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1-[1-(4-Fluorophenyl)-2-methyl-5-phenyl-1*H*-pyrrol-3-yl]ethanone

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Key indicators

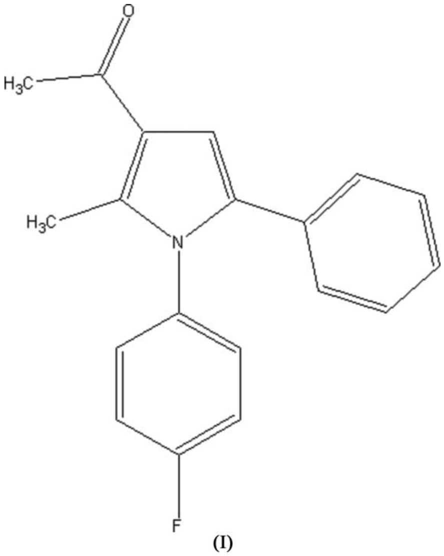
Single-crystal X-ray study
T = 290 K
Mean σ(C–C) = 0.002 Å
R factor = 0.042
wR factor = 0.120
Data-to-parameter ratio = 11.7

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

The title compound, $C_{19}H_{16}FNO$, crystallizes with two crystallographically independent molecules in the asymmetric unit. The dihedral angles between the pyrrole ring and fluorophenyl and unsubstituted phenyl rings are 44.9 (1) and 54.5 (2)°, respectively, in the first molecule, and 72.8 (3) and 30.7 (3)° in the second molecule. The crystal structure is stabilized by intermolecular C—H···O and C—H···π interactions.

Comment

Molecular organization and molecular interactions are the features that are responsible for molecules exhibiting different functional properties. An understanding of non-covalent interactions becomes essential for interpreting and predicting relationships between chemical structure and function (Hunter *et al.*, 2001). Crystal engineering *via* manipulation of hydrogen bonding has gained a lot of interest in the recent literature (Aakeröy, 1997; Desiraju, 2000). Weak intermolecular forces of the type C—H···π play an important role in various systems of biological and chemical interest (Nishio, 2004). Intramolecular C—H···π interactions are often responsible for the molecule adopting a particular conformation in the solid state (Jennings *et al.*, 2001). We report here the stucture of the title compound, (I) (Fig. 1 and Table 1), which displays both types of interaction.



(I)

The molecular conformation is stabilized by intramolecular C—H···O interactions, involving H18*A* and H33*B*, having graph-set motif *S*(6) (Bernstein *et al.*, 1995). This prevents conformational flexibility. In addition, intermolecular C—

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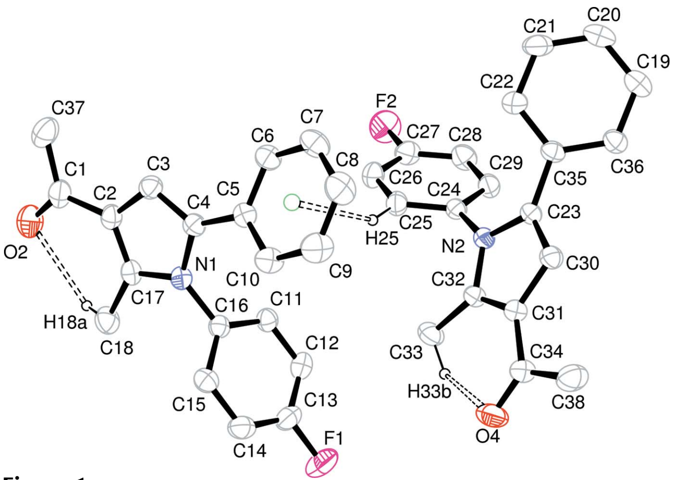

Figure 1
The asymmetric unit of the title compound, drawn with 50% probability displacement ellipsoids. Dashed lines indicate intramolecular C—H···O interactions and one C—H···π intermolecular contact. The green open circle is the center of gravity of the phenyl ring. H atoms other than those involved in the hydrogen bonds and the C—H···π contact have been omitted.

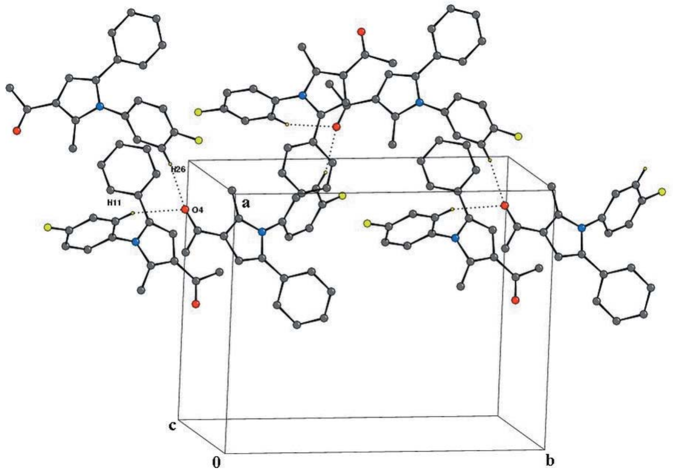

Figure 2
C—H···O chains along the [010] direction. Hydrogen bonds are drawn as dotted lines and H atoms not involved in these interactions have been omitted.

H···π interactions also link the molecules in the asymmetric unit (Fig. 1). Bifurcated hydrogen bonds between atoms O4, H11 and H26 form chains along the crystallographic *b* axis [graph-set symbol *C*(9); Fig. 2]. Finally, additional stability is provided by C—H···π interactions utilizing atom H12 of the 4-fluorophenyl ring, which form molecular chains along the crystallographic *c*-glide plane (Fig. 3).

Experimental

The title compound was synthesized according to the procedure reported in the literature (Nagarajan *et al.*, 1985) and subsequently tested for anti-implantation activity. The compound was crystallized from solutions in dichloromethane and hexane (2:1, *v*/*v*) by slow evaporation at 278 K.

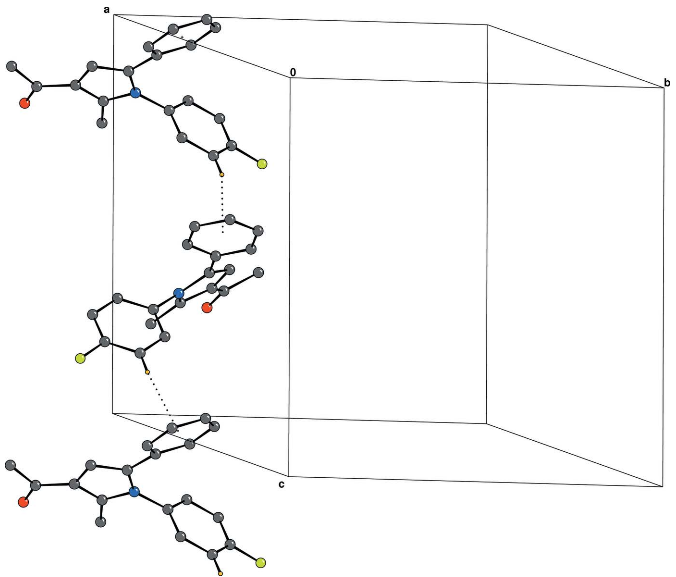

Figure 3
C—H···π interactions (represented by dotted lines) along the [001] direction. H atoms not involved in these interactions have been omitted.

Crystal data

$C_{19}H_{16}FNO$
$M_r = 293.33$
Monoclinic, $P2_1/c$
$a = 13.398$ (6) Å
$b = 15.838$ (7) Å
$c = 14.680$ (7) Å
$\beta = 101.979$ (8)°
$V = 3047$ (2) Å^3
$Z = 8$
$D_x = 1.279$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 290$ (2) K
Block, colorless
0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.974$, $T_{\max} = 0.991$
24441 measured reflections
6143 independent reflections
4748 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.018$
$\theta_{\max} = 26.4°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.120$
$S = 1.03$
6143 reflections
525 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0691P)^2 + 0.4133P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.22$ e Å^{-3}
$\Delta\rho_{\min} = -0.16$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C17	1.3723 (19)	N2—C24	1.4340 (19)
N1—C16	1.4350 (19)	F2—C27	1.3541 (19)
N2—C32	1.3737 (18)	O4—C34	1.2143 (19)
C30—C23—C35—C22	−133.36 (18)	C32—N2—C24—C29	−123.10 (16)
C16—N1—C4—C3	167.83 (13)	C30—C31—C34—O4	−176.33 (16)
C17—N1—C4—C5	175.62 (13)	C3—C2—C1—O2	−179.97 (17)

Table 2

Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C18—H18A···O2	0.95 (3)	2.44 (3)	3.012 (3)	119 (2)
C33—H33B···O4	0.96	2.47	3.020 (2)	116
C11—H11···O4^{i}	0.96 (2)	2.57 (2)	3.477 (3)	157 (1)
C25—H25···$Cg2^{ii}$	0.96 (2)	2.66 (2)	3.514 (2)	148 (1)
C12—H12···$Cg2^{iii}$	0.92 (2)	2.80 (2)	3.687 (3)	162 (2)
C26—H26···O4^{i}	0.93 (2)	2.36 (2)	3.213 (3)	152 (2)

Symmetry codes: (i) $-x+2, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x+1, y, z$; (iii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

The H atoms on the methyl atoms C33, C37 and C38 were positioned geometrically and refined as riding, with C—H = 0.96 Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C). The remaining H atoms were located in a difference Fourier map and refined isotropically. The C—H bond distances are in the range 0.90 (4) Å to 0.98 (2) Å.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 2003).

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