organic papers

Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(3-Fluorophenyl)-9*H*-xanthen-9-ylideneamine

Deepak Chopra,[a]* K. Nagarajan[b] and T. N. Guru Row[a]

[a]Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560 012, Karnataka, India, and [b]HIKAL India Limited, Banerghatta Road, Bangalore 560 078, Karnataka, India

Correspondence e-mail: deepak@sscu.iisc.ernet.in

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.082
wR factor = 0.157
Data-to-parameter ratio = 11.5

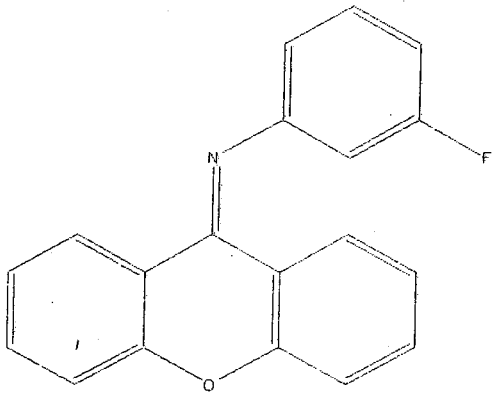
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e

In the title compound, $C_{19}H_{12}FNO$, the dihedral angle between the mean planes of the 9*H*-xanthene moiety and the 3-fluorophenyl group is 82.5 (1)°. An intramolecular C—H···π interaction stabilizes the molecular conformation.

Received 8 November 2004
Accepted 15 November 2004
Online 20 November 2004

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 C—H···π play an important role in various systems of biological and chemical interest (Nishio, 2004). Intramolecular C—H···π 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.



(I)

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 C12—N1—C14 of 126.7 (2)° is greater than the ideal bond angle value of 120° to avoid steric repulsion between atoms H15 and H1. Rotation of the 3-fluorophenyl group takes place and this is favoured because it leads to the formation of an intramolecular C—H···π interaction (Table 2) involving H1, which stabilizes the molecular conformation (Fig. 1).

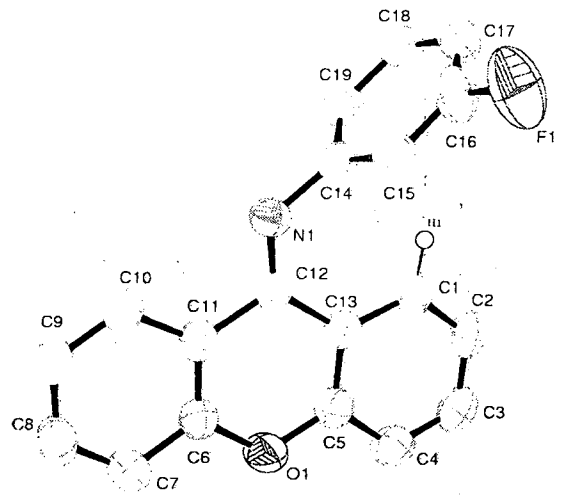


Figure 1
The molecular structure of (I), showing 40% probability ellipsoids. H atoms have been omitted for clarity, except for H1. The dashed line indicates the intramolecular C—H···π interaction.

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) Å
b = 5.0634 (9) Å
c = 19.912 (3) Å
β = 102.794 (4)°
V = 1393.6 (4) Å^3
Z = 4
D_x = 1.379 Mg m^{-3}
MoKa radiation
Cell parameters from 757 reflections
θ = 1.3–24.4°
μ = 0.10 mm^{-1}
T = 293 (2) K
Prism, orange–yellow
0.60 × 0.60 × 0.56 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_{int} = 0.069
θ_{max} = 26.4°
$h = -17 \rightarrow 17$
$k = -6 \rightarrow 6$
$l = -24 \rightarrow 24$

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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

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 (Å, °).

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) Å.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (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).

We thank the Department of Science and Technology, India, for data collection on the CCD facility set up under the IRFA–DST program. D. Chopra thanks CSIR, India, for a Junior Research Fellowship.

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.* pp. 3745–3751.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Hunter, C. A., Lawson, K. R., Perkins, J. & Urch, C. J. (2001). *J. Chem. Soc. Perkin Trans.* 2, pp. 651–669.
Jennings, W. B., Farell, B. M. & Malone, J. F. (2001). *Acc. Chem. Res.* **34**, 885–894.
Nagarajan, K., Kulkarni, C. L. & Venkateswarlu, A. (1974). *Indian J. Chem.* **12**, 247–251.
Nishio, M. (2004). *CrystEngComm*, **6**, 130–158.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL*97. 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.