Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-Benzoyl-*N*′-(3-pyridyl)thiourea

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.106
Data-to-parameter ratio = 13.9

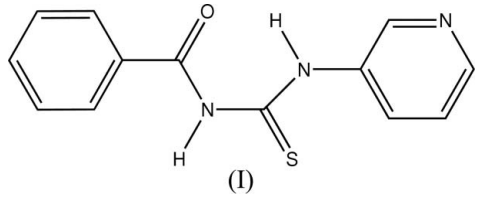
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 12 June 2006
Accepted 16 July 2006

The molecule of the title compound, $C_{13}H_{11}N_3OS$, is non-planar; the dihedral angles between the thiourea and pyridine planes and between the thiourea and benzene planes are 41.28 (8) and 27.47 (8)°, respectively.

Comment

Thiourea and its derivatives have attracted much attention because of their applications in fields such as herbicides, insecticides and plant-growth regulators (Anthiline & Taketa, 1982).



(I)

The molecular structure of the title thiourea derivative, (I), is shown in Fig. 1. The molecule is non-planar; the dihedral angles between the thiourea and pyridine planes and between the thiourea and benzene planes are 41.28 (8) and 27.47 (8)°, respectively. The carbonyl and thiocarbonyl groups are located on the opposite sides of the N3—C6 bond. The carbonyl group forms an intramolecular hydrogen bond with the N2-imino group (Table 1). This is similar to that found in *N*-benzoyl-*N*′-(2-hydroxyethyl)thiourea (Zhang *et al.*, 2006).

π–π stacking is observed in the crystal structure of (I) (Fig. 2). The centroid-to-centroid separation between parallel benzene rings related by an inversion center at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ is 3.7275 (17) Å; the centroid-to-centroid separation between parallel pyridine rings related by an inversion center at $(0, -\frac{1}{2}, 0)$ is 3.7767 (18) Å.

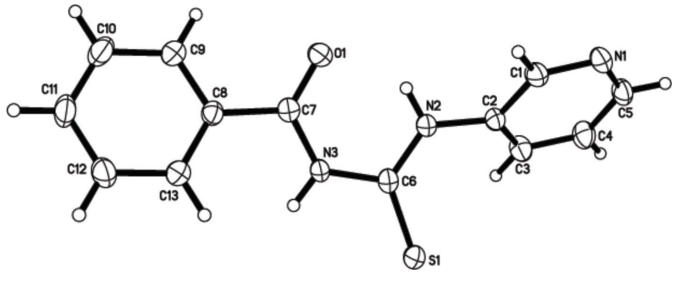


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

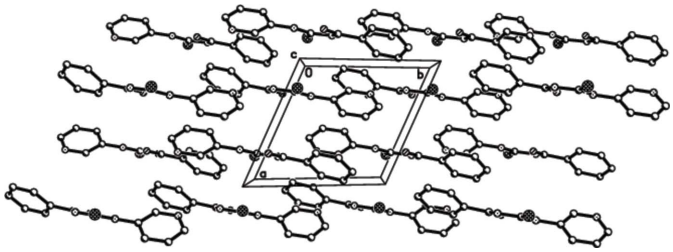


Figure 2
The packing of (I); H atoms have been omitted for clarity.

Experimental

The reaction of 2.82 g (0.02 mol) of benzoyl chloride, 2.29 g (0.03 mol) of ammonium thiocyanate and 1.70 g (0.02 mol) of 3-aminopyridine in 25 ml of CH_2Cl_2 under solid–liquid phase-transfer catalysis conditions (0.37 g of 3% polyethylene glycol-400) gave the title compound. The solid product was filtered off, washed with CH_2Cl_2 and water in turn, and dried under reduced pressure. Recrystallization from chloroform solution gave single crystals of (I).

Crystal data

$C_{13}H_{11}N_3OS$
M_r = 257.31
Triclinic, $P\overline{1}$
a = 7.828 (2) Å
b = 8.688 (2) Å
c = 10.892 (3) Å
α = 111.785 (3)°
β = 92.152 (4)°
γ = 111.499 (4)°
V = 627.0 (3) Å^3
Z = 2
D_x = 1.363 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 293 (2) K
Prism, colorless
0.25 × 0.15 × 0.06 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.930, T_{max} = 0.985
3239 measured reflections
2263 independent reflections
1879 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 25.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.106
S = 1.01
2263 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0512P)^2 + 0.1913P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O1	0.86	1.87	2.597 (2)	141
N3—H3A···N1^{i}	0.86	2.34	3.164 (3)	162

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

H atoms were placed in calculated positions with C—H = 0.93 Å and N—H = 0.86 Å, and refined in riding mode with U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); 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*.

This work was supported by the Natural Science Foundation of Gansu (ZS031-1325-003-*Z*) and the Qinglan Talent Foundation of Lanzhou Jiaotong University.

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