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2-(Benzothiazol-2-ylsulfanyl)acetic acid

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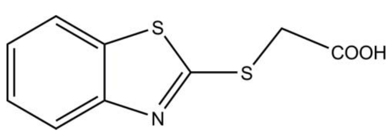
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.030; wR factor = 0.079; data-to-parameter ratio = 13.1.

In the title compound, $C_9H_7NO_2S_2$, the benzine 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 O—H···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 S···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 S···S contacts in similar compounds, see: Dai *et al.* (1997).



Experimental

Crystal data

$C_9H_7NO_2S_2$
M_r = 225.28
Monoclinic, $P2_1/c$
a = 6.0374 (5) Å
b = 19.2450 (17) Å
c = 8.1250 (7) Å
β = 90.419 (1)°
V = 944.02 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.53 mm^{-1}
T = 296 K
0.23 × 0.21 × 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_{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^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.82	1.89	2.686 (2)	165

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

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*.

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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.* A**64**, 112–122.
Zhu, J.-Q., Fang, H.-C., Chen, B.-Y., Feng, M.-S. & Li, J.-N. (2009). *Acta Cryst.* E**65**, o1640.

supporting information

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2-(Benzothiazol-2-ylsulfanyl)acetic acid

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S1. 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).

S2. 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}(parent atom) for carboxylic H atom and to 1.2U_{eq}(parent atom)for all other H atoms.

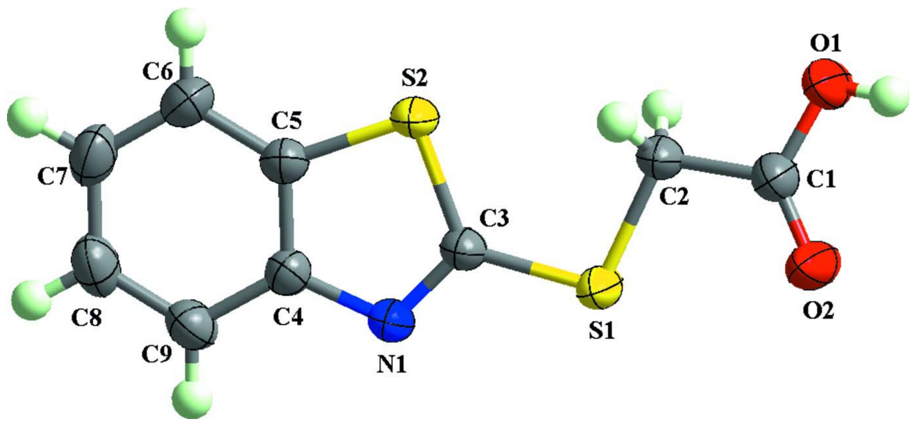

Figure 1

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

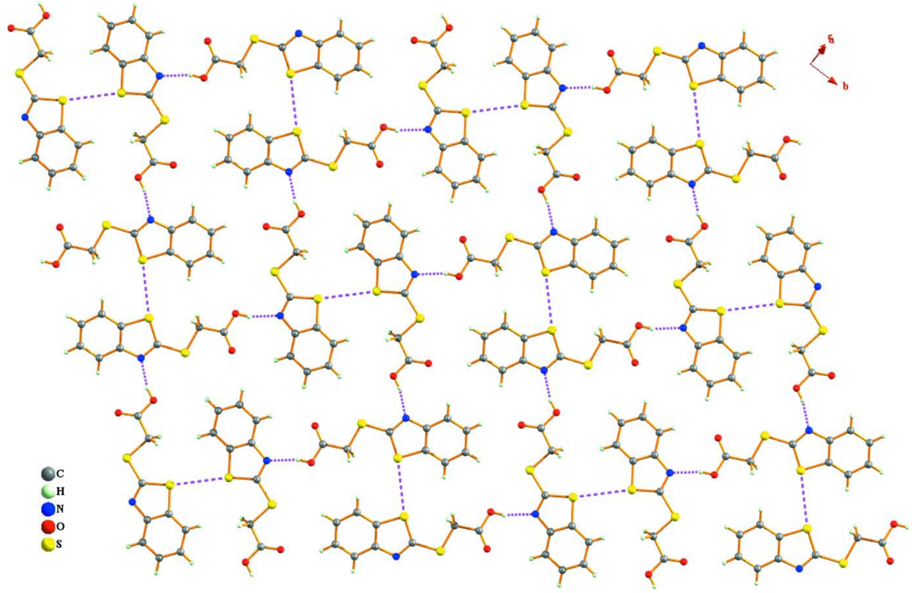

Figure 2

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

2-(Benzothiazol-2-ylsulfanyl)acetic acid

Crystal data

$C_9H_7NO_2S_2$	$F(000) = 464$
$M_r = 225.28$	$D_x = 1.585$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 2101 reflections
$a = 6.0374$ (5) Å	$\theta = 2.7$–27.5°
$b = 19.2450$ (17) Å	$\mu = 0.53$ mm^{-1}
$c = 8.1250$ (7) Å	$T = 296$ K
$\beta = 90.419$ (1)°	Block, pink
$V = 944.02$ (14) Å^3	0.23 × 0.21 × 0.17 mm
$Z = 4$	

Data collection

Bruker APEXII CCD diffractometer	4800 measured reflections
Radiation source: fine-focus sealed tube	1695 independent reflections
Graphite monochromator	1439 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.021$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 25.2°$, $\theta_{min} = 2.1°$
$T_{min} = 0.885$, $T_{max} = 0.914$	$h = -4 \rightarrow 7$
	$k = -22 \rightarrow 23$
	$l = -9 \rightarrow 9$

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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-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 (Å²)

	x	y	z	U_{iso}*/U_{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 (Å^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 (Å, º)

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
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 (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.82	1.89	2.686 (2)	165

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