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## Key indicators

Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$   
 $R$  factor = 0.056  
 $wR$  factor = 0.125  
Data-to-parameter ratio = 15.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## 5-Amino-1,3-benzothiazole-2(3H)-thione

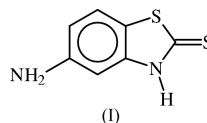
The two independent molecules of the title compound,  $\text{C}_7\text{H}_6\text{N}_2\text{S}_2$ , are linked by two secondary amino–thione hydrogen bonds [3.344 (3) and 3.376 (3) Å] to form a flat pseudo-centrosymmetric dimer.

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## Comment

Mercaptobenzothiazole exists in the thione form in the solid state (Chesick & Donohue, 1971; Radha, 1985). The deprotonated anion forms a large number of *N,S*-chelated metal complexes, *e.g.* cadmium di(benzothiazolyl-2-thiolate) (Hursthouse *et al.*, 1990) and tetramethylammonium tris-(benzothiazolyl-2-thiolate)nickelate (Rasper *et al.*, 1990); the diorganotin derivatives show cytotoxicity (Xanthopoulou *et al.*, 2003). Among the substituted compounds, the 5-chloro derivative has been extensively studied in view of its use as a drug (Antoniadis *et al.*, 2003).

The 5-amino-substituted compound, (I), exists with two molecules per asymmetric unit; these are linked by a pair of hydrogen bonds to form a pseudo-centrosymmetric dimer (Fig. 1 and Table 2). The parent compound, mercaptobenzothiazole, also exists as a hydrogen-bonded dimer (Chesick & Donohue, 1971; Radha, 1985). The molecules feature both long [ $\text{S1}-\text{C1}$  1.740 (3) Å and  $\text{S1}-\text{C2}$  1.751 (3) Å;  $\text{S1a}-\text{C1a}$  1.753 (3) Å and  $\text{S1a}-\text{C2a}$  1.762 (3) Å] and short [ $\text{S2}-\text{C1}$  1.688 (3) Å and  $\text{S2a}-\text{C1a}$  1.672 (3) Å] C–S bonds (Table 1).

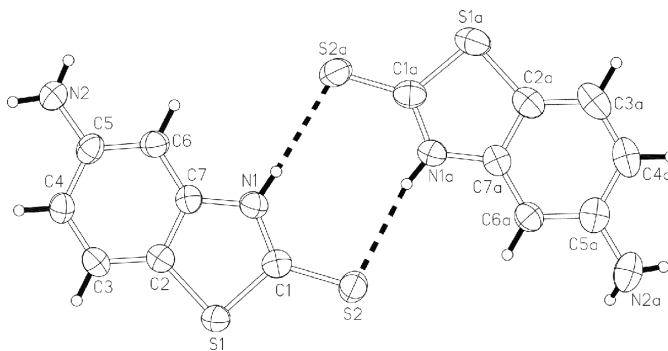


Figure 1

ORTEP II (Johnson, 1976) plot of the asymmetric unit of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii. Hydrogen bonds are indicated by dashed lines.

Hence, the title compound can be regarded as the thione tautomer in the solid state.

In the crystal structure the 'dimers' are hydrogen bonded to symmetry-related molecules, forming a zigzag sheet-like structure (Table 2).

## Experimental

An ethanol solution (50 ml) of *m*-phenylenediamine (0.22 g, 2 mmol) and carbon disulfide (15 ml, 2.4 mmol), kept at 273 K, was stirred for 2 h. The solution was then heated at reflux for 12 h. The reaction was carried out under an N<sub>2</sub> atmosphere. The solution was poured into water to afford a solid material that was recrystallized from ethanol.

### Crystal data

C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> S <sub>2</sub>	$D_x = 1.526 \text{ Mg m}^{-3}$
$M_r = 182.26$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 1662 reflections
$a = 5.1041$ (2) Å	$\theta = 2.4\text{--}23.3^\circ$
$b = 20.3859$ (7) Å	$\mu = 0.60 \text{ mm}^{-1}$
$c = 15.3378$ (5) Å	$T = 298$ (2) K
$\beta = 96.279$ (2)°	Block, yellow
$V = 1586.4$ (1) Å <sup>3</sup>	$0.32 \times 0.12 \times 0.09 \text{ mm}$
$Z = 8$	

### Data collection

Bruker SMART APEX area-detector diffractometer	2332 reflections with $I > 2\sigma(I)$
$\varphi$ and $\omega$ scans	$R_{\text{int}} = 0.046$
Absorption correction: none	$\theta_{\text{max}} = 27.5^\circ$
9371 measured reflections	$h = -5 \rightarrow 6$
3531 independent reflections	$k = -26 \rightarrow 19$
	$l = -19 \rightarrow 19$

### Refinement

Refinement on $F^2$	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.056$	$w = 1/[\sigma^2(F_o^2) + (0.0557P)^2]$
$wR(F^2) = 0.125$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.95$	$(\Delta/\sigma)_{\text{max}} = 0.001$
3531 reflections	$\Delta\rho_{\text{max}} = 0.34 \text{ e \AA}^{-3}$
223 parameters	$\Delta\rho_{\text{min}} = -0.24 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

S1—C1	1.740 (3)	S1a—C1a	1.753 (3)
S1—C2	1.751 (3)	S1a—C2a	1.762 (3)
S2—C1	1.688 (3)	S2a—C1a	1.672 (3)
N1—C1	1.344 (4)	N1a—C1a	1.350 (4)
N1—C7	1.402 (4)	N1a—C7a	1.392 (4)
N2—C5	1.391 (4)	N2a—C5a	1.410 (4)
C1—S1—C2	92.1 (1)	C1a—S1a—C2a	92.5 (2)
C1—N1—C7	116.8 (3)	C1a—N1a—C7a	117.5 (3)
N1—C1—S1	109.8 (2)	N1a—C1a—S1a	108.7 (2)
N1—C1—S2	128.2 (2)	N1a—C1a—S2a	127.4 (2)
S1—C1—S2	122.0 (2)	S1a—C1a—S2a	123.9 (2)

**Table 2**

Hydrogen-bonding geometry (Å, °).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
N1—H1n <sup>i</sup> ···S2a	0.86 (1)	2.52 (1)	3.376 (3)	177 (3)
N2—H2n1 <sup>i</sup> ···N2a <sup>i</sup>	0.86 (1)	2.39 (1)	3.223 (5)	163 (3)
N2—H2n2 <sup>i</sup> ···S2a <sup>ii</sup>	0.85 (1)	2.87 (2)	3.641 (3)	151 (3)
N1a—H1na <sup>i</sup> ···S2	0.86 (1)	2.51 (1)	3.344 (3)	164 (2)
N2a—H2nb <sup>i</sup> ···S2 <sup>iii</sup>	0.86 (1)	2.96 (2)	3.685 (3)	143 (3)
N2a—H2nb <sup>i</sup> ···S1a <sup>iv</sup>	0.86 (1)	3.11 (3)	3.726 (4)	130 (3)

Symmetry codes: (i)  $1 - x, y - \frac{1}{2}, \frac{3}{2} - z$ ; (ii)  $-x, 1 - y, 1 - z$ ; (iii)  $1 + x, y, z$ ; (iv)  $1 + x, \frac{3}{2} - y, \frac{1}{2} + z$ .

The aromatic H atoms were placed at calculated positions (C—H = 0.93 Å) in the riding-model approximation; the  $U_{\text{iso}}(\text{H})$  values were set equal to 1.2 $U_{\text{eq}}$ (parent C atom). The N-bound H atoms were located and refined with an N—H = 0.86 (1) Å distance restraint.

Data collection: SMART (Bruker, 2001); cell refinement: SMART; data reduction: SAINT (Bruker, 2001); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXL97.

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