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Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$
 R factor = 0.055
 wR factor = 0.125
Data-to-parameter ratio = 13.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

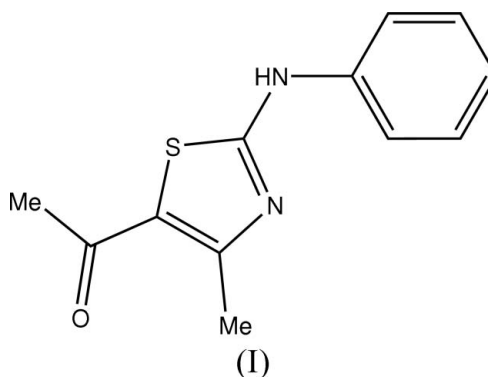
5-Acetyl-4-methyl-2-phenylamino-1,3-thiazole

The asymmetric unit of the title compound, $\text{C}_{12}\text{H}_{12}\text{N}_2\text{OS}$, contains two crystallographically independent molecules. Both molecules are essentially planar and stabilized by intra- and intermolecular hydrogen-bonding interactions to form one-dimensional zigzag polymeric chains parallel to the c 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) and 5-acetyl-4-methyl-2-(2-fluorophenylamino)-1,3-thiazole (Kasim *et al.*, 2005). The asymmetric unit consist of two molecules (Fig. 1). The bond lengths and angles of the molecules are in normal ranges (Allen *et al.*, 1987) and in agreement with the above two compounds. Both molecules are essentially planar, with a maximum deviation of 0.216 (2) Å for atom O1 in the first molecule and 0.154 (4) Å for atom C16 in the second molecule. In the *ortho*-fluorophenylamino analogue, the maximum deviation is 0.127 (3) Å for the methyl C atom of the acetyl group. There are intramolecular C1—H1A···N2 and C13—H13···N4 interactions (Table 2). In the crystal structure, the molecules are linked by intermolecular hydrogen-bonding interactions (N1—H1···O2ⁱ, N3—H3···O1ⁱⁱ and C5—H5···O2ⁱ; symmetry codes as in Table 2) to form one-dimensional zigzag polymeric chains parallel to the c axis (Fig. 2).



Experimental

A solution of aniline (0.93 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 1 h. The light-yellow solution was filtered off and some colourless crystals were obtained after five days of evaporation (yield 80%, m.p. 430.6–431.3 K).

Crystal data

$C_{12}H_{12}N_2OS$
 $M_r = 232.30$
 Monoclinic, $P2_1/c$
 $a = 12.932$ (6) Å
 $b = 7.532$ (3) Å
 $c = 24.322$ (11) Å
 $\beta = 101.236$ (9)°
 $V = 2323.6$ (18) Å³
 $Z = 8$

$D_x = 1.328$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 1480 reflections
 $\theta = 1.6$ – 26.0 °
 $\mu = 0.26$ mm⁻¹
 $T = 293$ (2) K
 Block, colourless
 $0.31 \times 0.19 \times 0.12$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2000)
 $T_{\min} = 0.924$, $T_{\max} = 0.969$
 11081 measured reflections

4065 independent reflections
 2637 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.049$
 $\theta_{\text{max}} = 25.0$ °
 $h = -15 \rightarrow 14$
 $k = -7 \rightarrow 8$
 $l = -28 \rightarrow 28$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.125$
 $S = 1.02$
 4065 reflections
 293 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + 0.0551P]^2 + 0.1476P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.18$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.20$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

S1–C7	1.734 (3)	N1–C6	1.414 (4)
S1–C8	1.742 (3)	N2–C7	1.317 (3)
S2–C19	1.731 (3)	N2–C9	1.371 (3)
S2–C20	1.744 (3)	N3–C19	1.364 (3)
O1–C11	1.219 (3)	N3–C18	1.406 (4)
O2–C23	1.223 (3)	N4–C19	1.309 (3)
N1–C7	1.354 (4)	N4–C21	1.372 (3)
C7–S1–C8	88.65 (14)	C7–N2–C9	110.3 (2)
C19–S2–C20	88.56 (14)	C19–N4–C21	109.9 (2)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1–H1A \cdots N2 ⁱ	0.93	2.37	2.991 (4)	124
C13–H13 \cdots N4 ⁱ	0.93	2.30	2.917 (4)	123
N1–H1 \cdots O2 ⁱⁱ	0.86	1.95	2.788 (4)	166
N3–H3 \cdots O1 ⁱⁱⁱ	0.86	2.02	2.872 (4)	171
C5–H5 \cdots O2 ⁱⁱ	0.93	2.57	3.288 (4)	135

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

After their location in a difference map, all H atoms were repositioned geometrically at ideal positions and allowed to ride on the parent C atoms with C–H distances of 0.93–0.96 Å, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl and $1.2U_{\text{eq}}(\text{C}, \text{N})$ for aromatic and amine groups.

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

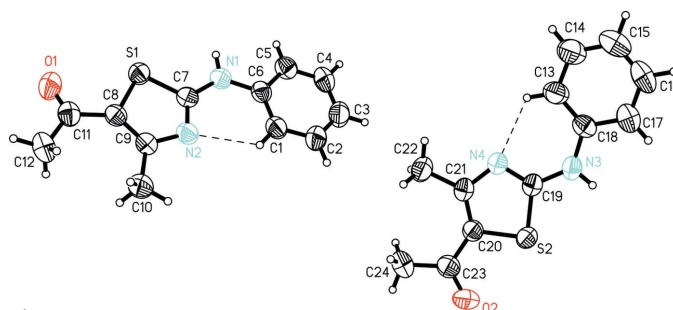


Figure 1

The asymmetric unit of (I), with 50% probability displacement ellipsoids. Hydrogen bonds are shown as dashed lines.

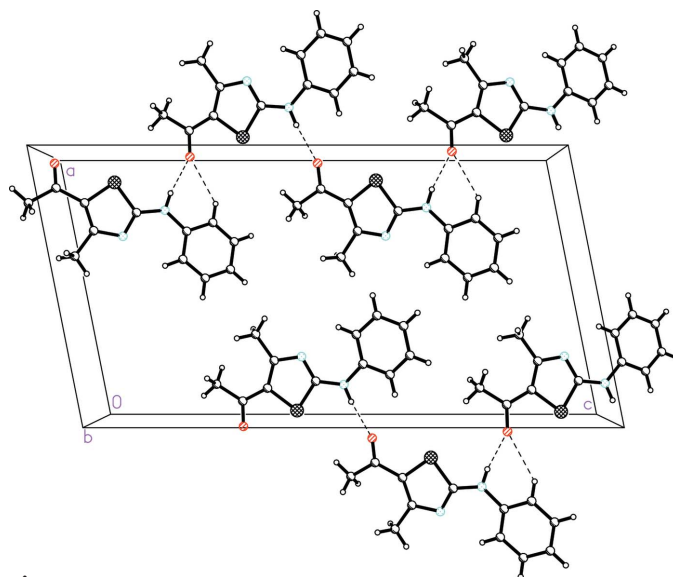


Figure 2

Packing diagram of (I), viewed down the b axis. The dashed lines denote the N–H \cdots O and C–H \cdots O interactions.

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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