

Acta Crystallographica Section E  
Structure Reports  
Online  
ISSN 1600-5368

# N-[(9E)-2-Chloro-9-thia-9H-xanthen-9-ylidene]-N-(4-fluorophenyl)amine

Deepak Chopra,<sup>a\*</sup> K. Nagarajan<sup>b</sup>  
and T. N. Guru Row<sup>a</sup>

<sup>a</sup>Solid State and Structural Chemistry Unit,  
Indian Institute of Science, Bangalore 560 012,  
Karnataka, India, and <sup>b</sup>HIKAL India Limited,  
Bannerghatta 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  $\sigma(\text{C}-\text{C}) = 0.007 \text{ \AA}$   
R factor = 0.092  
wR factor = 0.244  
Data-to-parameter ratio = 16.2

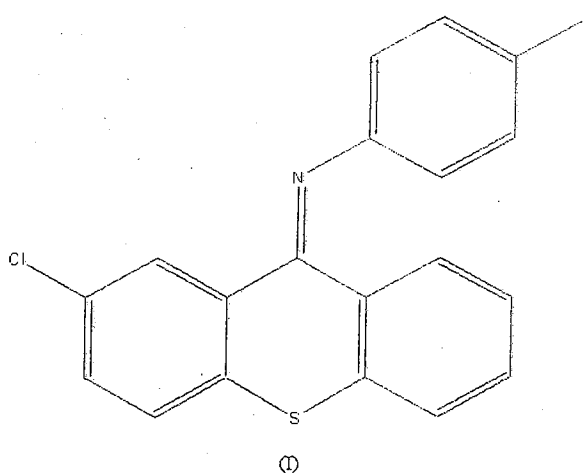
For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>

In the title compound,  $\text{C}_{19}\text{H}_{11}\text{ClFNS}$ , the central 4*H*-thiapyran ring of the 9*H*-thioxanthene moiety shows a roof-shaped structure, with a dihedral angle of  $34.3(2)^\circ$ . The molecules pack in the crystal structure *via* aromatic  $\pi-\pi$  interactions.

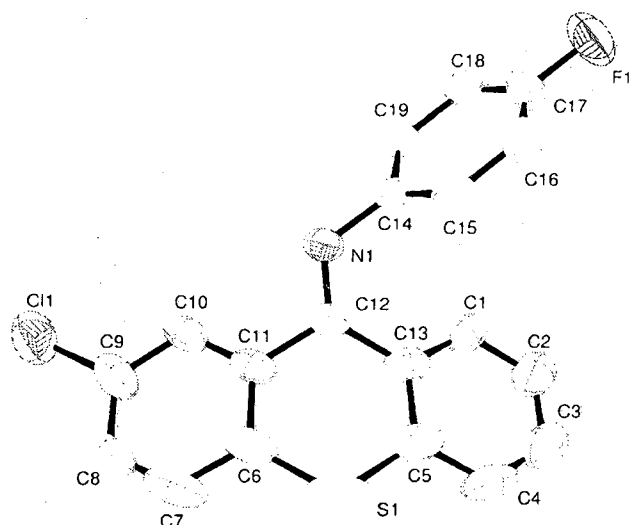
Received 8 November 2004  
Accepted 16 November 2004  
Online 27 November 2004

### 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* the manipulation of hydrogen bonding has attracted much interest in the recent literature (Aakeröy, 1997; Desiraju, 2000). Aromatic interactions involving  $\pi-\pi$  stacking are an important feature in molecules which contain aromatic groups. 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 is hence thought to be suitable for the study of weak intermolecular interactions.



A molecular view of (I) with the atom-labelling scheme is shown in Fig. 1. The 9*H*-thioxanthene unit is significantly distorted from planarity, as seen from the torsion angles (Table 1). The central 4*H*-thiapyran ring shows a roof-shaped structure, the dihedral angle between  $\text{S1/C6/C11/C12}$  and  $\text{S1/C5/C13/C12}$  being  $34.3(2)^\circ$ . The 9*H*-thioxanthene unit bends away from the 4-fluorophenyl group, precluding the formation of a possible intramolecular  $\text{C}-\text{H}\cdots\pi$  interaction. The dihedral angle between the rings  $\text{C1}-\text{C5/C13}$  and  $\text{C14}-\text{C19}$  is  $62.1(1)^\circ$ . This feature also decreases the steric repulsion between atoms H15 and H1 (bonded to C15 and C1, respec-



**Figure 1**  
The molecular structure of (I), showing 40% probability ellipsoids. H atoms have been omitted for clarity.

tively), which is indicated by the bond angle C12–N1–C14 [122.6 (4)°] being only slightly distorted from the ideal value of 120°.

There are no weak intermolecular interactions involving the halogen atoms (Cl1 and F1). The packing features  $\pi$ – $\pi$  stacks along the *c* axis involving the aromatic ring carrying the Cl atom, the separation between the stacks being 3.779 (3) Å (Fig. 2).

## Experimental

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

### Crystal data

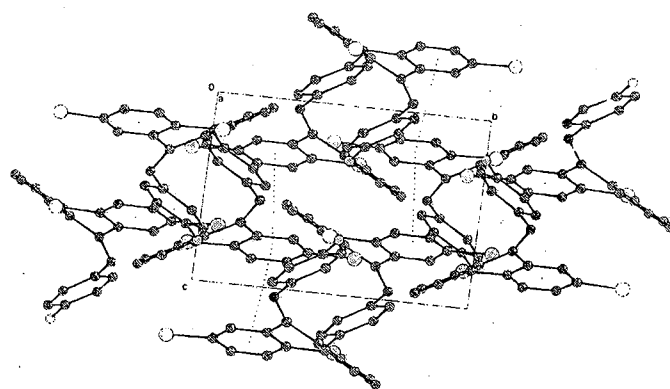
$C_{19}H_{11}ClFNS$	$D_x = 1.461 \text{ Mg m}^{-3}$
$M_r = 339.81$	Mo $K\alpha$ radiation.
Monoclinic, $P2_1/c$	Cell parameters from 964 reflections
$a = 20.052 (4) \text{ \AA}$	$\theta = 1.7\text{--}25.6^\circ$
$b = 10.3835 (19) \text{ \AA}$	$\mu = 0.39 \text{ mm}^{-1}$
$c = 7.5229 (14) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 99.375 (3)^\circ$	Block, yellow
$V = 1545.4 (5) \text{ \AA}^3$	$0.46 \times 0.24 \times 0.18 \text{ mm}$
$Z = 4$	

### Data collection

Bruker SMART CCD area-detector diffractometer	3378 independent reflections
$\varphi$ and $\omega$ scans	2107 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{int} = 0.031$
$T_{min} = 0.841$ , $T_{max} = 0.933$	$\theta_{max} = 28.0^\circ$
12 306 measured reflections	$h = -26 \rightarrow 25$
	$k = -12 \rightarrow 12$
	$l = -9 \rightarrow 9$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.1619P)^2 + 1.1895P]$
$R[F^2 > 2\sigma(F^2)] = 0.092$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.244$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.03$	$\Delta\rho_{max} = 0.94 \text{ e \AA}^{-3}$
3378 reflections	$\Delta\rho_{min} = -0.37 \text{ e \AA}^{-3}$
208 parameters	
H-atom parameters constrained	



**Figure 2**  
Packing diagram of (I), indicating the aromatic  $\pi$ – $\pi$  interactions by dashed lines. H atoms have been omitted for clarity.

**Table 1**

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

N1–C12	1.271 (5)	N1–C14	1.408 (5)
C12–N1–C14	122.6 (4)		
C12–N1–C14–C15	–62.1 (5)	C5–S1–C6–C11	–28.0 (4)
C14–N1–C12–C13	7.7 (6)	C6–S1–C5–C13	28.5 (4)

All H atoms were constrained to ride on their parent atom, with  $C\text{--}H = 0.93\text{--}0.97 \text{ \AA}$ , and  $U_{iso}(H) = 1.2U_{eq}(C)$ . The highest peak of the difference density is 1.06 Å from atom S1.

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).

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 the CSIR, India, for a Junior Research Fellowship.

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