

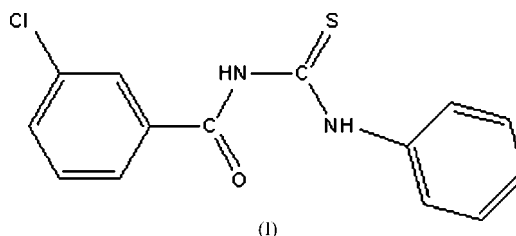
1-(3-Chlorobenzoyl)-3-phenylthiourea

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Key indicators

Single-crystal X-ray study
 $T = 173$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.037
 wR factor = 0.102
Data-to-parameter ratio = 14.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.The phenyl and benzoyl groups in the title compound, $\text{C}_{14}\text{H}_{11}\text{ClN}_2\text{OS}$, are *cis* and *trans*, respectively, with respect to the $\text{C}=\text{S}$ bond. The crystal packing is characterized by $\text{N}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{S}$ hydrogen bonds.Received 29 March 2006
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Comment

 N,N' -Disubstituted thiourea derivatives have attracted attention due to their coordination behaviour with transition metals (Schuster *et al.*, 1990). The biological activities, such as antibacterial, antifungal, antitubercular, antithyroid and insecticidal, of complexes with thiourea derivatives have also been studied (Madan & Taneja, 1991; Frech *et al.*, 1970). We present here the crystal structure of the title thiourea compound, (I).The structure of (I) (Fig. 1) possesses an intramolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bond (Table 2), which appears to control the essentially planar conformation of the central thiourea unit.In the crystal structure, independent molecules are linked by two intermolecular $\text{N}-\text{H}\cdots\text{S}$ hydrogen bonds to form dimers which are stacked along [100] (Fig. 2).The 3-chloro substitution on the benzoyl ring in (I) does not lead to any significant changes in geometric or conformational parameters compared with the molecular structures of related compounds (Khawar Rauf *et al.*, 2006).

Experimental

A solution of 3-chlorobenzoyl chloride (1.75 g, 10 mmol) in acetone (30 ml) was added to a suspension of KSCN (1.00 g, 10 mmol) in acetone (30 ml). The reaction mixture was heated under reflux for a few minutes, and then aniline (0.93 g, 10 mmol) was added and the resulting mixture was stirred for 1 h. The reaction mixture was then poured into water and stirred well. The solid product was separated, washed with water and purified by recrystallization from toluene to give crystals of the title compound in an overall yield of 85%. Full spectroscopic and physical characterization will be reported elsewhere.

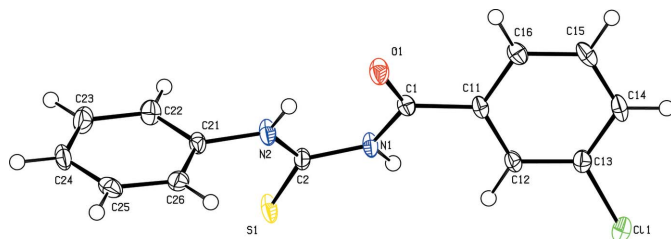


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

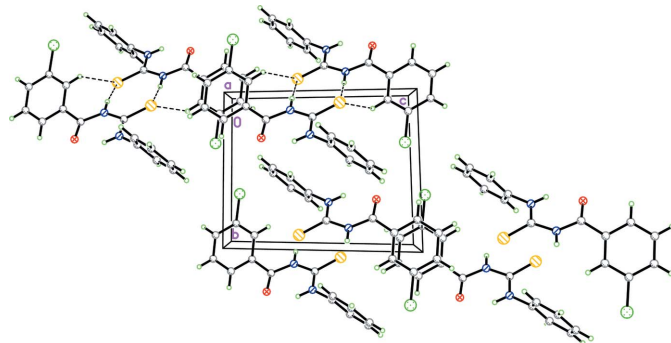


Figure 2
The crystal packing of (I), viewed along [100], with hydrogen bonds indicated as dashed lines.

Crystal data

$C_{14}H_{11}ClN_2OS$
 $M_r = 290.76$
 Triclinic, $P\bar{1}$
 $a = 7.6340$ (12) Å
 $b = 8.8940$ (14) Å
 $c = 11.0219$ (18) Å
 $\alpha = 83.129$ (13)°
 $\beta = 70.328$ (12)°
 $\gamma = 71.382$ (12)°
 $V = 667.74$ (18) Å³
 $Z = 2$
 $D_x = 1.446$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.43$ mm⁻¹
 $T = 173$ (2) K
 Block, colourless
 $0.47 \times 0.44 \times 0.42$ mm

Data collection

Stoe IPDS-II two-circle diffractometer
 ω scans
 Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995)
 $T_{\min} = 0.822$, $T_{\max} = 0.839$
 5414 measured reflections
 2471 independent reflections
 2242 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.045$
 $\theta_{\text{max}} = 25.6^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.102$
 $S = 1.04$
 2471 reflections
 173 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0614P)^2 + 0.294P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.31$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.40$ e Å⁻³
 Extinction correction: SHELXL97 (Sheldrick, 1997)
 Extinction coefficient: 0.081 (7)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1\cdots S1^i$	0.88	2.60	3.4465 (16)	161
$N2-H2\cdots O1$	0.88	1.95	2.6516 (19)	136

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

H atoms were included in calculated positions, with $C-H = 0.95$ Å and $N-H = 0.88$ Å, and refined as riding on their parent C or N atoms, with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C,N)$.

Data collection: X-AREA (Stoe & Cie, 2001); cell refinement: X-AREA; data reduction: X-AREA; program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: XP in SHELXTL-Plus (Sheldrick, 1991) and PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97 and PLATON.

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