

5-Benzyl-1-(4-fluorophenyl)-2-phenyl-4,5,6,7-tetrahydro-1H-pyrrolo[3,2-c]pyridine

Deepak Chopra,^{a*} K. Nagarajan^b
and T. N. Guru Row^a^aSolid State and Structural Chemistry Unit,
Indian Institute of Science, Bangalore 560 012,
Karnataka, India, and ^bHIKAL India Limited,
Banerghatta Road, Bangalore 560 078
Karnataka, IndiaCorrespondence e-mail:
deepak@sscu.iisc.ernet.in

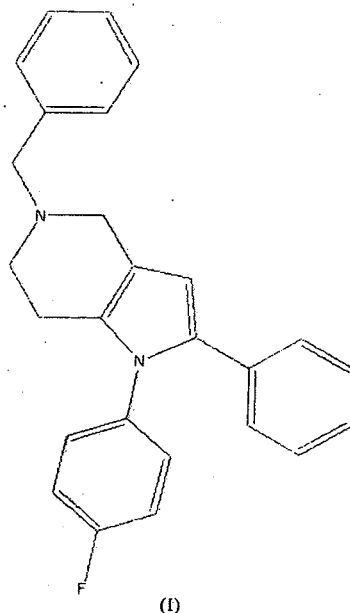
Key indicators

Single-crystal X-ray study
T = 290 K
Mean $\sigma(\text{C}-\text{C})$ = 0.004 Å
R factor = 0.082
wR factor = 0.137
Data-to-parameter ratio = 11.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

In the title compound, $\text{C}_{26}\text{H}_{23}\text{FN}_2$, the dihedral angle between the 4-fluorophenyl ring and the adjacent phenyl ring is $62.3(1)^\circ$. The crystal structure is stabilized by $\text{C}-\text{H}\cdots\pi$ 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* the manipulation of hydrogen bonding has attracted much attention 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 *et al.*, 2004). Intramolecular $\text{C}-\text{H}\cdots\pi$ interactions are responsible for a molecule adopting a particular conformation in the solid state (Jennings *et al.*, 2001). 4-Keto-4,5,6,7-tetrahydroindoles have been tested for anti-implantation agents in rats and have been found to exhibit potent biological activity. Against this background, we have studied the crystal structure of the title compound (1).



A molecular view of (1), with the atom-labelling scheme, is shown in Fig. 1. Relevant bond distances and torsion angles are given in Table 1. Atom N1 deviates by 0.604 (2) Å from

the least-squares plane passing through atoms C5/C3/C4/C7/C6. The crystal structure is stabilized by C—H... π intermolecular interactions (Table 2), forming molecular dimers (Fig. 2).

Experimental

The compound (I) was synthesized according to the procedure reported in the literature (Nagarajan *et al.*, 1985), and crystallized by slow evaporation of a chloroform/hexane (2:1 *v/v*) solution at 278 K.

Crystal data

$C_{26}H_{23}FN_2$
 $M_r = 382.46$
 Monoclinic, $P2_1/c$
 $a = 13.220$ (8) Å
 $b = 18.431$ (11) Å
 $c = 8.475$ (5) Å
 $\beta = 103.223$ (11)°
 $V = 2010$ (2) Å³
 $Z = 4$

$D_x = 1.264$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 650 reflections
 $\theta = 1.4$ – 25.8 °
 $\mu = 0.08$ mm⁻¹
 $T = 290$ (2) K
 Block, colourless
 0.25 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEX CCD area detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{min} = 0.939$, $T_{max} = 0.988$
 15238 measured reflections

3975 independent reflections
 2935 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.043$
 $\theta_{max} = 26.4$ °
 $h = -16 \rightarrow 16$
 $k = -22 \rightarrow 22$
 $l = -10 \rightarrow 10$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.082$
 $wR(F^2) = 0.137$
 $S = 1.23$
 3975 reflections
 354 parameters
 All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0366P)^2 + 0.563P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 0.17$ e Å⁻³
 $\Delta\rho_{min} = -0.15$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

N2—C4	1.392 (3)	N1—C20	1.461 (3)
N2—C1	1.393 (3)	N1—C5	1.467 (3)
N2—C8	1.431 (3)	N1—C6	1.473 (3)
F1—C11	1.356 (3)		
C5—N1—C20—C26	60.4 (3)	C20—N1—C6—C7	169.2 (2)
C6—N1—C20—C26	-176.4 (3)	C5—N1—C6—C7	-67.5 (3)
C19—C14—C1—C2	-144.7 (3)		

Table 2

Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
C9—H9...Cg1 ¹	0.95 (3)	2.79 (3)	3.648 (4)	150 (2)

Symmetry code: (i) $-x, -y + 1, -z + 1$. Cg1 is the centroid of the five-membered ring C1—C4/N2

All H atoms were located in difference Fourier maps and refined isotropically. The C—H bond distances are in the range 0.92 (3) Å to 1.02 (2) Å.

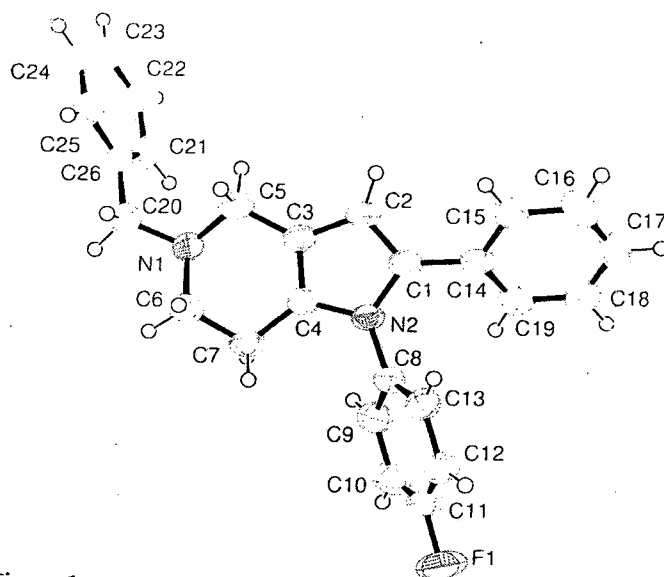


Figure 1
 Molecular structure of (I), showing 50% probability displacement ellipsoids.

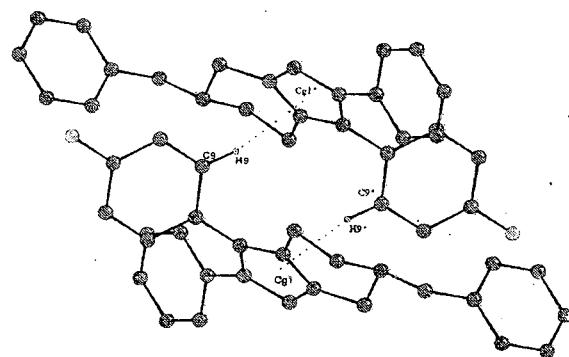


Figure 2
 A molecular dimer. Dashed lines indicate C—H... π interactions. Atoms labelled with an asterisk (*) are at the symmetry position ($-x, 1 - y, 1 - z$).

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, 1999) and CAMERON (Watkin *et al.*, 1993); software used to prepare material for publication: PLATON (Spek, 2003).

We thank the Department of Science and Technology, India for data collection on the CCD facility set up under the IRFA-DST programme. DC thanks CSIR, India for a JRF.

References

- Aakeröy, C. B. (1997). *Acta Cryst.* B53, 569–586.
 Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* 26, 343–350.
 Bruker (2000). SMART (Version 5.628) and SAINT (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
 Desiraju, G. R. (2000). *J. Chem. Soc. Dalton Trans.* 21, 3745–3751.
 Farrugia, L. J. (1999). *J. Appl. Cryst.* 32, 837–838.

- Hunter, C. A., Lawson, K. R., Perkins, J. & Urch, C. J. (2001). *Perkin Trans.* 2, pp. 651–669.
- Jennings, W. B., Farrell, B. M. & Malone, J. F. (2001). *Acc. Chem. Res.* 34, 885–894.
- Nagarajan, K., Talwalker, P. K., Shah, R. K., Mehta, S. R. & Nayak, G. V. (1985). *Indian J. Chem.* 24, 98–111.
- Nishio, M. (2004). *CrystEngComm*, 6, 130–158.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
- Spek, A. L. (2003). *J. Appl. Cryst.* 36, 7–13.
- Watkin, D. M., Pearce, L. & Prout, C. K. (1993). *CAMERON*. Chemical Crystallography Laboratory, University of Oxford, England.