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## Structure Reports

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## 1,3-Benzothiazol-2-amine

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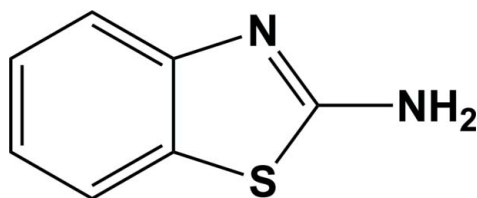
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Key indicators: single-crystal X-ray study;  $T = 173$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.052;  $wR$  factor = 0.143; data-to-parameter ratio = 11.9.

In the crystal structure of the title compound,  $\text{C}_7\text{H}_6\text{N}_2\text{S}$ , molecules related by an inversion center are linked *via*  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bonds involving the amino groups, forming dimers. In turn, these dimers are linked *via* a second  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bond, forming an infinite two-dimensional network parallel to (011).

### Related literature

For the original powder diffraction study of the title compound, see: Goubitz *et al.* (2001). For related structures containing the title compound, see: Martínez-Martínez *et al.* (2003); Padilla-Martínez *et al.* (2003); Wang *et al.* (2008). For a description of the Cambridge Structural Database, see: Allen (2002).



### Experimental

#### Crystal data

$\text{C}_7\text{H}_6\text{N}_2\text{S}$   
 $M_r = 150.20$   
 Monoclinic,  $P2_1/c$

$a = 14.606$  (4) Å  
 $b = 3.997$  (1) Å  
 $c = 11.565$  (4) Å

$\beta = 94.47$  (2)°  
 $V = 673.1$  (3) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation

$\mu = 0.39$  mm<sup>-1</sup>  
 $T = 173$  K  
 $0.50 \times 0.50 \times 0.50$  mm

#### Data collection

Stoe IPDS-2 diffractometer  
 Absorption correction: none  
 2783 measured reflections

1181 independent reflections  
 1061 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.086$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$   
 $wR(F^2) = 0.143$   
 $S = 1.06$   
 1181 reflections  
 99 parameters  
 2 restraints

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.38$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.31$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N2}-\text{H2B}\cdots\text{N1}^i$	0.83 (2)	2.14 (2)	2.964 (3)	172 (2)
$\text{N2}-\text{H2A}\cdots\text{N2}^{ii}$	0.80 (2)	2.46 (2)	3.217 (3)	157 (2)

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

Data collection: *X-Area* (Stoe & Cie, 2006); cell refinement: *X-Area*; data reduction: *X-RED32* (Stoe & Cie, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

This work was supported by the Swiss National Science Foundation.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JH2090).

### References

- Allen, F. H. (2002). *Acta Cryst.* **B58**, 380–388.  
 Goubitz, K., Sonneveld, E. J. & Schenk, H. (2001). *Z. Kristallogr.* **216**, 176–181.  
 Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.  
 Martínez-Martínez, F. J., García-Báez, E. V., Höpfl, H. & Padilla-Martínez, I. I. (2003). *Acta Cryst.* **E59**, o1628–o1630.  
 Padilla-Martínez, I. I., García-Báez, E. V., Höpfl, H. & Martínez-Martínez, F. J. I. (2003). *Acta Cryst.* **C59**, o544–o546.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.  
 Stoe & Cie (2006). *X-Area* and *X-RED32*. Stoe & Cie, Darmstadt, Germany.  
 Wang, Y.-Y., Hu, R.-D. & Wang, Y.-J. (2008). *Acta Cryst.* **E64**, o1442.

**supplementary materials**

*Acta Cryst.* (2009). E65, o1894 [ doi:10.1107/S1600536809027561 ]

## 1,3-Benzothiazol-2-amine

M. Altaf and H. Stoeckli-Evans

### Comment

The first reference to the crystal structure of the title compound appeared in a study by (Goubitz *et al.*, 2001) on the crystal structure determination of a series of small organic molecules from powder diffraction data. The analysis, using Guinier photographic data, was successful but the final Reitveld refinement gave an  $R_f$  value of only 16.4%. Herein, we report on a single-crystal low temperature analysis (173 K) of the title compound.

A search of the Cambridge Structural Database (Allen, 2002; CSD version 5.30, last update May 2009) revealed the presence of the title compound in a number of co-crystals, for example, with *rac*-7-oxabicyclo[2.2.1]heptane-2,3-dicarboxylic acid (Wang *et al.*, 2008), and in some (1/1) donor-acceptor complexes, for example, with *N*-benzyl-2-oxo-2*H*-1-benzopyran-3-carboximide (Martínez-Martínez *et al.*, 2003) and ethyl-coumarin-3-carboxylate (Padilla-Martínez *et al.*, 2003).

The molecular structure of the title compound is illustrated in Fig. 1. The geometric parameters are available in the archived CIF and are similar to those in the above mentioned compounds.

In the crystal of the title compound molecules related by an inversion center are linked by  $N2-H2B \cdots N1^i$  [symmetry operation: (i)  $-x, -y + 1, -z$ ] hydrogen bonds to form centrosymmetric dimers (Table 1 and Fig. 2). These dimers are further linked *via*  $N2-H2A \cdots N1^{ii}$  [symmetry operation: (ii)  $-x, y - 1/2, -z + 1/2$ ] interactions to form infinite two-dimensional networks lying parallel to the (011) plane, and stacking along the [100] direction.

### Experimental

Single crystals of the title compound were obtained by recrystallization from methanol of a reagent grade sample.

### Refinement

All the H-atoms could be located in difference electron-density maps. The amino H-atoms were refined isotropically with distance restraints:  $N-H = 0.82$  (2) Å. The aromatic H-atoms were included in calculated positions and treated as riding atoms:  $C-H = 0.95$  Å with  $U_{iso}(H) = 1.2U_{eq}(\text{parent C-atom})$ .

### Figures

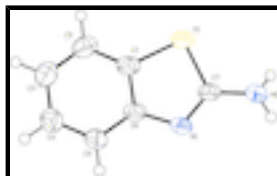


Fig. 1. A view of the molecular structure of the title compound, with the displacement ellipsoids drawn at the 50% probability level.

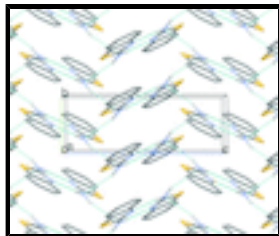


Fig. 2. A view along the  $a$  axis of the crystal packing of the title compound, illustrating the formation of the centrosymmetric hydrogen bonded dimers and the two-dimensional hydrogen bonded network (see Table 1 for details; the hydrogen bonds are shown as pale-blue dashed lines; H-atoms not involved in hydrogen bonding have been omitted for clarity).

## 1,3-Benzothiazol-2-amine

### Crystal data

$C_7H_6N_2S$

$M_r = 150.20$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 14.606$  (4) Å

$b = 3.997$  (1) Å

$c = 11.565$  (4) Å

$\beta = 94.47$  (2)°

$V = 673.1$  (3) Å<sup>3</sup>

$Z = 4$

$F_{000} = 312$

$D_x = 1.482$  Mg m<sup>-3</sup>

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

Cell parameters from 42133 reflections

$\theta = 3.5$ – $25.6$ °

$\mu = 0.39$  mm<sup>-1</sup>

$T = 173$  K

Block, colourless

$0.50 \times 0.50 \times 0.50$  mm

### Data collection

Stoe IPDS-2  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 173$  K

$\varphi$  and  $\omega$  scans

Absorption correction: none

2783 measured reflections

1181 independent reflections

1061 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.086$

$\theta_{\text{max}} = 25.2$ °

$\theta_{\text{min}} = 3.5$ °

$h = -17 \rightarrow 15$

$k = -4 \rightarrow 4$

$l = -13 \rightarrow 13$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.052$

$wR(F^2) = 0.143$

$S = 1.06$

1181 reflections

99 parameters

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

$$w = 1/[\sigma^2(F_o^2) + (0.1031P)^2 + 0.0494P]$$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 0.38$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.31$  e Å<sup>-3</sup>

2 restraints

Extinction correction: none

Primary atom site location: structure-invariant direct methods

*Special details*

**Geometry.** Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**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>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.17155 (4)	0.19806 (15)	0.24812 (4)	0.0406 (3)
N1	0.12810 (12)	0.4914 (5)	0.04966 (13)	0.0373 (5)
N2	0.00290 (14)	0.2707 (6)	0.14135 (17)	0.0427 (7)
C1	0.25983 (15)	0.3777 (6)	0.17558 (17)	0.0391 (7)
C2	0.35252 (17)	0.3886 (7)	0.2091 (2)	0.0481 (8)
C3	0.40994 (17)	0.5406 (7)	0.1364 (2)	0.0523 (8)
C4	0.37475 (18)	0.6870 (6)	0.0321 (2)	0.0492 (8)
C5	0.28136 (17)	0.6797 (6)	-0.0011 (2)	0.0435 (7)
C6	0.22260 (15)	0.5222 (5)	0.07108 (17)	0.0381 (6)
C7	0.09342 (15)	0.3274 (5)	0.13327 (18)	0.0367 (7)
H2	0.37610	0.29340	0.28060	0.0580*
H2A	-0.009 (2)	0.116 (6)	0.182 (2)	0.062 (9)*
H2B	-0.0377 (18)	0.328 (7)	0.091 (2)	0.063 (9)*
H3	0.47420	0.54640	0.15710	0.0630*
H4	0.41550	0.79300	-0.01660	0.0590*
H5	0.25790	0.78020	-0.07170	0.0520*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0458 (5)	0.0516 (5)	0.0240 (4)	0.0062 (2)	0.0010 (3)	0.0025 (2)
N1	0.0421 (10)	0.0481 (10)	0.0218 (8)	0.0010 (8)	0.0038 (7)	-0.0002 (7)
N2	0.0419 (11)	0.0582 (12)	0.0282 (11)	-0.0013 (9)	0.0048 (8)	0.0087 (8)
C1	0.0429 (12)	0.0467 (11)	0.0278 (11)	0.0062 (9)	0.0038 (9)	-0.0062 (8)
C2	0.0472 (13)	0.0581 (14)	0.0376 (12)	0.0064 (11)	-0.0050 (10)	-0.0080 (10)
C3	0.0391 (12)	0.0645 (16)	0.0526 (15)	0.0011 (11)	-0.0001 (11)	-0.0144 (12)
C4	0.0458 (14)	0.0573 (15)	0.0456 (14)	-0.0084 (10)	0.0103 (11)	-0.0114 (10)
C5	0.0454 (13)	0.0546 (14)	0.0310 (11)	-0.0034 (10)	0.0067 (9)	-0.0056 (9)
C6	0.0443 (12)	0.0456 (11)	0.0242 (10)	0.0010 (9)	0.0023 (8)	-0.0057 (8)
C7	0.0425 (12)	0.0459 (13)	0.0215 (10)	0.0039 (9)	0.0017 (9)	-0.0031 (8)

## supplementary materials

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

S1—C1	1.747 (2)	C2—C3	1.375 (4)
S1—C7	1.760 (2)	C3—C4	1.402 (3)
N1—C6	1.389 (3)	C4—C5	1.388 (4)
N1—C7	1.303 (3)	C5—C6	1.393 (3)
N2—C7	1.352 (3)	C2—H2	0.9500
N2—H2B	0.83 (2)	C3—H3	0.9500
N2—H2A	0.80 (2)	C4—H4	0.9500
C1—C6	1.410 (3)	C5—H5	0.9500
C1—C2	1.380 (3)		
C1—S1—C7	88.64 (10)	N1—C6—C1	115.36 (18)
C6—N1—C7	110.53 (17)	N1—C6—C5	125.68 (19)
H2A—N2—H2B	117 (3)	S1—C7—N1	116.18 (16)
C7—N2—H2B	123.7 (18)	S1—C7—N2	118.60 (16)
C7—N2—H2A	115 (2)	N1—C7—N2	125.1 (2)
C2—C1—C6	122.2 (2)	C1—C2—H2	121.00
S1—C1—C6	109.29 (16)	C3—C2—H2	121.00
S1—C1—C2	128.54 (17)	C2—C3—H3	120.00
C1—C2—C3	118.3 (2)	C4—C3—H3	120.00
C2—C3—C4	120.7 (2)	C3—C4—H4	119.00
C3—C4—C5	121.0 (2)	C5—C4—H4	120.00
C4—C5—C6	118.8 (2)	C4—C5—H5	121.00
C1—C6—C5	119.0 (2)	C6—C5—H5	121.00
C7—S1—C1—C2	-179.8 (2)	S1—C1—C6—N1	0.0 (2)
C7—S1—C1—C6	0.41 (17)	S1—C1—C6—C5	-179.83 (17)
C1—S1—C7—N1	-0.79 (18)	C2—C1—C6—N1	-179.8 (2)
C1—S1—C7—N2	-176.53 (19)	C2—C1—C6—C5	0.4 (3)
C7—N1—C6—C1	-0.6 (3)	C1—C2—C3—C4	1.4 (4)
C7—N1—C6—C5	179.2 (2)	C2—C3—C4—C5	-0.6 (4)
C6—N1—C7—S1	0.9 (2)	C3—C4—C5—C6	-0.3 (4)
C6—N1—C7—N2	176.3 (2)	C4—C5—C6—N1	-179.4 (2)
S1—C1—C2—C3	179.0 (2)	C4—C5—C6—C1	0.4 (3)
C6—C1—C2—C3	-1.2 (4)		

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2B $\cdots$ N1 <sup>i</sup>	0.83 (2)	2.14 (2)	2.964 (3)	172 (2)
N2—H2A $\cdots$ N2 <sup>ii</sup>	0.80 (2)	2.46 (2)	3.217 (3)	157 (2)

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

Fig. 1

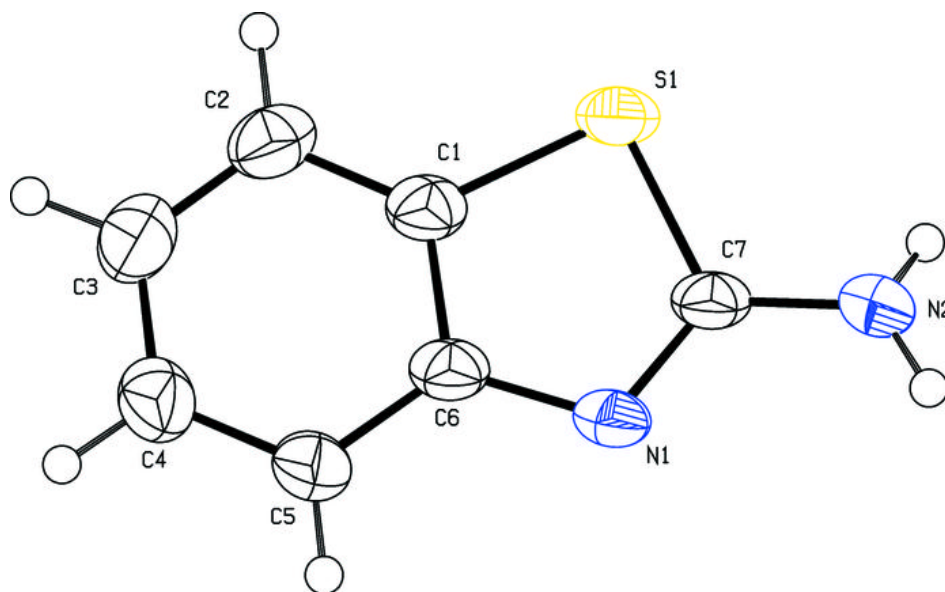


Fig. 2

