

## Phenylthiourea

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## Key indicators

Single-crystal X-ray study  
 $T = 295$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.037  
 $wR$  factor = 0.091  
Data-to-parameter ratio = 17.3For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

In the title compound,  $\text{C}_7\text{H}_8\text{N}_2\text{S}$ , the C–N(imino) and C–N(amino) bond distances within the thiourea moiety are 1.3395 (18) and 1.321 (2) Å, respectively. This significant difference in magnitude is also observed for some halogen-phenylthiourea compounds.

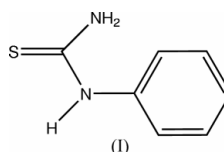
Received 2 June 2004

Accepted 9 June 2004

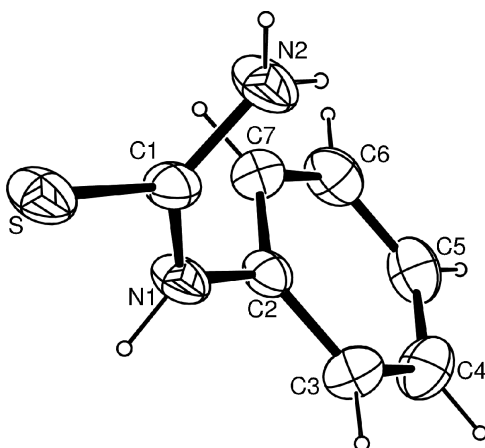
Online 19 June 2004

## Comment

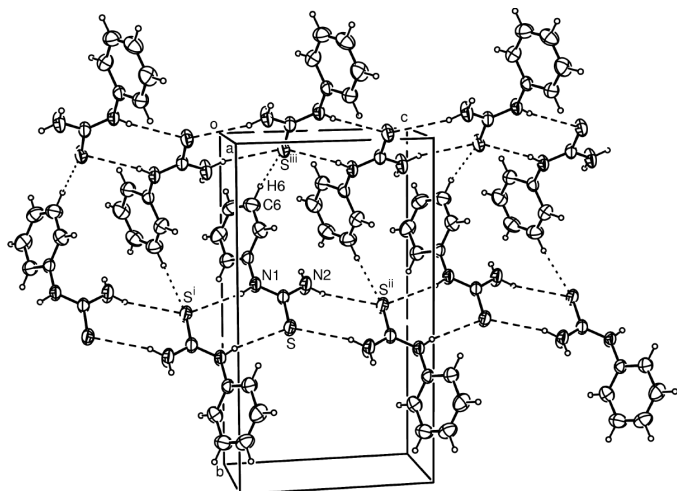
Thiourea and phenylthiourea have been used in preparing aminobithiazole (AT) and phenylaminobithiazole (PAT) in our laboratory, as metal complexes incorporating AT or PAT have shown potential application in the field of soft magnetic materials (Liu, 2003). We determined the crystal structure of phenylthiourea, (I), to compare the molecular structure with its derivatives.



The molecular structure of (I) is presented in Fig. 1. The electron delocalization within the thiourea moiety is clearly shown by both the C1–N1 and C1–N2 bond distances and the C1–S bond distance (Table 1). The phenyl ring is tilted from the plane of the thiourea moiety, with a dihedral angle of  $64.54(7)^\circ$ , which implies there is no conjugation effect between the phenyl group and the thiourea moiety. The C1–N2(amino) bond distance in (I) is essentially the same as the C–N(amino) bond distances found in the phenylthiourea complex of  $\text{Cd}^{\text{II}}$  (Yang *et al.*, 2001), which range from 1.315 (5)



**Figure 1**  
The molecular structure of (I), shown with 30% probability displacement ellipsoids.



**Figure 2**  
The hydrogen-bonded supramolecular structure of (I). [Symmetry codes: (i)  $2 - x, 1 - y, -z$ ; (ii)  $2 - x, 1 - y, 1 - z$ ; (iii)  $2 - x, y - \frac{1}{2}, \frac{1}{2} - z$ .]

to 1.322 (7) Å. It is noteworthy that the C1–N1(imino) bond in (I) is 0.019 (3) Å longer than the C1–N2(amino) bond. A search of the Cambridge Structural Database (Version 5.25; Allen, 2002) revealed that a significant difference between C–N(imino) and C–N(amino) bonds also occurs in reported halogen–phenylthiourea structures, *viz.* 0.026 (3) Å in fluorophenylthiourea (Steiner, 1998), 0.022 (4) Å in chlorophenylthiourea (Mao *et al.*, 1993) and 0.024 (4) Å in bromophenylthiourea (Wang *et al.*, 1991). This may be due to the induction effect of the phenyl group on the N1 imino group.

In the crystal structure, phenylthiourea molecules form a supramolecular ribbon *via* N–H...S hydrogen bonding (Table 2) along the crystallographic *c* axis, with adjacent ribbons linked by weak C–H...S hydrogen bonds, forming a two-dimensional network, as shown in Fig. 2.

## Experimental

Phenylthiourea is commercially available. Well shaped single crystals were obtained by recrystallization from an ethanol/water solution.

### Crystal data

$C_7H_8N_2S$	$D_x = 1.331 \text{ Mg m}^{-3}$
$M_r = 152.21$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 5560 reflections
$a = 5.6991(4) \text{ \AA}$	$\theta = 2.7\text{--}27.0^\circ$
$b = 15.2962(10) \text{ \AA}$	$\mu = 0.35 \text{ mm}^{-1}$
$c = 8.7352(8) \text{ \AA}$	$T = 295(2) \text{ K}$
$\beta = 93.7430(16)^\circ$	Prism, yellow
$V = 759.86(10) \text{ \AA}^3$	$0.26 \times 0.24 \times 0.22 \text{ mm}$
$Z = 4$	

### Data collection

Rigaku R-AXIS RAPID diffractometer	1428 reflections with $I > 2\sigma(I)$
$\omega$ scans	$R_{\text{int}} = 0.022$
Absorption correction: none	$\theta_{\text{max}} = 27.5^\circ$
6947 measured reflections	$h = -7 \rightarrow 7$
1734 independent reflections	$k = -19 \rightarrow 19$
	$l = -10 \rightarrow 11$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0425P)^2 + 0.1385P]$
$R[F^2 > 2\sigma(F^2)] = 0.037$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.091$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.17 \text{ e \AA}^{-3}$
1734 reflections	$\Delta\rho_{\text{min}} = -0.24 \text{ e \AA}^{-3}$
100 parameters	
H atoms treated by a mixture of independent and constrained refinement	

**Table 1**

Selected geometric parameters (Å, °).

S–C1	1.6915 (16)	N1–C2	1.4276 (19)
N1–C1	1.3395 (18)	N2–C1	1.321 (2)
C1–N1–C2	126.33 (13)	N2–C1–S	121.08 (12)
N2–C1–N1	117.93 (15)	N1–C1–S	120.99 (11)

**Table 2**

Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1–H1...S <sup>i</sup>	0.827 (18)	2.646 (17)	3.4480 (14)	163.8 (16)
N2–H2B...S <sup>ii</sup>	0.838 (18)	2.676 (17)	3.4925 (14)	164.9 (16)
C6–H6...S <sup>iii</sup>	0.93	2.94	3.702 (2)	140

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

H atoms on N atoms were located in a difference Fourier map and refined with fixed isotropic displacement parameters of  $0.06 \text{ \AA}^2$ . All other H atoms were placed in calculated positions (C–H =  $0.93 \text{ \AA}$ ) and refined using a riding model, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The project was supported by the National Natural Science Foundation of China (29973036).

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