

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

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## Key indicators

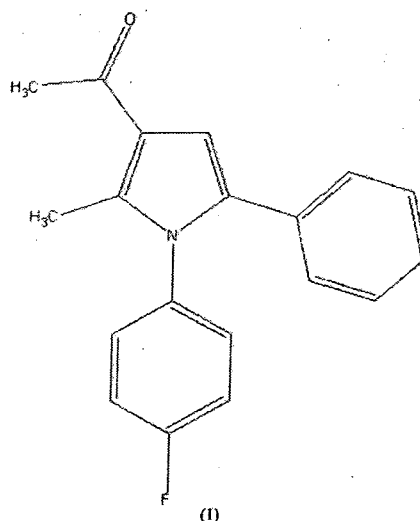
Single-crystal X-ray study  
T = 290 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$   
R factor = 0.042  
wR factor = 0.120  
Data-to-parameter ratio = 11.7For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

The title compound,  $\text{C}_{19}\text{H}_{16}\text{FNO}$ , 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  $54.5 (2)^\circ$ , respectively, in the first molecule, and  $72.8 (3)$  and  $30.7 (3)^\circ$  in the second molecule. The crystal structure is stabilized by intermolecular  $\text{C}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\pi$  interactions.

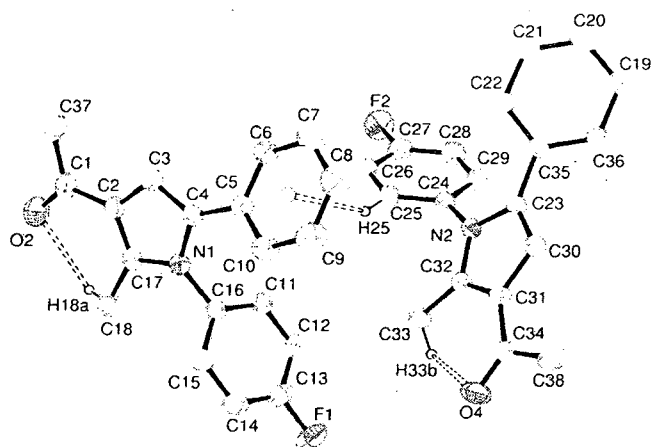
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## Comment

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  $\text{C}-\text{H}\cdots\pi$  play an important role in various systems of biological and chemical interest (Nishio, 2004). Intramolecular  $\text{C}-\text{H}\cdots\pi$  interactions are often responsible for the molecule adopting a particular conformation in the solid state (Jennings *et al.*, 2001). We report here the structure of the title compound, (I) (Fig. 1 and Table 1), which displays both types of interaction.

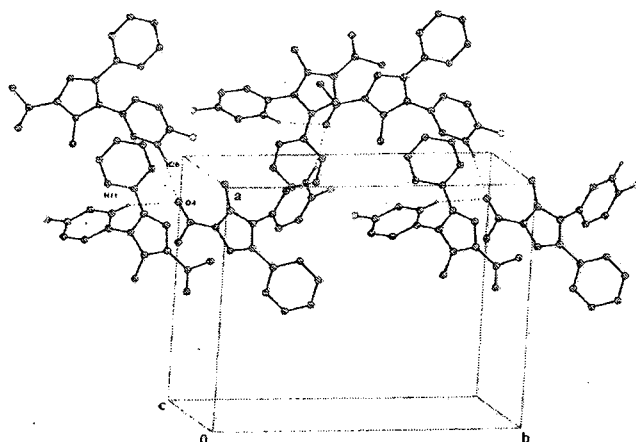


The molecular conformation is stabilized by intramolecular  $\text{C}-\text{H}\cdots\text{O}$  interactions, involving H18A and H33B, having graph-set motif  $S(6)$  (Bernstein *et al.*, 1995). This prevents conformational flexibility. In addition, intermolecular  $\text{C}-$



**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... $\pi$  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... $\pi$  contact have been omitted.



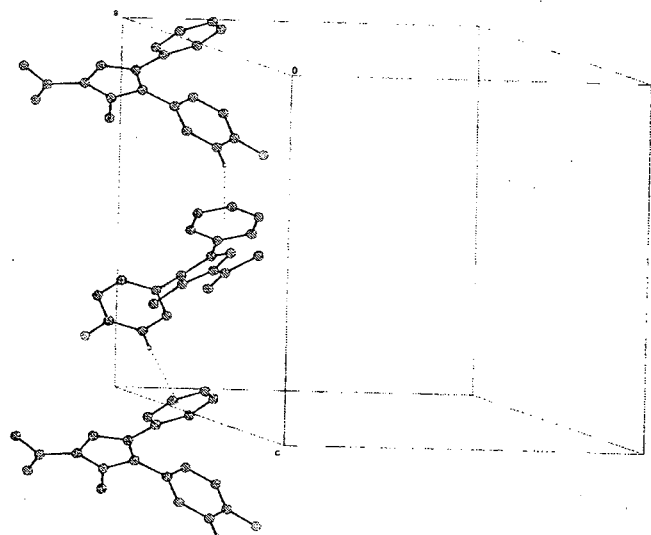
**Figure 2**

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... $\pi$  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... $\pi$  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... $\pi$  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<sup>3</sup>

$Z = 8$   
 $D_x = 1.279$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 290$  (2) K  
 Block, colorless  
 $0.30 \times 0.25 \times 0.20$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  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  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.018$   
 $\theta_{\text{max}} = 26.4^\circ$

## 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  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.22$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.16$  e Å<sup>-3</sup>

**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, °).

<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>
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 <sup>i</sup>	0.96 (2)	2.57 (2)	3.477 (3)	157 (1)
C25—H25...Cg2 <sup>ii</sup>	0.96 (2)	2.66 (2)	3.514 (2)	148 (1)
C12—H12...Cg2 <sup>iii</sup>	0.92 (2)	2.80 (2)	3.687 (3)	162 (2)
C26—H26...O4 <sup>j</sup>	0.93 (2)	2.36 (2)	3.213 (3)	152 (2)

Symmetry codes: (i)  $-x+2, y+\frac{1}{2}, -z+\frac{1}{2}$ ; (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  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ . 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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