

Shashidhar,^a Vijay
Thiruvengatam,^b
S. A. Shivashankar,^a M. B. Halli^c
and T. N. Guru Row^{b*}^aMaterials Research Centre, Indian Institute of Science, Bangalore 560 012, Karnataka, India, ^bSolid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560 012, Karnataka, India, and ^cDepartment of Chemistry, Gulbarga University, Gulbarga 585106, Karnataka, IndiaCorrespondence e-mail:
sctng@sscu.iisc.ernet.in

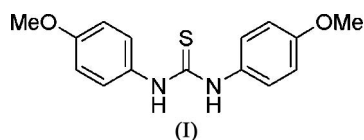
Key indicators

Single-crystal X-ray study
 $T = 290$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.054
 wR factor = 0.127
Data-to-parameter ratio = 12.5For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

1,3-Bis(4-methoxyphenyl)thiourea

In the crystal structure of the title compound, $\text{C}_{15}\text{H}_{16}\text{N}_2\text{O}_2\text{S}$, the $\text{C}=\text{S}$ group lies on a mirror plane. The molecules are packed in a centrosymmetric manner through intermolecular $\text{N}-\text{H}\cdots\text{S}$ hydrogen bonds.Received 23 February 2006
Accepted 14 March 2006

Comment

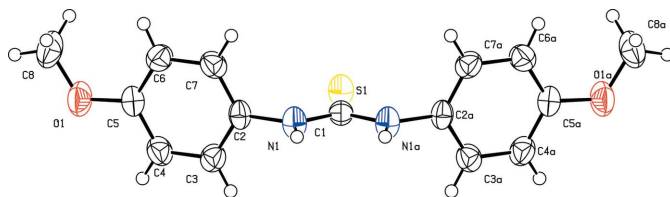
Compounds containing the thiourea unit show strong anti-fungal and antibacterial activity and find applications in medicine and agriculture (Lin *et al.*, 2004). The title compound, (I), crystallized in the space group $Pnma$ with $Z = 4$. The $\text{C}=\text{S}$ group lies on a mirror plane and thus there is one half-molecule in the asymmetric unit.The molecule of (I) is shown in Fig. 1 and a packing diagram is shown in Fig. 2. The dihedral angle between the planes formed by $\text{N1}/\text{C1}/\text{S1}$ and $\text{C2}-\text{C7}$ is $90.26(1)^\circ$, resulting in a bent 'butterfly-like' molecular shape. The molecules are arranged parallel to each other and extend along the long b axis *via* purely due to purely van der Waals interactions. Two well defined $\text{N}-\text{H}\cdots\text{S}$ hydrogen bonds involving the S atom lying on the mirror plane generate the packing motif in the ac plane [$\text{N}-\text{H}\cdots\text{S}:\text{N}\cdots\text{S} = 3.551(3)$ Å]. As a result, alternate molecules generated by the glide planes are held perpendicular to each other, as shown in Fig. 2.

Experimental

To a solution of *p*-anisidine (37 g), carbon disulfide (24 ml) and rectified spirit (40 ml) kept at 283–287 K, a small amount of aqueous ammonia (41 ml) was added, accompanied by constant shaking. The intermediate thiocarbamate was recovered and washed with small amounts of diethyl ether. It was subjected to steam distillation after adding lead nitrate and water. The compound which separated was further distilled and crystallized. The NMR data for the compound have been reported previously (Natarajan *et al.*, 2005).

Crystal data

 $\text{C}_{15}\text{H}_{16}\text{N}_2\text{O}_2\text{S}$
 $M_r = 288.37$
Orthorhombic, $Pnma$
 $a = 8.427(5)$ Å
 $b = 31.628(19)$ Å
 $c = 5.292(3)$ Å
 $V = 1410.3(14)$ Å³
 $Z = 4$
 $D_x = 1.358$ Mg m⁻³Mo $K\alpha$ radiation
Cell parameters from 732
reflections
 $\theta = 2.6-27.4^\circ$
 $\mu = 0.23$ mm⁻¹
 $T = 290(2)$ K
Prism, colourless
 $0.45 \times 0.40 \times 0.35$ mm

**Figure 1**

View of the molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radii. [Symmetry code: (a) $x, \frac{1}{2} - y, z$.]

Data collection

Bruker SMART CCD area-detector diffractometer	1572 independent reflections
φ and ω scans	1433 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.022$
$T_{\text{min}} = 0.903, T_{\text{max}} = 0.923$	$\theta_{\text{max}} = 27.4^\circ$
11344 measured reflections	$h = -10 \rightarrow 10$
	$k = -40 \rightarrow 39$
	$l = -6 \rightarrow 6$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 0.7475P]$
$R[F^2 > 2\sigma(F^2)] = 0.054$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.127$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.21$	$\Delta\rho_{\text{max}} = 0.33 \text{ e } \text{\AA}^{-3}$
1572 reflections	$\Delta\rho_{\text{min}} = -0.19 \text{ e } \text{\AA}^{-3}$
126 parameters	
All H-atom parameters refined	

Table 1

Selected geometric parameters (\AA , $^\circ$).

S1—C1	1.693 (3)	N1—C1	1.339 (2)
O1—C5	1.375 (3)	N1—C2	1.431 (3)
O1—C8	1.417 (4)		
C5—O1—C8	117.5 (2)	N1—C2—C3	119.41 (19)
C1—N1—C2	124.68 (18)	N1—C2—C7	120.56 (18)
N1—C1—N1 ⁱ	114.7 (2)	O1—C5—C6	124.4 (2)
S1—C1—N1	122.66 (12)	O1—C5—C4	115.5 (2)

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

Table 2

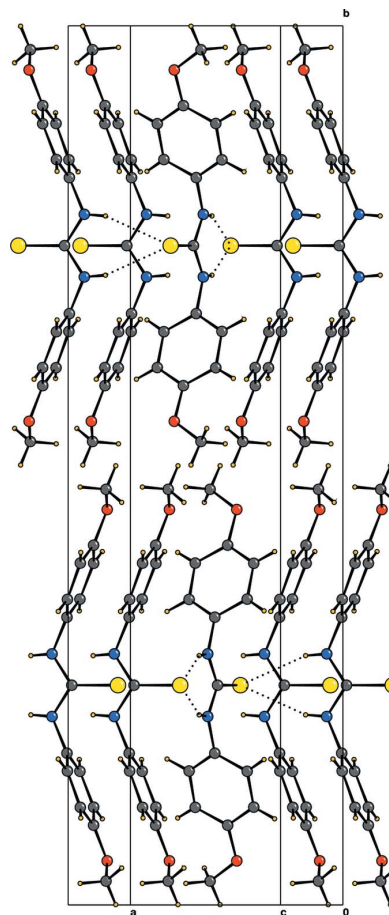
Hydrogen-bond geometry (\AA , $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N1—H1 ⁱ \cdots S1 ⁱⁱ	0.80 (3)	2.79 (3)	3.551 (3)	160 (2)

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

All the H atoms were located and refined isotropically. The C—H bond lengths are 0.89 (3)–1.05 (3) \AA and the N—H bond length is 0.80 (3) \AA .

Data collection: SMART (Bruker, 1998); cell refinement: SMART; data reduction: SAINT (Bruker, 1998); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics:

**Figure 2**

Packing diagram of (I), viewed down the c axis. The dotted lines indicate intermolecular N—H \cdots S hydrogen bonds.

ORTEP-3 for Windows (Farrugia, 1997) and CAMERON (Watkin *et al.*, 1993); software used to prepare material for publication: PLATON (Spek, 2003).

We thank the Department of Science and Technology, India, for use of the CCD facility set up under the IRHPA-DST programme at IISc.

References

- Bruker (1998). SMART (Version 5.628) and SAINT (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 6362–6368.
- Lin, Q., Zhang, Y.-M., Wei, T.-B. & Wang, H. (2004). *Acta Cryst.* **E60**, o580–o582.
- Natarajan, A., Guo, Y.-H., Arthanari, H., Wagner, G., Halperin, J. A. & Choev, M. (2005). *J. Org. Chem.* **70**, 6362–6368.
- Sheldrick, G. M. (1996). SADABS. University of Gottingen, Germany.
- Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Gottingen, Germany.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
- Watkin, D. M., Pearce, L. & Prout, C. K. (1993). Chemical Crystallography Laboratory, University of Oxford, England.