

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

## 2-(Benzothiazol-2-ylsulfanyl)acetic acid

Zhi-li Fang<sup>a\*</sup> and Jun Wang<sup>b</sup>

<sup>a</sup>School of Basic Science, East China Jiaotong University, Nanchang 330013, People's Republic of China, and <sup>b</sup>Zhongshan Polytechnic, Zhongshan, Guangdong 528404, People's Republic of China  
Correspondence e-mail: fhcgdfz@yahoo.cn

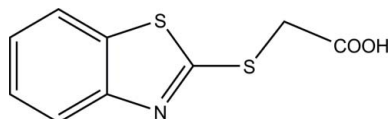
Received 18 September 2010; accepted 15 October 2010

Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.030;  $wR$  factor = 0.079; data-to-parameter ratio = 13.1.

In the title compound,  $\text{C}_9\text{H}_7\text{NO}_2\text{S}_2$ , the benzene ring is essentially co-planar with the thiazole ring, making a dihedral angle of  $0.36$  (7)°. In the crystal structure, molecules are linked by intermolecular  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bonds between the carboxy group and the thiazole N atom into chains along  $[10\bar{1}]$ . The chains are assembled into a supermolecular layer structure by thiazole ring  $\text{S}\cdots\text{S}$  contacts [ $3.5679$  (7) Å].

### Related literature

For the structure of tris(2-hydroxyethyl)ammonium 3-benzothiazole-2-thiolate, see: Zhu *et al.* (2009). For  $\text{S}\cdots\text{S}$  contacts in similar compounds, see: Dai *et al.* (1997).



### Experimental

#### Crystal data

$\text{C}_9\text{H}_7\text{NO}_2\text{S}_2$   
 $M_r = 225.28$   
Monoclinic,  $P2_1/c$   
 $a = 6.0374$  (5) Å

$b = 19.2450$  (17) Å  
 $c = 8.1250$  (7) Å  
 $\beta = 90.419$  (1)°  
 $V = 944.02$  (14) Å<sup>3</sup>

$Z = 4$   
Mo  $K\alpha$  radiation  
 $\mu = 0.53$  mm<sup>-1</sup>

$T = 296$  K  
 $0.23 \times 0.21 \times 0.17$  mm

#### Data collection

Bruker APEXII CCD diffractometer  
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.885$ ,  $T_{\max} = 0.914$

4800 measured reflections  
1695 independent reflections  
1439 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.021$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$   
 $wR(F^2) = 0.079$   
 $S = 1.04$   
1695 reflections

129 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.25$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.16$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1}\cdots\text{N1}^i$	0.82	1.89	2.686 (2)	165

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; 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.

The authors acknowledge South China Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DS2058).

### References

- Bruker (2004). APEX2 and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.  
Dai, J., Munakata, M., Kuroda-Sowa, T., Suenaga, Y., Wu, L. P. & Yamamoto, M. (1997). *Inorg. Chim. Acta*, **258**, 65–69.  
Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.  
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
Zhu, J.-Q., Fang, H.-C., Chen, B.-Y., Feng, M.-S. & Li, J.-N. (2009). *Acta Cryst.* **E65**, o1640.

**supplementary materials**

*Acta Cryst.* (2010). E66, o2912 [ doi:10.1107/S1600536810041796 ]

## 2-(Benzothiazol-2-ylsulfanyl)acetic acid

Z. Fang and J. Wang

### Experimental

A solution of benzothiazole-2-thiol (167.2 mg, 1.00 mmol) and  $K_2CO_3$  (207.0 mg, 1.50 mmol) in  $CH_3OH$  (15 ml) was slowly added to a solution of 2-chloroacetic acid (113.4 mg, 1.20 mmol) in  $CH_3OH$  (10 ml). The resultant solution was stirred and refluxed for 20 h and then filtered. Colorless crystals suitable for X-ray diffraction were obtained in about a week by slow diffusion of diethyl ether into a dilute solution of the title compound in methanol. yield: ca 82.3% (based on benzothiazole-2-thiol).

### Refinement

The structure was solved using direct methods followed by Fourier synthesis. Non-H atoms were refined anisotropically. All of H atoms were placed in idealized positions ( $C-H = 0.93$  or  $0.97$  Å,  $O-H = 0.82$  Å), forced to ride on the atom to which they are bonded, and were included in the refinement in the riding-model approximation.  $U_{iso}$  values were set equal to  $1.5U_{eq}(\text{parent atom})$  for carboxylic H atom and to  $1.2U_{eq}(\text{parent atom})$  for all other H atoms.

### Figures

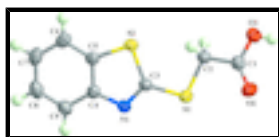


Fig. 1. The structure of the title compound with 50% probability displacement ellipsoids.

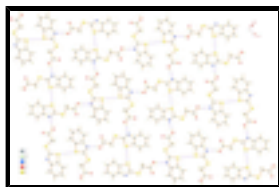


Fig. 2. Two-dimensional supramolecular layer which is connected by  $O-H\cdots N$  [ $O\cdots N$  2.686 (2) Å,  $H\cdots N$  1.89 Å,  $O-H\cdots N$  165.3°, symmetry code:  $x + 1, -y + 3/2, z + 1/2$ ] hydrogen bonds and  $S\cdots S$  [ $S\cdots S$  3.568 Å, symmetry code:  $1-x, 1-y, 1-z$ ] contacts.

## 2-(Benzothiazol-2-ylsulfanyl)acetic acid

### Crystal data

$C_9H_7NO_2S_2$

$M_r = 225.28$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P 2ybc$

$a = 6.0374$  (5) Å

$b = 19.2450$  (17) Å

$c = 8.1250$  (7) Å

$F(000) = 464$

$D_x = 1.585$  Mg m $^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2101 reflections

$\theta = 2.7-27.5^\circ$

$\mu = 0.53$  mm $^{-1}$

$T = 296$  K

# supplementary materials

---

$\beta = 90.419 (1)^\circ$   
 $V = 944.02 (14) \text{ \AA}^3$   
 $Z = 4$

Block, pink  
 $0.23 \times 0.21 \times 0.17 \text{ mm}$

## Data collection

Bruker APEXII CCD diffractometer  
Radiation source: fine-focus sealed tube graphite  
 $\varphi$  and  $\omega$  scans  
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.885$ ,  $T_{\max} = 0.914$   
4800 measured reflections

1695 independent reflections  
1439 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.021$   
 $\theta_{\max} = 25.2^\circ$ ,  $\theta_{\min} = 2.1^\circ$   
 $h = -4 \rightarrow 7$   
 $k = -22 \rightarrow 23$   
 $l = -9 \rightarrow 9$

## Refinement

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.030$   
 $wR(F^2) = 0.079$   
 $S = 1.04$   
1695 reflections  
129 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0386P)^2 + 0.2852P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.25 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.16 \text{ e \AA}^{-3}$

## 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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.5666 (3)	0.77360 (10)	0.5938 (3)	0.0446 (5)
C2	0.4631 (3)	0.70448 (10)	0.5538 (3)	0.0424 (5)
H2A	0.4289	0.6798	0.6546	0.051*

H2B	0.5654	0.6764	0.4906	0.051*
C3	0.1497 (3)	0.63490 (9)	0.3747 (2)	0.0367 (4)
C4	-0.0451 (3)	0.55193 (10)	0.2515 (2)	0.0371 (4)
C5	0.1331 (3)	0.51163 (10)	0.3081 (2)	0.0391 (4)
C6	0.1436 (4)	0.44073 (10)	0.2773 (3)	0.0509 (5)
H6	0.2624	0.4143	0.3154	0.061*
C7	-0.0259 (4)	0.41063 (11)	0.1894 (3)	0.0556 (6)
H7	-0.0223	0.3632	0.1677	0.067*
C8	-0.2024 (4)	0.45021 (12)	0.1327 (3)	0.0531 (6)
H8	-0.3154	0.4287	0.0732	0.064*
C9	-0.2144 (3)	0.52022 (11)	0.1620 (2)	0.0458 (5)
H9	-0.3337	0.5461	0.1228	0.055*
N1	-0.0309 (3)	0.62213 (8)	0.2909 (2)	0.0396 (4)
O1	0.7348 (3)	0.76603 (7)	0.6956 (2)	0.0557 (4)
H1	0.7911	0.8041	0.7140	0.084*
O2	0.5039 (3)	0.82751 (8)	0.5396 (2)	0.0736 (5)
S1	0.21328 (9)	0.71923 (3)	0.43642 (7)	0.04900 (19)
S2	0.31920 (8)	0.56396 (2)	0.41411 (7)	0.04382 (18)

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0430 (11)	0.0378 (11)	0.0528 (12)	0.0004 (9)	-0.0105 (10)	-0.0021 (9)
C2	0.0413 (11)	0.0343 (10)	0.0515 (12)	0.0031 (8)	-0.0147 (9)	0.0004 (8)
C3	0.0340 (10)	0.0336 (10)	0.0422 (11)	0.0021 (8)	-0.0077 (8)	0.0014 (8)
C4	0.0402 (10)	0.0332 (10)	0.0378 (10)	-0.0017 (8)	-0.0033 (8)	0.0011 (8)
C5	0.0420 (11)	0.0354 (10)	0.0398 (10)	0.0014 (8)	-0.0068 (9)	0.0023 (8)
C6	0.0621 (14)	0.0344 (11)	0.0560 (13)	0.0066 (9)	-0.0087 (11)	0.0005 (9)
C7	0.0772 (16)	0.0335 (11)	0.0562 (13)	-0.0083 (11)	-0.0032 (12)	-0.0042 (10)
C8	0.0589 (14)	0.0514 (13)	0.0489 (12)	-0.0166 (11)	-0.0080 (10)	-0.0046 (10)
C9	0.0410 (11)	0.0495 (12)	0.0468 (12)	-0.0027 (9)	-0.0099 (9)	0.0009 (9)
N1	0.0387 (9)	0.0344 (8)	0.0455 (9)	0.0022 (7)	-0.0121 (7)	0.0010 (7)
O1	0.0507 (9)	0.0409 (8)	0.0751 (11)	-0.0069 (7)	-0.0270 (8)	0.0023 (7)
O2	0.0777 (12)	0.0336 (9)	0.1090 (14)	-0.0015 (8)	-0.0464 (10)	0.0066 (8)
S1	0.0454 (3)	0.0309 (3)	0.0703 (4)	0.0053 (2)	-0.0231 (3)	-0.0041 (2)
S2	0.0415 (3)	0.0336 (3)	0.0560 (3)	0.00667 (19)	-0.0177 (2)	-0.0010 (2)

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

C1—O2	1.188 (2)	C4—C5	1.401 (3)
C1—O1	1.313 (2)	C5—C6	1.389 (3)
C1—C2	1.504 (3)	C5—S2	1.7332 (19)
C2—S1	1.8012 (19)	C6—C7	1.372 (3)
C2—H2A	0.9700	C6—H6	0.9300
C2—H2B	0.9700	C7—C8	1.386 (3)
C3—N1	1.304 (2)	C7—H7	0.9300
C3—S2	1.7345 (18)	C8—C9	1.370 (3)
C3—S1	1.7407 (18)	C8—H8	0.9300
C4—N1	1.391 (2)	C9—H9	0.9300

## supplementary materials

C4—C9	1.391 (3)	O1—H1	0.8200
O2—C1—O1	124.99 (19)	C4—C5—S2	109.55 (14)
O2—C1—C2	124.15 (19)	C7—C6—C5	118.3 (2)
O1—C1—C2	110.86 (17)	C7—C6—H6	120.9
C1—C2—S1	108.66 (14)	C5—C6—H6	120.9
C1—C2—H2A	110.0	C6—C7—C8	120.7 (2)
S1—C2—H2A	110.0	C6—C7—H7	119.7
C1—C2—H2B	110.0	C8—C7—H7	119.7
S1—C2—H2B	110.0	C9—C8—C7	121.6 (2)
H2A—C2—H2B	108.3	C9—C8—H8	119.2
N1—C3—S2	115.97 (14)	C7—C8—H8	119.2
N1—C3—S1	120.51 (14)	C8—C9—C4	118.9 (2)
S2—C3—S1	123.51 (11)	C8—C9—H9	120.6
N1—C4—C9	126.16 (18)	C4—C9—H9	120.6
N1—C4—C5	114.61 (16)	C3—N1—C4	110.65 (15)
C9—C4—C5	119.22 (18)	C1—O1—H1	109.5
C6—C5—C4	121.37 (18)	C3—S1—C2	100.82 (9)
C6—C5—S2	129.08 (16)	C5—S2—C3	89.21 (9)
O2—C1—C2—S1	-7.7 (3)	C5—C4—C9—C8	0.4 (3)
O1—C1—C2—S1	172.54 (15)	S2—C3—N1—C4	0.0 (2)
N1—C4—C5—C6	-179.50 (19)	S1—C3—N1—C4	178.49 (14)
C9—C4—C5—C6	-0.3 (3)	C9—C4—N1—C3	-179.45 (19)
N1—C4—C5—S2	0.5 (2)	C5—C4—N1—C3	-0.3 (2)
C9—C4—C5—S2	179.69 (15)	N1—C3—S1—C2	176.73 (16)
C4—C5—C6—C7	0.0 (3)	S2—C3—S1—C2	-4.87 (16)
S2—C5—C6—C7	-179.96 (17)	C1—C2—S1—C3	170.23 (15)
C5—C6—C7—C8	0.2 (3)	C6—C5—S2—C3	179.6 (2)
C6—C7—C8—C9	-0.1 (4)	C4—C5—S2—C3	-0.40 (15)
C7—C8—C9—C4	-0.2 (3)	N1—C3—S2—C5	0.25 (16)
N1—C4—C9—C8	179.49 (19)	S1—C3—S2—C5	-178.21 (14)

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 $\cdots$ N1 <sup>i</sup>	0.82	1.89	2.686 (2)	165

Symmetry codes: (i)  $x+1, -y+3/2, z+1/2$ .

Fig. 1

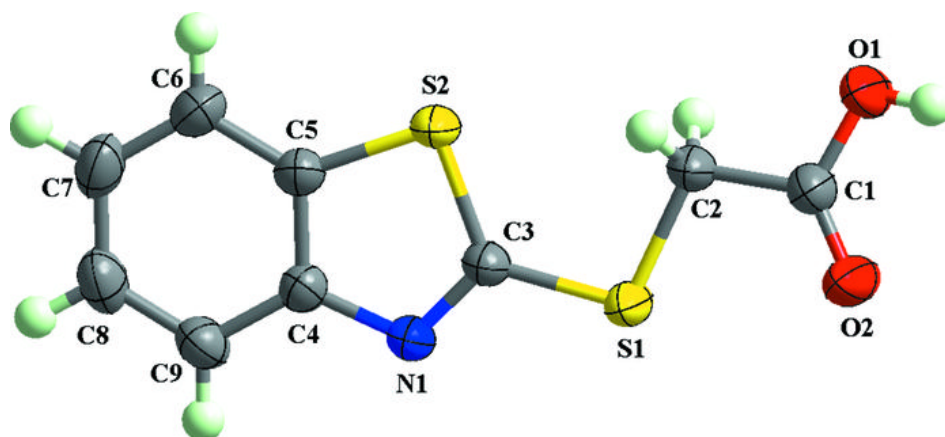


Fig. 2

