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Key indicators

Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.045
 wR factor = 0.132
Data-to-parameter ratio = 13.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

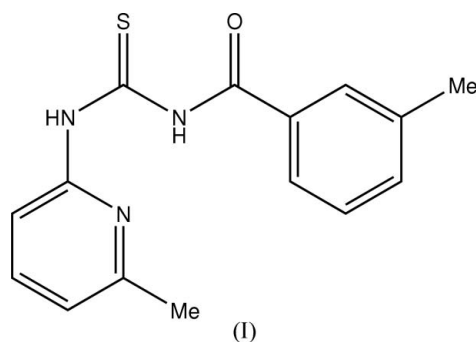
1-(3-Methylbenzoyl)-3-(6-methyl-2-pyridyl)-thiourea

The title molecule, $\text{C}_{15}\text{H}_{15}\text{N}_3\text{OS}$, adopts a *cis-trans* configuration with respect to the positions of the 3-methylbenzoyl and 6-methyl-2-pyridyl groups relative to the S atom across the thiourea C—N bonds. In the crystal structure, the molecules are linked by intermolecular N—H···S hydrogen bonds, forming centrosymmetric dimers.

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Comment

In our earlier X-ray crystallographic study, the molecule of 1-benzoyl-3-(6-methyl-2-pyridyl)thiourea (Yusof *et al.*, 2006) was shown to display a *cis-trans* configuration with respect to the position of the benzoyl and 6-methyl-2-pyridyl groups relative to the S atom across the thiourea C—N bonds. The same configuration is also adopted in the title compound, (I), with the presence of a methyl group at the 3-position of the benzene ring (Fig. 1). The bond lengths and angles (Table 1) are comparable and in normal ranges (Allen *et al.*, 1987). The (6-methyl-2-pyridyl)thiourea fragment (C7/C8/S1/N1/N2/N3/C9—C13/C15) is essentially planar, with a maximum deviation of 0.066 (1) Å for atom N1. The least-squares plane for this fragment is inclined by 30.29 (8)° with respect to the benzene ring C1—C6 plane.



There is an intramolecular hydrogen bond, N1—H1A···N3 (Fig. 1 and Table 2) and, as a result, a pseudo-six-membered ring, N3···H1A—N1—C8—N2—C9, is formed. In the crystal structure, the molecules are not linked to form a one-dimensional chain as in the closely related molecule previously reported (Yusof *et al.*, 2006), but instead form centrosymmetric dimers through N—H···S intermolecular interactions (Fig. 2, Table 2).

Experimental

An equimolar amount of 2-amino-6-methylpyridine (1.78 g, 11 mmol) in 20 ml acetone was added dropwise to a stirred acetone

solution (75 ml) containing 3-methylbenzoyl chloride (2.0 g, 11 mmol) and ammonium thiocyanate (0.82 g, 11 mmol). The mixture was refluxed for 1 h and the resulting solution was poured into a beaker containing some ice blocks. The white precipitate was filtered off and washed with distilled water and cold ethanol and then dried under vacuum. Good quality crystals were obtained by recrystallization from acetone [yield 67% (2.73 g); m.p. 489.3–491.7 K].

Crystal data

$C_{15}H_{15}N_3OS$
 $M_r = 285.36$
 Monoclinic, $P2_1/n$
 $a = 7.1981$ (19) Å
 $b = 10.092$ (3) Å
 $c = 19.372$ (5) Å
 $\beta = 95.826$ (5)°
 $V = 1399.9$ (6) Å³

$Z = 4$
 $D_x = 1.354$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.23$ mm⁻¹
 $T = 298$ (2) K
 Block, colourless
 $0.50 \times 0.32 \times 0.28$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2000)
 $T_{\min} = 0.893$, $T_{\max} = 0.938$

6913 measured reflections
 2459 independent reflections
 1995 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$
 $\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.132$
 $S = 1.04$
 2459 reflections
 183 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0823P)^2 + 0.2335P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.26$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.14$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

S1–C8	1.665 (2)	N1–C8	1.363 (2)
O1–C7	1.211 (2)	N1–C7	1.388 (2)
C8–N1–C7	129.14 (17)	N2–C8–S1	119.47 (14)
N2–C8–N1	115.07 (17)	N1–C8–S1	125.46 (15)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1–H1A \cdots N3	0.86	1.94	2.657 (2)	140
N2–H2A \cdots S1 ⁱ	0.86	2.60	3.4478 (19)	169

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

All H atoms were positioned geometrically and allowed to ride on their parent C or N atoms, with C–H bond lengths constrained to 0.93 (aromatic CH) or 0.96 Å (methyl CH₃), and N–H bond lengths constrained to 0.86 Å. Isotropic displacement parameters for H atoms were set at $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier atom})$ for aromatic CH and NH groups, and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{carrier atom})$ for methyl groups.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 1997); program(s) used to refine

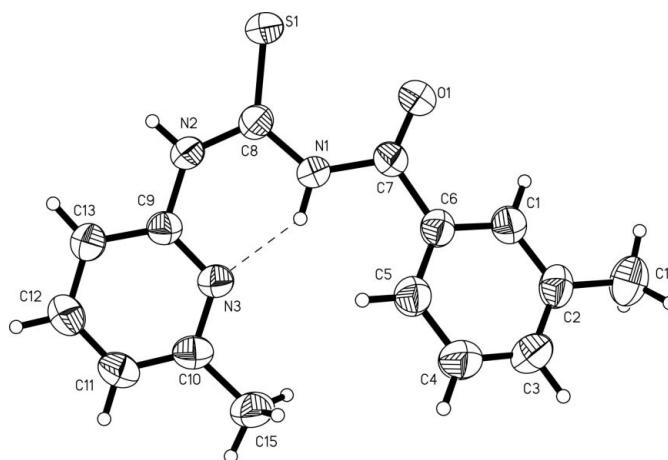


Figure 1

The molecular structure of (I), with 50% probability displacement ellipsoids for non-H atoms. The dashed line indicates the intramolecular N–H \cdots N hydrogen bond.

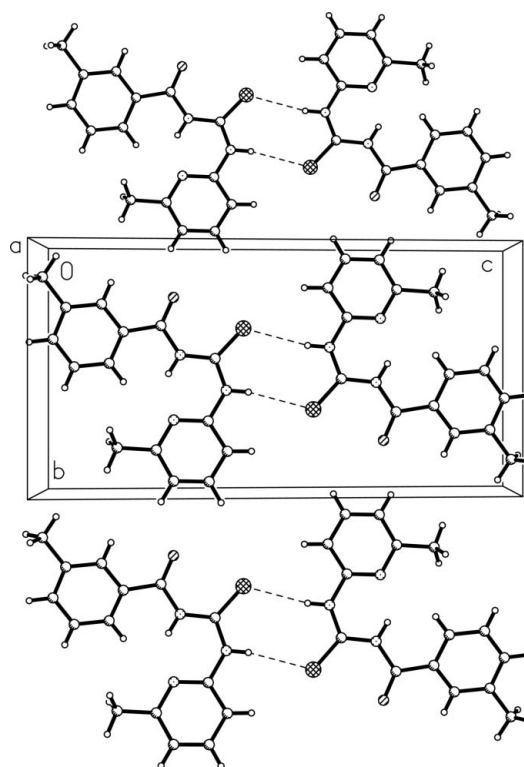


Figure 2

Packing diagram for (I), viewed down the a axis. The dashed lines denote the N–H \cdots S hydrogen bonds, which form dimers.

structure: SHELXTL (Sheldrick, 1997); molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL, PARST95 (Nardelli, 1995) and PLATON (Spek, 2003).

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