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N-Benzoyl-*N*′-phenylthiourea

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The phenyl and benzoyl groups in the title compound, $C_{14}H_{12}N_2OS$, lie *cis* and *trans*, respectively, to the S atom across the thiourea C—N bonds. The molecules are packed as dimers, *via* N—H···S intermolecular hydrogen bonds, and arranged parallel to the *a* and *c* axes.

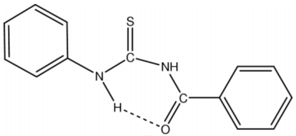
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.125
Data-to-parameter ratio = 17.9

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

Comment

Although some arylbenzoylthioureas such as 3,4-dimethylphenylbenzoylthiourea (Shanmuga Sundara Raj *et al.*, 1999) and 2,6-dimethylphenylbenzoylthiourea (Usman *et al.*, 2002) have been reported, the structure of the unsubstituted phenyl analogue is still not available. Therefore the X-ray crystallographic investigation of the title compound, (I), was carried out.



(I)

The C—C bond lengths and bond angles of the phenyl and the benzoyl groups are in the normal ranges (Allen *et al.*, 1987). The geometry of the central carbonyl-thiourea moiety, (S1/C8/N1/N2/C7/O1) is also in agreement with most benzoylthiourea derivatives (Shanmuga Sundara Raj *et al.*, 1999; Usman *et al.*, 2002; Kaminsky *et al.*, 2002). However, the N2—C9 bond length of 1.408 (2) Å is shorter than in the bulky 2,6-dimethylphenylbenzoylthiourea [1.436 (2) Å] and the C8—N2—C9 bond angle of 133.16 (14)° is larger compared to 123.2 (2)° and 127.9 (2)° in 2,6- (Usman *et al.*, 2002) and 3,4-dimethylphenylbenzoylthiourea (Shanmuga Sundara Raj *et al.*, 1999), respectively. The phenyl and the benzoyl substituents in the molecule lie *cis* and *trans*, respectively, to S atom across the thiourea C—N bonds.

The O1/C7/N1/C8/N2 plane has a maximum deviation of 0.035 (1) Å at atom N1. However, the central carbonyl-thiourea (S1/C8/N1/N2/C7/O1) moiety connecting the two phenyl rings is slightly less planar, with atom S1 deviating by 0.145 (1) Å. The phenyl (C1–C6 and C9–C14) rings are essentially planar. The two rings make dihedral angles of 28.78 (9)° and 7.52 (9)°, respectively, with the carbonyl-thiourea plane. The dihedral angle between the two aromatic rings is 33.3 (1)°.

As in most benzoylthiourea derivatives, intramolecular hydrogen bonding N2—H2*B*···O1 maintains the six-membered ring formation of the N2/C8/N1/C7/O1 plane; there is also a weak interaction of C14—H14*A*···S1 (Table 2). In the

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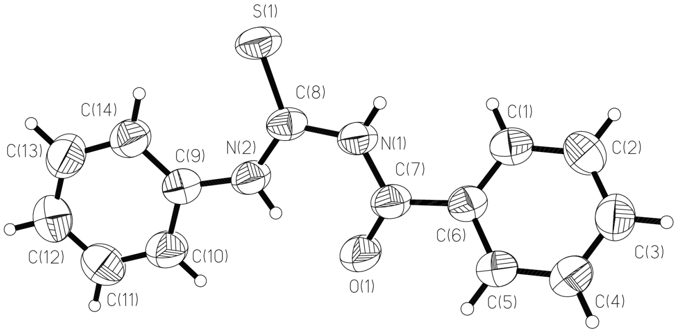

Figure 1
Molecular structure of the title compound (I), with 50% probability displacement ellipsoids for non-H atoms.

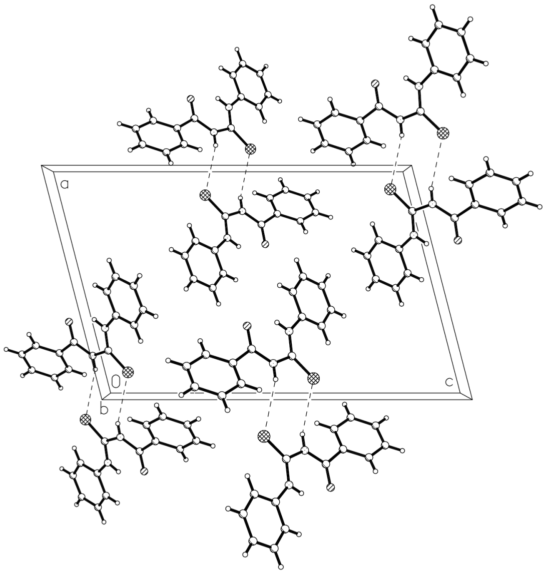

Figure 2
Packing diagram of (I), viewed down the *b* axis. Dashed lines denote N—H···S hydrogen bonds.

crystal structure, the molecules are packed as dimers, *via* weak N1—H1*B*···S1′ interactions, and arranged parallel to the *a* and *c* axes (Fig. 2).

Experimental

A solution of aniline (0.16 g, 1.40 mmol) in acetone (50 ml) was added dropwise to 50 ml of an acetone solution containing an equimolar amount of benzoyl thiocyanate in a two-neck round-bottomed flask. The solution was refluxed for about 1 h and then cooled in ice. The white precipitate which formed was filtered off and washed with ethanol-distilled water, then dried in a vacuum (yield 79%). Recrystallization from DMSO yielded single crystals of (I) suitable for X-ray analysis.

Crystal data

$C_{14}H_{12}N_2OS$
$M_r = 256.32$
Monoclinic, $P2_1/c$
$a = 12.8492$ (11) Å
$b = 5.1963$ (5) Å
$c = 19.5971$ (18) Å
$\beta = 104.484$ (2)°
$V = 1266.9$ (2) Å^3
$Z = 4$

$D_x = 1.344$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2753 reflections
$\theta = 1.6$–27.6°
$\mu = 0.24$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.46 × 0.33 × 0.30 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.896$, $T_{\max} = 0.930$
8234 measured reflections

2917 independent reflections
2304 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.017$
$\theta_{\max} = 27.6°$
$h = -16 \rightarrow 16$
$k = -5 \rightarrow 6$
$l = -20 \rightarrow 25$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.125$
$S = 1.04$
2917 reflections
163 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0646P)^2 + 0.2031P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.24$ e Å^{-3}
$\Delta\rho_{\min} = -0.14$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C8	1.6567 (15)	C7—O1	1.222 (2)
N1—C7	1.3746 (19)	C8—N2	1.326 (2)
N1—C8	1.393 (2)	C9—N2	1.408 (2)
C7—N1—C8	128.58 (14)	N2—C8—S1	127.73 (13)
O1—C7—N1	121.83 (16)	N1—C8—S1	117.88 (12)
N2—C8—N1	114.38 (14)	C8—N2—C9	133.16 (14)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*B*···S1$^{\rm i}$	0.86	2.87	3.6544 (14)	152
N2—H2*B*···O1	0.86	1.86	2.599 (2)	143
C14—H14*A*···S1	0.93	2.59	3.237 (2)	127

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

After checking their presence in a difference map, all H atoms were fixed geometrically and allowed to ride on the parent C or N atoms, with C—H = 0.93 Å and N—H = 0.86 Å.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL, PARST* (Nardelli, 1995) and *PLATON* (Spek, 1990).

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