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N-Benzoyl-*N*′-(3-hydroxyphenyl)thiourea

Hamza Milad Abosadiya, Bohari M. Yamin and Nurziana Ngah*

School of Chemical Sciences and Food Technology, Universiti Kebangsaan Malaysia, 43600 Bangi, Selangor, Malaysia

Correspondence e-mail: nurziana_ngah@yahoo.com

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.102
Data-to-parameter ratio = 13.2

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

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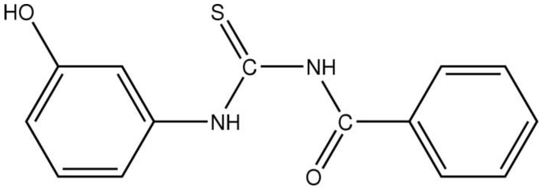
In the title compound, $C_{14}H_{12}N_2O_2S$, the benzoyl and 3-hydroxyphenyl fragments adopt *trans–cis* positions with respect to the S atom across their C—N bonds. The dihedral angle between the 3-hydroxyphenyl and N_2CS thiourea groups is 72.09 (8)°. The crystal structure is stabilized by O—H···S and N—H···S hydrogen bonds, forming a polymeric chain along the *c* axis.

Comment

The title compound (I), $C_{14}H_{12}N_2O_2S$, is analogous with *N*-benzoyl-*N*′-phenylthiourea, (II) (Yamin & Yusof, 2003), except for the presence of a hydroxyl group at the *meta* position of the benzene ring.



(I)

The molecule of (I) adopts a *trans–cis* configuration with respect to the positions of the benzoyl and 3-hydroxyphenyl groups relative to the thiono S atom across the C8—N1 and C8—N2 bonds, respectively (Fig. 1). The bond lengths and angles are in normal ranges (Allen *et al.*, 1987). The phenyl [C1–C6 (*A*)], central thiourea [S1/N1/N2/C8 (*B*)] and 3-hydroxyphenyl [C9–C14/O2 (*C*)] fragments are each essentially planar. The maximum deviation is 0.013 (2) Å for atom N2 from the thiourea mean plane. The presence of the hydroxyl group at the *meta* position causes the *C*/*B* dihedral angle to increase from 7.52 (9)° in the unsubstitued phenylthiourea, (II), to 72.09 (8)° in (I). Rings *A* and *C* are almost perpendicular to each other, with an angle of 79.95 (9)°.

There is an intramolecular N2—H2*A*···O1 hydrogen bond (Table 2), resulting in the formation of a pseudo-six-membered ring (N2/H2*A*/O1/C7/N1/C8). The crystal structure of (I) is stabilized by intermolecular N1—H1···O2^{i} and O2—H2···S1^{ii} hydrogen bonds (Table 2), forming polymeric chains along the *c* axis; this contrasts with the dimeric form in (II).

Experimental

An acetone solution (50 ml) of 3-aminophenol (3.273 g, 0.03 mol) was added dropwise to a two-necked round-bottomed flask containing an acetone solution (50 ml) of an equimolar quantity of benzoyl isothiocyanate (4.896 g, 0.03 mol). The mixture was refluxed for about 5 h and then filtered into a beaker containing ice cubes. The white precipitate obtained was washed with cold distilled water before drying and kept in a desiccator. Recrystallization from ethanol yielded colourless crystals of (I) suitable for X-ray analysis (yield 85%; m.p. 446.4–447.2 K).

Crystal data

$C_{14}H_{12}N_2O_2S$
$M_r = 272.32$
Monoclinic, $P2_1/c$
$a = 12.209\ (3)$ Å
$b = 7.3126\ (17)$ Å
$c = 15.710\ (4)$ Å
$\beta = 112.133\ (4)^\circ$
$V = 1299.2\ (5)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.25$ mm^{-1}
$T = 298\ (2)$ K
$0.50 \times 0.40 \times 0.30$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{\min} = 0.886$, $T_{\max} = 0.929$
6357 measured reflections
2289 independent reflections
1997 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.022$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.102$
$S = 1.05$
2289 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{\max} = 0.20$ e Å^{-3}
$\Delta\rho_{\min} = -0.31$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C8	1.6725 (18)	N1—C8	1.388 (2)
O1—C7	1.217 (2)	N2—C8	1.316 (2)
N1—C7	1.377 (2)	N2—C9	1.433 (2)
C8—N2—C9	125.91 (15)	N2—C8—S1	124.68 (13)
O1—C7—N1	122.27 (15)	N1—C8—S1	119.48 (12)
N2—C8—N1	115.83 (15)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1	0.86	1.93	2.621 (2)	137
N1—H1···O2$^{\rm i}$	0.86	2.20	2.961 (2)	147
O2—H2···S1$^{\rm ii}$	0.82	2.48	3.2002 (17)	148

Symmetry codes: (i) $x, -y + \frac{5}{2}, z - \frac{1}{2}$; (ii) $x, -y + \frac{5}{2}, z + \frac{1}{2}$.

All H atoms were positioned geometrically in ideal positions and allowed to ride on their parent atoms, with C—H = 0.93 Å, N—H = 0.86 Å and O—H = 0.82 Å, and with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C,N) for CH, CH_2 and NH or $1.5U_{\rm eq}$(O) for (OH).

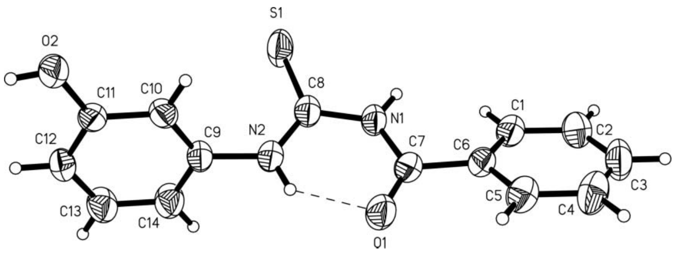


Figure 1
The molecular structure of (I), with 50% probability displacement ellipsoids. The dashed line indicates the intramolecular hydrogen bond.

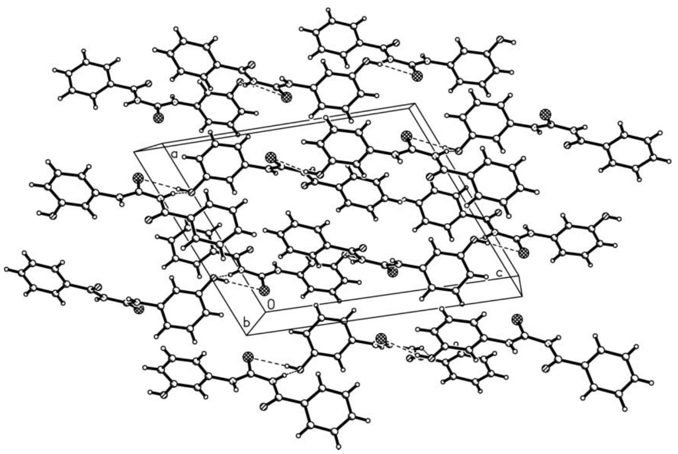


Figure 2
A packing diagram for (I), viewed down the b axis. Dashed lines denote N—H···O and O—H···S hydrogen bonds.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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