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1-Benzoyl-3-(3-chlorophenyl)thiourea

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.002 Å
R factor = 0.040
wR factor = 0.091
Data-to-parameter ratio = 18.3

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

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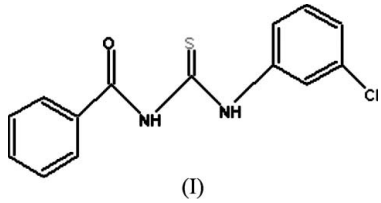
In the molecule of the title compound, $C_{14}H_{11}ClN_2OS$, the dihedral angle between the two aromatic rings is 19.02 (9)°. In the crystal packing, the molecules are linked by intermolecular C—H···S and N—H···S hydrogen bonds into centrosymmetric dimers stacked along the [010] direction.

Comment

Transition metal complexes of *N*,*N*-disubstituted thiourea have attracted much attention, due to their coordination properties (Schuster *et al.*, 1990) and biological activities (Frech *et al.*, 1970). In addition, thiourea derivatives have been shown to possess antibacterial, antifungal, antitubercular, antithyroid and insecticidal properties (Madan *et al.*, 1991).



(I)

The title compound, (I) (Fig. 1), is a typical *N*,*N*′-disubstituted thiourea derivative with normal geometric parameters. The C7—S1 and C8—O1 bonds (Table 1) both show the expected double-bond character. The short values of the C1—N1, C7—N1, C7—N2 and C8—N2 bond lengths also indicate partial double-bond character. Compared with *N*-benzoyl-*N*′-phenylthiourea (Yamin & Yusof, 2003; refcode HURYAU in the Cambridge Structural Database; *MOGUL*, Version 1.0; Allen, 2002), the Cl substituent at C5 has no significant effect on these bond lengths.

In (I), both benzene rings are essentially planar. Their dihedral angle is 19.02 (9)°, and the corresponding angles to the thiourea plane are 4.3 (1)° for the *m*-chlorophenyl group and 22.84 (8)° for the phenyl group.

An intramolecular N—H···O hydrogen bond is present (Table 2), forming a six-membered ring commonly observed in this class of compounds. As in most benzylthiourea derivatives (Arslan *et al.*, 2004; Yamin & Yusof, 2003), in the crystal packing of (I), intermolecular N—H···S and C—H···S hydrogen bonds link the molecules into centrosymmetric dimers stacked along the [010] direction (Fig. 2).

Experimental

A solution of benzoyl chloride (1.41 g, 10 mmol) in acetone (50 ml) was added dropwise to a suspension of KSCN ((1.00 g, 10 mmol) in acetone (30 ml). The reaction mixture was heated under reflux for

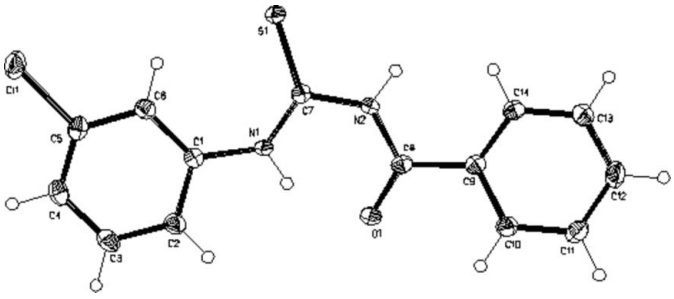


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level.

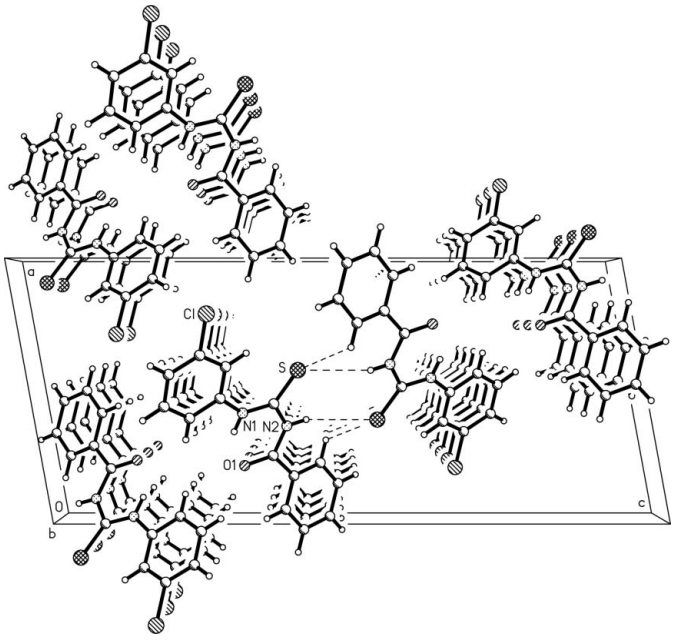


Figure 2
The crystal packing for (I), viewed along the [010] direction, with hydrogen bonds shown as dashed lines.

45 min and then cooled to room temperature. Afterwards, a solution of *m*-chloroaniline (1.28 g, 10 mmol) in acetone (15 mmol) was added and the resulting mixture was stirred for 3 h. The reaction mixture was then poured into crushed ice and stirred well. The solid product was separated, washed with deionized water and purified by recrystallization from toluene to give fine crystals of the title compound, in an overall yield of 85%. Full spectroscopic and physical characterization will be reported elsewhere.

Crystal data

$C_{14}H_{11}ClN_2OS$
M_r = 290.76
Monoclinic, $P2_1/n$
a = 11.2191 (9) Å
b = 4.5955 (4) Å
c = 25.631 (2) Å
β = 100.438 (2)°
V = 1299.61 (19) Å^3
Z = 4
D_x = 1.486 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3339 reflections
θ = 2.3–28.1°
μ = 0.45 mm^{-1}
T = 120 (2) K
Prism, colourless
0.44 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.828, T_{max} = 0.932
12106 measured reflections
3144 independent reflections
2510 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 28.1°
$h = -13 \rightarrow 14$
$k = -5 \rightarrow 6$
$l = -33 \rightarrow 33$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.091
S = 0.96
3144 reflections
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0488P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl1—C5	1.7398 (17)	N1—C1	1.413 (2)
S1—C7	1.6594 (16)	N2—C8	1.376 (2)
O1—C8	1.2295 (18)	N2—C7	1.399 (2)
N1—C7	1.3367 (19)		
C7—N1—C1	132.41 (14)	N1—C7—N2	114.12 (13)
C8—N2—C7	128.36 (13)	N2—C8—C9	117.65 (13)
C7—N1—C1—C6	5.6 (3)	N2—C8—C9—C10	158.45 (14)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1	0.88	1.83	2.592 (2)	143
N2—H2B···S1^{i}	0.88	2.82	3.607 (1)	150
C14—H14A···S1^{i}	0.95	2.76	3.330 (2)	119

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

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.95 Å and N—H = 0.88 Å, and with U_{iso}(H) = 1.2U_{eq}(C,*N*).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2002); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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