Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(3-Chloro-4-fluorophenyl)thiourea

Mohd Mustaqim Rosli,[a] Mari Sithambaram Karthikeyan,[b] Hoong-Kun Fun,[a]* Ibrahim Abdul Razak[a] and P. S. Patil[c]

[a]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, [b]Department of P. G. Studies and Research in Chemistry, Mangalore University, Mangalagangotri, Mangalore 574 199, India, and [c]Department of Studies in Physics, Mangalore University, Mangalagangotri, Mangalore 574 199, India

Correspondence e-mail: hkfun@usm.my

Received 21 November 2006
Accepted 22 November 2006

In the title compound, $C_7H_6ClFN_2S$, the dihedral angle between the benzene ring and the thiourea group is 63.62 (3)°. The crystal structure is stabilized by intermolecular N—H$\cdots$Cl/S hydrogen bonds.

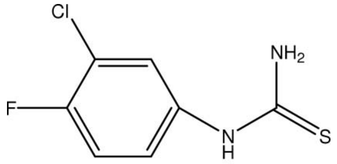
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.001 Å
R factor = 0.026
wR factor = 0.074
Data-to-parameter ratio = 25.1

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

Comment

Thiourea and its derivatives are known to have numerous applications, including complexation with several metal cations (Ali *et al.*, 2005). They are used as corrosion inhibitors for steel and as antioxidants (Alshkel *et al.*, 1987). The anti-irradiation characteristics of thiourea and its derivatives have also been reported (Elsabee *et al.*, 1991). Introducing a thiourea system as a pendant group to a polymer backbone could have several uses. As part of our study of thiourea derivatives (Teh *et al.*, 2006), we report here the crystal structure of the title compound, (I) (Fig. 1).



(I)

All bond lengths and angles in (I) show normal values (Allen *et al.*, 1987) and are comparable to those of a related structure (Teh *et al.*, 2006). The thiourea portion of the molecule is planar, with a mean deviation from the N1/N2/C7/S2 plane of 0.0003 Å. The dihedral angle between the benzene ring and the thiourea group is 63.62 (3)°. The crystal structure

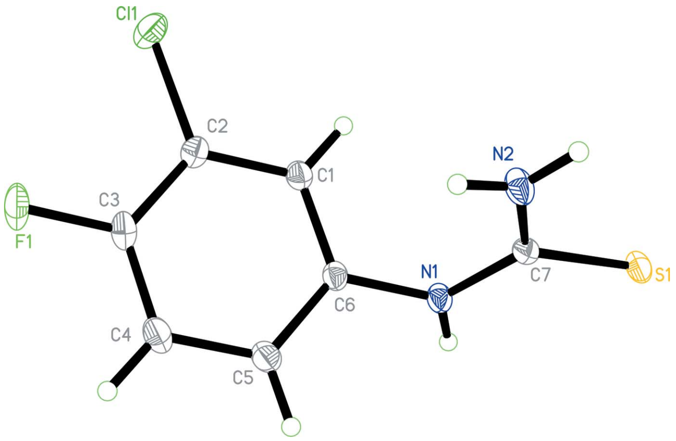


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering.

© 2007 International Union of Crystallography
All rights reserved

is stabilized by intermolecular N—H···S and N—H···Cl hydrogen bonds (Table 1), forming an infinite two-dimensional network parallel to the (101) plane (Fig. 2).

Experimental

The title compound was synthesized following the method reported in the literature (Teh *et al.*, 2006), using 3-chloro-4-fluoroaniline, in a yield of 83%. The compound was purified by recrystallization from ethanol. Crystals were obtained by the slow evaporation of an ethanol solution.

Crystal data

$C_7H_6ClFN_2S$
$M_r = 204.65$
Triclinic, $P\bar{1}$
$a = 5.4642$ (1) Å
$b = 8.3919$ (1) Å
$c = 9.6469$ (2) Å
$\alpha = 105.228$ (1)°
$\beta = 94.455$ (1)°
$\gamma = 95.321$ (1)°
$V = 422.58$ (1) Å^3
$Z = 2$
$D_x = 1.608$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.66$ mm^{-1}
$T = 100.0$ (1) K
Block, colourless
0.68 × 0.57 × 0.18 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{\min} = 0.666$, $T_{\max} = 0.891$
9586 measured reflections
3041 independent reflections
2894 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.018$
$\theta_{\max} = 32.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.074$
$S = 1.09$
3041 reflections
121 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0392P)^2 + 0.1257P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.44$ e Å^{-3}
$\Delta\rho_{\min} = -0.53$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N1···S1$^{\rm i}$	0.85 (2)	2.462 (17)	3.3011 (8)	167
N2—H1N2···Cl1$^{\rm ii}$	0.86 (2)	2.664 (17)	3.4433 (9)	152
N2—H2N2···S1$^{\rm iii}$	0.84 (2)	2.508 (16)	3.3375 (9)	168

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+2, -y, -z$; (iii) $-x+1, -y, -z+1$.

N-bound H atoms were located in difference maps and refined isotropically. The remaining H atoms were positioned geometrically and treated as riding, with C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

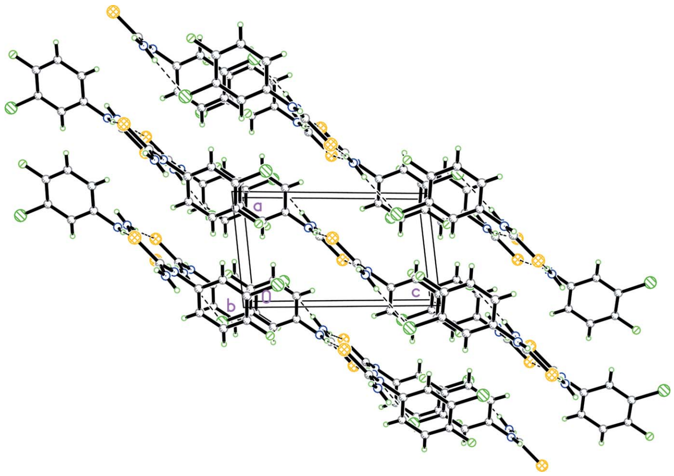


Figure 2
The crystal packing of (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

The authors thank the Malaysian Government and Universiti Sains Malaysia for the Scientific Advancement Grant Allocation (SAGA) grant No. 304/PFIZIK/653003/A118. MSK is grateful to CSIR, New Delhi, for providing a Senior Research Fellowship (SRF).

References

Ali, A. M., El-Sawy, N. M. & Sagheer, F. A. (2005). *Int. J. Polym. Mat.* **54**, 359–373.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Alshkel, A. G., Hefny, M. M., Ismail, A. R. & El-Basiouny, M. A. (1987). *Corros. Prev. Contr.*, **34**, 155–159.
Bruker (2005). *APEX2* (Version 1.27), *SAINT* (Version 7.12A) and *SADABS* (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.
Elsabee, M. Z., Naguib, H. F., Mikhael, M. G., Sabaa, M. W. & Furuhata, K. (1991). *Macromolecules*, **24**, 1962–1968.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sheldrick, G. M. (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Teh, J. B.-J., Karthikeyan, M. S., Fun, H.-K., Patil, P. S., Razak, I. A., Holla, B. S. & Dharmaprakash, S. M. (2006). *Acta Cryst.* E**62**, o4693–o4694.

o68 Rosli *et al.* • $C_7H_6ClFN_2S$ *Acta Cryst.* (2007). E**63**, o67–o68