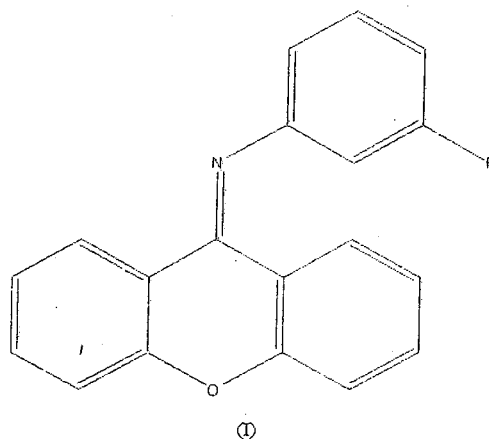


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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.082
 wR factor = 0.157
Data-to-parameter ratio = 11.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>*N*-(3-Fluorophenyl)-9*H*-xanthen-9-ylideneamineIn the title compound, $\text{C}_{19}\text{H}_{12}\text{FNO}$, the dihedral angle between the mean planes of the 9*H*-xanthene moiety and the 3-fluorophenyl group is $82.5(1)^\circ$. An intramolecular $\text{C}-\text{H}\cdots\pi$ interaction stabilizes the molecular conformation.Received 8 November 2004
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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 attracted 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 responsible for molecules adopting a particular conformation in the solid state (Jennings *et al.*, 2001). A structural study of the title compound, (I), has been carried out as a case study where there is no possibility of formation of hydrogen bonds and hence it is thought to be suitable for the study of weak interactions.

A view of (I) with the atom-labelling scheme is shown in Fig. 1. The 9*H*-xanthene unit is almost planar, as indicated by the torsion angles (Table 1). The bond angle $\text{C}12-\text{N}1-\text{C}14$ of $126.7(2)^\circ$ is greater than the ideal bond angle value of 120° to avoid steric repulsion between atoms $\text{H}15$ and $\text{H}1$. Rotation of the 3-fluorophenyl group takes place and this is favoured because it leads to the formation of an intramolecular $\text{C}-\text{H}\cdots\pi$ interaction (Table 2) involving $\text{H}1$, which stabilizes the molecular conformation (Fig. 1).

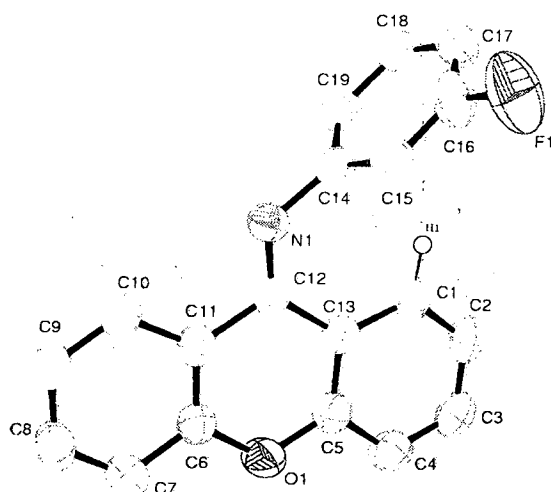


Figure 1
The molecular structure of (I), showing 40% probability ellipsoids. H atoms have been omitted for clarity, except for H1. The dashed line indicates the intramolecular C—H... π interaction.

Experimental

Compound (I) was synthesized according to a procedure reported in the literature (Nagarajan *et al.*, 1974). The compound was crystallized from a solution in ethyl acetate and hexane, by slow evaporation at ca 278 K.

Crystal data

$C_{19}H_{12}FNO$
 $M_r = 289.30$
Monoclinic, $P2_1/n$
 $a = 14.175(3) \text{ \AA}$
 $b = 5.0634(9) \text{ \AA}$
 $c = 19.912(3) \text{ \AA}$
 $\beta = 102.794(4)^\circ$
 $V = 1393.6(4) \text{ \AA}^3$
 $Z = 4$

$D_x = 1.379 \text{ Mg m}^{-3}$
MoK α radiation
Cell parameters from 757 reflections
 $\theta = 1.3\text{--}24.4^\circ$
 $\mu = 0.10 \text{ mm}^{-1}$
 $T = 293(2) \text{ K}$
Prism, orange–yellow
 $0.60 \times 0.60 \times 0.56 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.902$, $T_{\max} = 0.949$
10501 measured reflections

2849 independent reflections
1600 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.069$
 $\theta_{\text{max}} = 26.4^\circ$
 $h = -17 \rightarrow 17$
 $k = -6 \rightarrow 6$
 $l = -24 \rightarrow 24$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.082$
 $wR(F^2) = 0.157$
 $S = 1.12$
2849 reflections
247 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0527P)^2 + 0.0746P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.16 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.17 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

N1—C12	1.283 (3)	N1—C14	1.403 (4)
C12—N1—C14	126.7 (2)		
C14—N1—C12—C13	−6.1 (5)	C6—O1—C5—C13	1.7 (4)
N1—C12—C11—C10	1.4 (4)	C12—N1—C14—C15	−82.4 (4)
N1—C12—C13—C1	−5.8 (5)	C5—O1—C6—C11	−0.8 (4)

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

D—H...A	D—H	H...A	D...A	D—H...A
C1—H1...Cg1	0.98 (3)	2.76 (3)	3.630 (5)	147 (2)

Cg1 is the centroid of the C14–C19 ring.

All H atoms were located in difference Fourier maps and refined isotropically. The C—H bond distances are in the range 0.89 (3)–1.08 (2) \AA .

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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