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Key indicators

Single-crystal X-ray study
 $T = 273\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.053
 wR factor = 0.133
Data-to-parameter ratio = 13.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

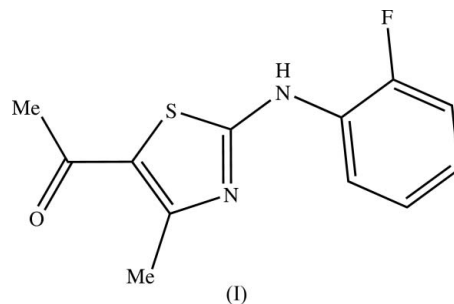
5-Acetyl-4-methyl-2-(2-fluorophenylamino)-1,3-thiazole

The molecule of the title compound, $\text{C}_{12}\text{H}_{11}\text{N}_2\text{FOS}$, is essentially planar, with a maximum deviation of $0.127(3)\text{ \AA}$ for the C atom of the methyl group attached to the thiazole ring. The structure is stabilized by intra- and intermolecular hydrogen bonds to form one-dimensional polymeric chains parallel to the b axis.

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Comment

The title compound, (I), is isostructural with 5-acetyl-4-methyl-2-(*o*-toluidinyl)-1,3-thiazole (Yamin *et al.*, 2005), except that the F atom is bonded at the *ortho* position of the phenylamino fragment. The whole molecule is essentially planar, with a maximum deviation for atom C12 of $0.127(3)\text{ \AA}$ from the least-squares plane; in the molecule of 5-acetyl-4-methyl-2-(*o*-toluidinyl)-1,3-thiazole, the benzene group is inclined to the thiazole ring by $73.44(10)^\circ$. All bond lengths and angles are in normal ranges (Allen *et al.*, 1987) and are comparable with those in the analogue.



There are weak intramolecular $\text{N1}-\text{H1}\cdots\text{F1}$, $\text{C10}-\text{H10B}\cdots\text{O1}$ and $\text{C5}-\text{H5}\cdots\text{N2}$ hydrogen bonds (Table 2). In the crystal structure, the molecules are linked by inter-

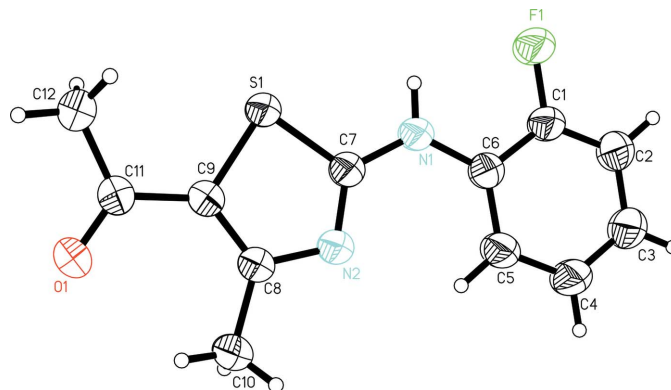


Figure 1
The molecular structure of (I), with 50% probability displacement ellipsoids.

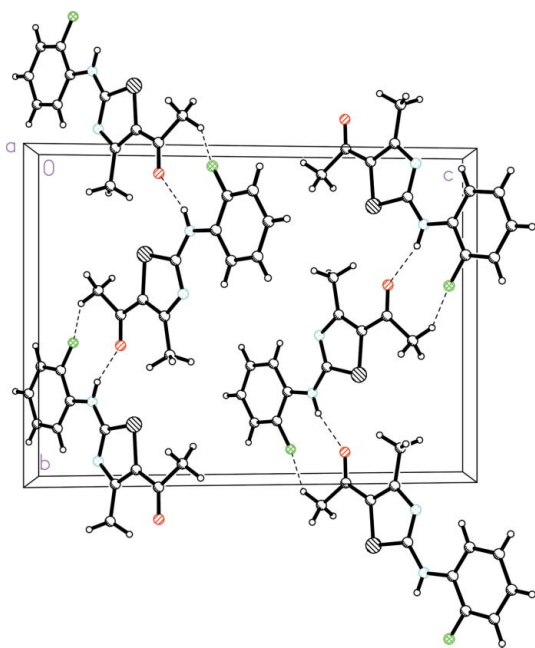


Figure 2
A packing diagram for (I), viewed down the *b* axis. Dashed lines denote the N—H···O and C—H···F hydrogen bonds.

molecular N1—H1···O1ⁱ and C12—H12C···F1ⁱⁱ hydrogen bonds (symmetry codes as in Table 2) to form one-dimensional zigzag polymeric chains parallel to the *b* axis (Fig. 2).

Experimental

A solution of *o*-fluoroaniline (1.11 g, 0.01 mol) in acetone (50 ml) was added dropwise to an acetone solution (50 ml) containing an equimolar amount of 3-chloroacetylacetone and ammonium thiocyanate in a two-necked round-bottomed flask. The solution was refluxed for about 2 h. The light-yellow solution was filtered off and colourless crystals of (I) were obtained after evaporation over a period of 5 d (yield 85%; m.p. 447.8–449.3 K).

Crystal data

C₁₂H₁₁FN₂OS
M_r = 250.29
 Monoclinic, *P*2₁/*c*
a = 5.0205 (11) Å
b = 13.081 (3) Å
c = 17.598 (4) Å
 β = 97.085 (4)°
V = 1146.9 (4) Å³
Z = 4

D_x = 1.450 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 2840 reflections
 θ = 1.9–26.5°
 μ = 0.28 mm⁻¹
T = 273 (2) K
 Block, colourless
 0.43 × 0.28 × 0.17 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2000)
T_{min} = 0.889, *T_{max}* = 0.954
 6015 measured reflections

2115 independent reflections
 1931 reflections with *I* > 2σ(*I*)
R_{int} = 0.018
 θ_{\max} = 25.5°
h = -6 → 5
k = -15 → 13
l = -13 → 21

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.053
wR (*F*²) = 0.133
S = 1.19
 2115 reflections
 160 parameters
 H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0582P)^2 + 0.5434P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.23 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.19 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

S1—C7	1.733 (3)	N1—C6	1.401 (3)
S1—C9	1.740 (2)	N2—C7	1.309 (3)
F1—C1	1.358 (3)	N2—C8	1.375 (3)
O1—C11	1.214 (3)	C8—C9	1.370 (4)
N1—C7	1.360 (3)		
C7—S1—C9	88.76 (11)	C7—N2—C8	110.8 (2)

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N1—H1···F1	0.87 (3)	2.27 (3)	2.653 (3)	107 (2)
C5—H5···N2	0.93	2.30	2.919 (4)	123
C10—H10B···O1	0.96	2.40	3.018 (4)	122
N1—H1···O1 ⁱ	0.87 (3)	2.18 (3)	3.010 (3)	158 (3)
C12—H12C···F1 ⁱⁱ	0.96	2.33	3.165 (3)	144

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

All H atoms were located in a difference map. The H atom on N1 was refined isotropically. All other H atoms were placed geometrically in ideal positions and allowed to ride on their parent C atoms, with C—H distances in the range 0.93–0.96 Å and with *U_{iso}*(H) = 1.5*U_{eq}*(methyl C), or 1.2*U_{eq}*(C) for CH 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 structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL, PARST (Nardelli, 1995) and PLATON (Spek, 2003).

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