

Jing-Han Hu,^{a*} De-Sheng Li,^b
Cheng Cao^c and Tai-Bao Wei^c

^aCollege of Chemical and Biological Engineering, Lanzhou Jiaotong University, Lanzhou, Gansu 730070, People's Republic of China, ^bCollege of Environmental Science & Municipal Engineering, Lanzhou Jiaotong University, Lanzhou, Gansu 730070, People's Republic of China, and ^cCollege of Chemistry and Chemical Engineering, Northwest Normal University, Lanzhou, Gansu 730070, People's Republic of China

Correspondence e-mail: hujinghan62@163.com

Key indicators

Single-crystal X-ray study
 $T = 296$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.039
 wR factor = 0.115
Data-to-parameter ratio = 14.7

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

1-(4-Ethoxybenzoyl)-3-*o*-tolylthiourea

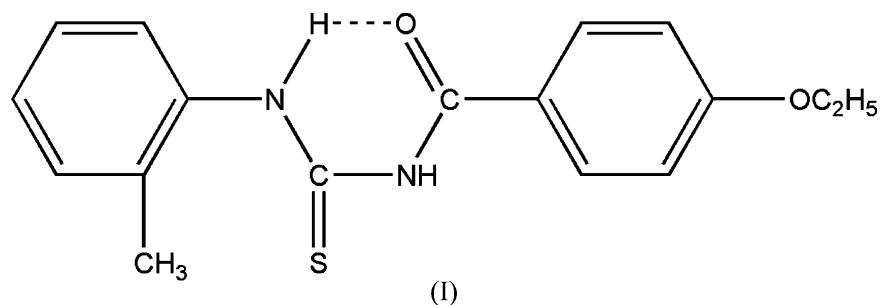
The molecule of the title compound, $\text{C}_{17}\text{H}_{18}\text{N}_2\text{O}_2\text{S}$, is not planar; the thiourea mean plane is twisted with respect to the benzene rings with dihedral angles of 65.95 (12) and 51.54 (10)°.

Received 30 June 2006

Accepted 13 July 2006

Comment

Thiourea derivatives have been studied for their potential use in agriculture, medicine and analytical chemistry (Schroeder, 1955; Antholine *et al.*, 1982). As part of our ongoing work on acylthiourea derivatives (Zhang *et al.*, 2003; Zhang *et al.*, 2006), we present here the structure of the title thiourea derivative, (I).



The molecular structure (Fig. 1) of (I) is similar to those of *N*-(*o*-nitrophenyl)-*N'*-methoxycarbonylthiourea and *N*-(*p*-nitrophenyl)-*N'*-ethoxycarbonylthiourea (Shen *et al.*, 1998). The O1-containing carbonyl and thiocarbonyl groups are located on opposite sides of the N2–C8 bond. The O1-carbonyl is intramolecularly hydrogen bonded with the neighbouring N1-imino group (Table 1). The molecule is not planar; the thiourea mean plane is twisted with respect to the benzene rings, the dihedral angles being 65.95 (12) (between thiourea and C2-benzene) and 51.54 (10)° (between thiourea and C10-benzene). Intermolecular N–H...S hydrogen bonding is observed in the crystal structure of (I), which helps to stabilize the crystal structure (Table 1).

Experimental

Potassium thiocyanate (7.5 mmol), 2-ethoxybenzoyl chloride (5 mmol), PEG-400 (3% with respect to ammonium thiocyanate) and dichloromethane (20 ml) were placed in a dried flask and stirred at room temperature for 1 h, then 2-methylbenzenamine (5 mmol) was added. The mixture was stirred for 0.5 h at room temperature and a precipitate was formed. This was filtered off, washed with water and dried. Colourless single crystals of (I) were obtained from an ethanol–dimethylformamide (1:1) solution.

Crystal data

$C_{17}H_{18}N_2O_2S$
 $M_r = 314.39$
 Triclinic, $P\bar{1}$
 $a = 7.734$ (1) Å
 $b = 10.198$ (2) Å
 $c = 12.314$ (2) Å
 $\alpha = 103.94$ (1)°
 $\beta = 103.09$ (1)°
 $\gamma = 112.03$ (1)°

$V = 817.9$ (3) Å³
 $Z = 2$
 $D_x = 1.277$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.21$ mm⁻¹
 $T = 296$ (2) K
 Block, colourless
 $0.58 \times 0.44 \times 0.24$ mm

Data collection

Siemens P4 diffractometer
 ω scans
 Absorption correction: multi-scan
 (*SHELXTL*; Bruker, 1998)
 $T_{\min} = 0.880$, $T_{\max} = 0.953$
 3332 measured reflections
 2975 independent reflections

2260 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.010$
 $\theta_{\text{max}} = 25.5^\circ$
 3 standard reflections
 every 97 reflections
 intensity decay: 3.4%

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.115$
 $S = 1.08$
 2975 reflections
 202 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0626P)^2 + 0.0506P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.38$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.18$ e Å⁻³
 Extinction correction: *SHELXL97*
 Extinction coefficient: 0.019 (4)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1\cdots O1$	0.86	1.99	2.649 (2)	133
$N2-H2\cdots S^i$	0.86	2.77	3.5712 (16)	156

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

Methyl H atoms were placed in calculated positions, with $C-H = 0.96$ Å, and torsion angles were refined to fit the electron density; $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$. Other H atoms were placed in calculated positions, with $C-H = 0.93$ (aromatic) or 0.97 Å (methylene) and $N-H = 0.86$ Å, and refined in riding mode, with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(N,C)$.

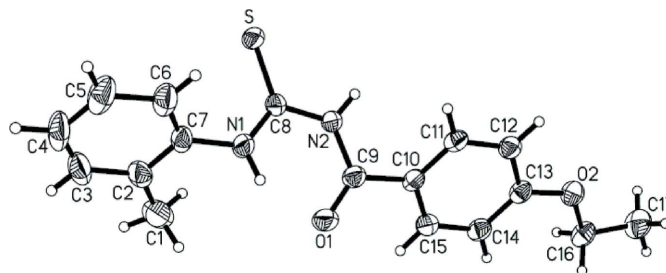


Figure 1

The molecular structure of (I), with 50% probability displacement ellipsoids (small spheres of arbitrary radii for H atoms).

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The work was supported by the Natural Science Foundation of China (grant No. 20371040), the Key Scientific and Technical Research Project of the Ministry of Education of China (grant No. 205161) and the Youth Foundation of Gansu province (grant No. 3YS051-A25-010).

References

- Antholine, W. & Taketa, F. (1982). *J. Inorg. Biochem.* **16**, 145–154.
 Bruker (1998). *SADABS* (Version 2.0) and *SHELXTL* (Version 6.1). Bruker AXS Inc., Madison, Wisconsin, USA.
 Schroeder, D. C. (1955). *Chem. Rev.* **50**, 181–228.
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
 Shen, X., Shi, X., Kang, B., Liu, Y., Jiang, H. & Chen, K. (1998). *Polyhedron*, **17**, 4049–4058.
 Siemens (1994). *XSCANS*. Version 2.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
 Zhang, Y.-M., Cao, C., Lin, Q., Yang, L.-Z. & Wei, T.-B. (2006). *Acta Cryst.* **E62**, o1791–o1792.
 Zhang, Y.-M., Xian, L. & Wei, T.-B. (2003). *Acta Cryst.* **C59**, m473–m474.