6	0.0091 (10)	0.0132 (10)	0.0160 (10)	−0.0037 (9)	0.0032 (8)	0.0004 (9)
C7	0.0125 (11)	0.0137 (10)	0.0133 (10)	−0.0043 (9)	0.0033 (9)	−0.0010 (9)
N2	0.0186 (11)	0.0117 (9)	0.0145 (9)	0.0011 (8)	−0.0009 (7)	0.0004 (8)
C3	0.0189 (13)	0.0231 (12)	0.0133 (10)	−0.0065 (9)	0.0009 (9)	−0.0015 (10)
C1	0.0113 (11)	0.0129 (11)	0.0129 (10)	0.0004 (9)	0.0005 (8)	0.0027 (8)
C8	0.0167 (13)	0.0162 (10)	0.0215 (11)	0.0010 (10)	−0.0008 (9)	0.0034 (9)

Geometric parameters (Å, º)

S1—C1	1.746 (2)	N1—C7	1.289 (2)
S1—C7	1.756 (2)	N1—C6	1.399 (2)
C5—C4	1.389 (3)	C4—C3	1.379 (3)
C5—C6	1.397 (3)	C4—H4	0.9500
C5—C8	1.516 (3)	C6—C1	1.407 (2)
N3—N2	1.420 (2)	C7—N2	1.375 (3)
N3—H3A	0.923 (9)	N2—H2	0.891 (9)
N3—H3B	0.903 (9)	C3—H3	0.9500
C2—C3	1.387 (3)	C8—H8A	0.9800
C2—C1	1.388 (2)	C8—H8B	0.9800
C2—H2A	0.9500	C8—H8C	0.9800

C1—S1—C7	87.97 (10)	N1—C7—S1	117.74 (15)
C4—C5—C6	117.47 (18)	N2—C7—S1	118.61 (15)
C4—C5—C8	121.90 (18)	C7—N2—N3	115.08 (15)
C6—C5—C8	120.64 (17)	C7—N2—H2	117.6 (16)
N2—N3—H3A	110.0 (13)	N3—N2—H2	110.2 (17)
N2—N3—H3B	110.7 (14)	C4—C3—C2	121.44 (19)
H3A—N3—H3B	109.6 (12)	C4—C3—H3	119.3
C3—C2—C1	117.26 (17)	C2—C3—H3	119.3
C3—C2—H2A	121.4	C2—C1—C6	121.80 (18)
C1—C2—H2A	121.4	C2—C1—S1	128.72 (15)
C7—N1—C6	109.43 (16)	C6—C1—S1	109.47 (14)
C3—C4—C5	121.98 (19)	C5—C8—H8A	109.5
C3—C4—H4	119.0	C5—C8—H8B	109.5
C5—C4—H4	119.0	H8A—C8—H8B	109.5
C5—C6—N1	124.57 (18)	C5—C8—H8C	109.5
C5—C6—C1	120.04 (17)	H8A—C8—H8C	109.5
N1—C6—C1	115.39 (17)	H8B—C8—H8C	109.5
N1—C7—N2	123.57 (18)		

C6—C5—C4—C3	0.6 (3)	N1—C7—N2—N3	−165.94 (18)
C8—C5—C4—C3	−179.61 (17)	S1—C7—N2—N3	17.4 (2)
C4—C5—C6—N1	179.46 (18)	C5—C4—C3—C2	−0.4 (3)
C8—C5—C6—N1	−0.3 (3)	C1—C2—C3—C4	0.5 (3)
C4—C5—C6—C1	−0.9 (3)	C3—C2—C1—C6	−0.9 (3)
C8—C5—C6—C1	179.27 (16)	C3—C2—C1—S1	−179.19 (14)
C7—N1—C6—C5	179.87 (19)	C5—C6—C1—C2	1.1 (3)
C7—N1—C6—C1	0.3 (2)	N1—C6—C1—C2	−179.26 (17)
C6—N1—C7—N2	−176.41 (18)	C5—C6—C1—S1	179.73 (15)
C6—N1—C7—S1	0.3 (2)	N1—C6—C1—S1	−0.6 (2)
C1—S1—C7—N1	−0.54 (17)	C7—S1—C1—C2	179.11 (18)
C1—S1—C7—N2	176.31 (16)	C7—S1—C1—C6	0.61 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N3^{i}	0.89 (1)	2.30 (2)	2.996 (3)	135 (2)
N3—H3*A*···N1^{ii}	0.92 (1)	2.21 (1)	3.077 (3)	156 (2)

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