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N′-(4-Chlorobenzoyl)-*N*,*N*-diphenylthiourea

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.041
wR factor = 0.122
Data-to-parameter ratio = 18.0

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

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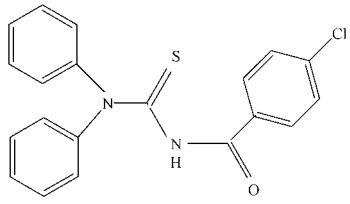
The crystal packing in the title compound, $C_{20}H_{15}ClN_2OS$, shows sheets of molecules stacked along [001].

Comment

Recently, we discussed a novel series of thiourea derivatives and their metal complexes (Arslan *et al.*, 2003). One of these new derivatives is the title compound, (I), reported here.



(I)

The bond lengths and angles in the thiourea moiety are typical for thiourea derivatives; the C8—S1 and C7—O1 bonds both show typical double-bond character. However, the C—N bond lengths C7—N1, C8—N1 and C8—N2 are shorter than the normal C—N single-bond length of about 1.48 Å. The shortening of these C—N bonds reveals the effects of resonance in this part of the molecule. All other bond lengths fall within the expected ranges; the terminal C3—Cl1 bond length is 1.735 (2) Å. The conformation of the molecule with respect to the thiocarbonyl and carbonyl moieties is twisted, as reflected by the torsion angles O1—C7—N1—C8 and C7—N1—C8—N2 of 4.9 (3) and 49.8 (3)°, respectively. Intermolecular hydrogen-bonding *D*—H···*A* parameters are: N1—H1*A*···S1($-x+1, -y+2, -z+1$) with H···*A* = 2.48 Å and a *D*—H···*A* angle of 153°; C2—H2*A*···O1($x+1, y, z$) with H···*A* = 2.32 Å and a *D*—H···*A* angle of 133°; a weak interaction C12—H12*A*···O1($-x, -y+2, -z+2$) with H···A = 2.68 Å and a *D*—H···*A* angle of 160° (values

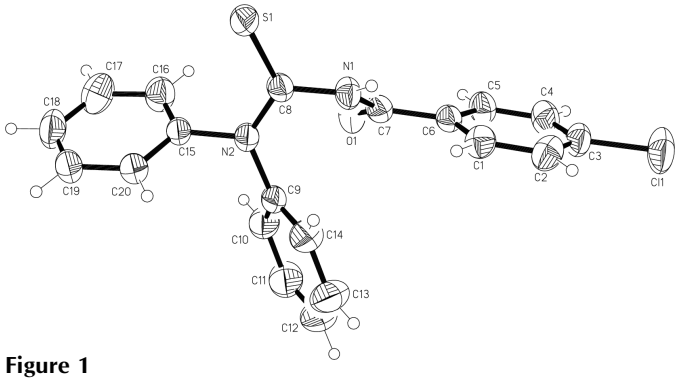


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

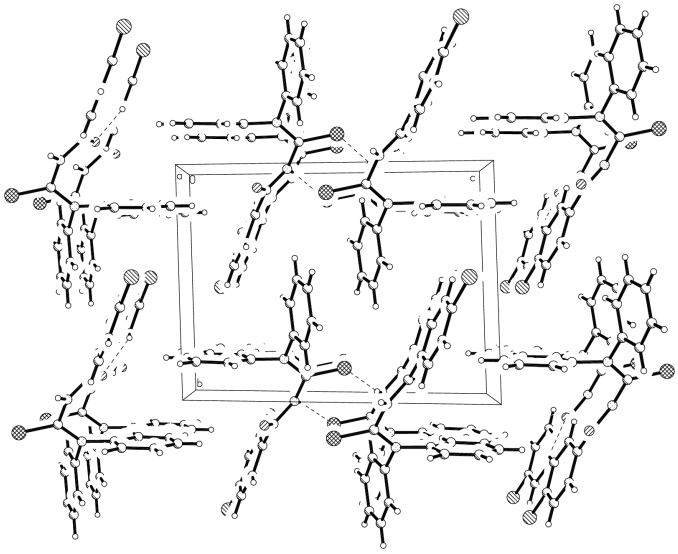


Figure 2
Packing diagram, viewed along [100]. Hydrogen bonding is indicated by dashed lines.

normalized for N—H = 1.03 and C—H = 1.08 Å). Accordingly, molecules are packed in parallel sheets along [001].

Experimental

The title compound was prepared according to the method of Arslan *et al.* (2003) by converting 4-chlorobenzoyl chloride into 4-chlorobenzoyl isothiocyanate and then condensing with the appropriate secondary amine. The compound was recrystallized from ethanol/dichloromethane (1:1).

Crystal data

$C_{20}H_{15}ClN_2OS$
M_r = 366.85
Triclinic, $P\overline{1}$
a = 6.811 (2) Å
b = 9.950 (1) Å
c = 13.442 (2) Å
α = 88.14 (1)°
β = 79.12 (2)°
γ = 89.54 (1)°
V = 894.1 (3) Å^3
Z = 2
D_x = 1.363 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 26 reflections
θ = 7.5–18.6°
μ = 0.34 mm^{-1}
T = 293 (2) K
Prism, pale yellow
0.38 × 0.25 × 0.14 mm

Data collection

Bruker $P4$ diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.811, T_{max} = 0.946
5122 measured reflections
4095 independent reflections
2774 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 27.5°
$h = -1 \rightarrow 8$
$k = -12 \rightarrow 12$
$l = -17 \rightarrow 17$
3 standard reflections every 397 reflections
intensity decay: <1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.122
S = 1.08
4095 reflections
227 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0433P)^2 + 0.3889P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.010 (2)

Table 1
Selected geometric parameters (Å, °).

Cl1—C3	1.735 (2)	N1—C7	1.389 (3)
S1—C8	1.664 (2)	N1—C8	1.393 (2)
O1—C7	1.213 (3)	N2—C8	1.346 (3)
C7—N1—C8	124.4 (2)	N2—C8—N1	116.1 (2)
O1—C7—N1	122.3 (2)	N2—C8—S1	123.6 (2)
O1—C7—C6	122.7 (2)	N1—C8—S1	120.3 (2)
N1—C7—C6	115.0 (2)		

H atoms were refined at calculated positions riding on the C atoms, with isotropic displacement parameters $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Bruker, 1998); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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