Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

1-Benzoyl-3-[3-(trifluoromethyl)phenyl]thiourea

M. Khawar Rauf,[a]* Amin Badshah[a] and Ulrich Flörke[b]

[a]Department of Chemistry, Quaid-i-Azam University, Islamabad 45320, Pakistan, and [b]Department Chemie, Fakultät für Naturwissenschaften, Universität Paderborn, Warburgerstrasse 100, D-33098 Paderborn, Germany

Correspondence e-mail:
aminbadshah@yahoo.com

Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.003 Å
R factor = 0.056
wR factor = 0.145
Data-to-parameter ratio = 17.2

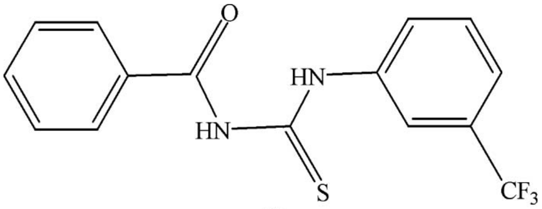
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 15 May 2006
Accepted 18 May 2006

In the title molecular structure, $C_{15}H_{11}F_3N_2OS$, the dihedral angle between the two benzene rings is 7.1 (1)°. In the crystal structure, molecules form centrosymmetric dimers *via* intermolecular N—H···S and C—H···S hydrogen bonds; the dimers are stacked along [010].

Comment

N-Substituted and *N*,*N*′-disubstituted thiourea derivatives have potential applications due to their coordination behavior towards transition metals (Schuster *et al.*, 1990) and also their biological activity (Frech *et al.*, 1970). In addition, thiourea derivatives have been shown to possess antitubercular, antibacterial, antifungal, antithyroid and insecticidal properties (Madan *et al.*, 1991). The title compound, (I) (Fig. 1), is a typical *N*,*N*′-disubstituted thiourea derivative with normal geometric parameters. The C8—S1 and C9—O1 bonds (Table 1) both show the expected double-bond character. The C1—N1, C8—N1, C8—N2 and C9—N2 bond lengths indicate the partial double-bond character typical for this type of compound. Compared to the unsubstituted (Yamin & Yusof, 2003) or the *m*-chloro-substituted (Khawar Rauf *et al.*, 2006) *N*-benzoyl-*N*′-phenylthioureas, the trifluoromethyl substitution at C3 does not result in any significant effect on these bond lengths. The dihedral angle formed by the aromatic rings C1–C6 and C10–C15 is 7.1 (1)°, and the corresponding angles with respect to the thiourea plane (N1/C8/S1/N2/C9/O1) are 10.6 (1)° for the C1–C6 ring and 17.3 (1)° for the C10–C15 ring.



(I)

An intramolecular N—H···O hydrogen bond (Table 2) may influence the planar conformation of the thiourea unit. In the crystal structure, molecules are linked by intermolecular N—H···S and C—H···S hydrogen bonds (Table 2), forming centrosymmetric dimers which are stacked along [010] (Fig. 2).

Experimental

Freshly prepared benzoyl chloride (1.50 g, 10 mmol) was added to a suspension of KSCN (1.00 g, 10 mmol) in acetone (30 ml). The reaction mixture was stirred for 15 min. Afterwards, neat 3-

doi:10.1107/S1600536806018630

(trifluoromethyl)aniline (1.61 g, 10 mmol) was added and the resulting mixture was stirred for 1 h. The reaction mixture was then poured into acidified water and stirred well. The solid product was separated, washed with deionized water and purified by recrystallization from methanol–dichloromethane (1:1) to give X-ray quality crystals of the title compound in an overall yield of 85%. Full spectroscopic and physical characterization will be reported elsewhere.

Crystal data

$C_{15}H_{11}F_3N_2OS$
M_r = 324.32
Monoclinic, $P2_1/n$
a = 15.8710 (13) Å
b = 4.5603 (4) Å
c = 19.6800 (16) Å
β = 95.477 (2)°
V = 1417.9 (2) Å^3

Z = 4
D_x = 1.519 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 120 (2) K
Needle, colorless
0.37 × 0.09 × 0.06 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{\min}$ = 0.909, $T_{\max}$ = 0.981

13559 measured reflections
3416 independent reflections
2473 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.058
$\theta_{\max}$ = 28.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.145
S = 1.06
3416 reflections
199 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0717P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.001
$\Delta\rho_{\max}$ = 0.57 e Å^{-3}
$\Delta\rho_{\min}$ = −0.64 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C8	1.657 (2)	N1—C1	1.410 (3)
O1—C9	1.231 (2)	N2—C9	1.380 (3)
N1—C8	1.344 (2)	N2—C8	1.395 (3)
C8—N1—C1	131.25 (18)	N1—C8—N2	114.67 (18)
C9—N2—C8	128.87 (17)	N2—C9—C10	117.59 (17)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1	0.88	1.86	2.611 (2)	142
N2—H2B···S1$^{\rm i}$	0.88	2.75	3.5680 (17)	155
C15—H15A···S1$^{\rm i}$	0.95	2.76	3.441 (2)	130

Symmetry code: (i) $-x+1, -y+2, -z$.

H atoms were located in difference Fourier maps and refined in idealized positions riding on the C and N atoms, with C—H = 0.95 Å, N—H = 0.88 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C,N). The anisotropic displacement parameters of the trifluoromethyl group indicate disorder (with respect to rotation about the C3—C7 bond) which, however, could not be resolved.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2002); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

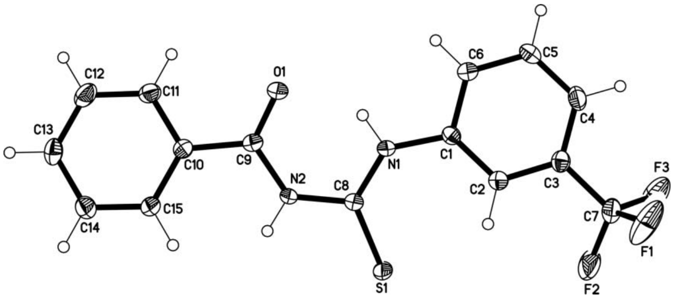


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

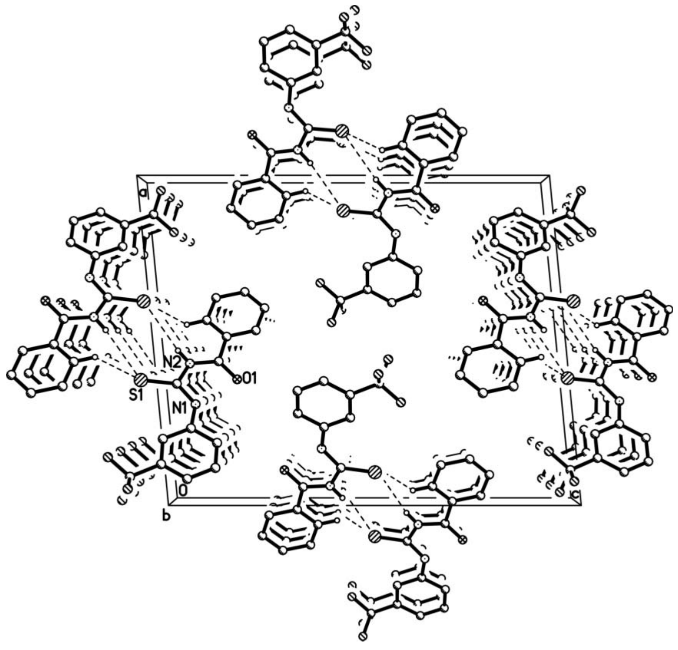


Figure 2
The crystal packing, viewed along [010], with hydrogen bonds indicated by dashed lines. H atoms not involved in hydrogen bonds have been omitted.

MKR is grateful to the Higher Education Commission of Pakistan for financial support for the PhD program (PIN) ILC (0363104).

References

Bruker (2002). *SMART* (Version 5.62), *SAINT* (Version 6.02), *SHELXTL* (Version 6.10) and *SADABS* (Version 2.03). Bruker AXS Inc., Madison, Wisconsin, USA.

Frech, F. A., Blanz, E. J., Amaral, J. R. D. & French, D. A. (1970). *J. Med. Chem.* **13**, 1117–1124.

Khawar Rauf, M., Badshah, A., Flörke, U. & Saeed, A. (2006). *Acta Cryst.* E**62**, o1060–o1061.

Madan, V. K., Taneja, A. D. & Kudesia, V. P (1991). *J. Indian Chem. Soc.* **68**, 471–472.

Schuster, M., Kugler, B. & Konig, K. H. (1990). *J. Anal. Chem.* **338**, 717–720.

Yamin, B. M. & Yusof, M. S. M. (2003). *Acta Cryst.* E**59**, o151–o152.