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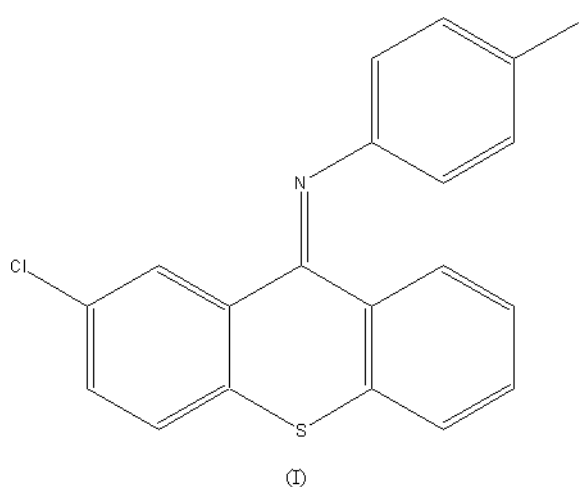
Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.007$ Å
 R factor = 0.092
 wR factor = 0.244
Data-to-parameter ratio = 16.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.***N*-[(9*E*)-2-Chloro-9-thia-9*H*-xanthen-9-ylidene]-*N*-(4-fluorophenyl)amine**

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 π - π 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 interest in the recent literature (Aakeröy, 1997; Desiraju, 2000). Aromatic interactions involving π - π 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 $\text{S1}/\text{C6}/\text{C11}/\text{C12}$ and $\text{S1}/\text{C5}/\text{C13}/\text{C12}$ 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 $\text{C1}-\text{C5}/\text{C13}$ 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-

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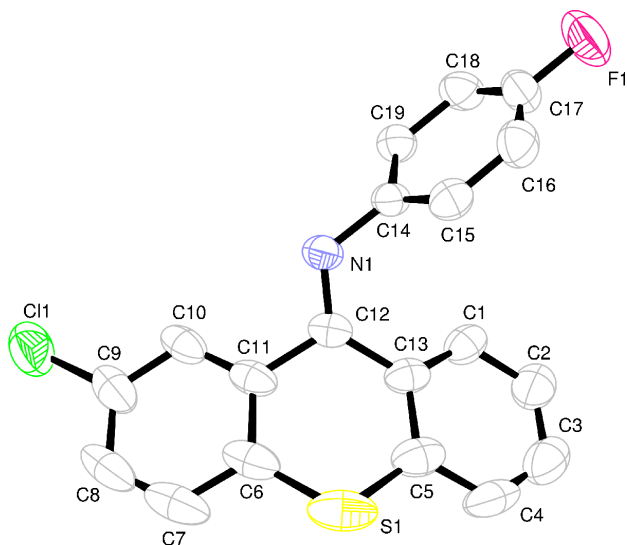


Figure 1
The molecular structure of (I), showing 40% probability ellipsoids. H atoms have been omitted for clarity.

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 π – π 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
$a = 20.052 (4) \text{ \AA}$	$\theta = 1.7\text{--}25.6^\circ$
$b = 10.3835 (19) \text{ \AA}$	$\theta_{\text{max}} = 28.0^\circ$
$c = 7.5229 (14) \text{ \AA}$	$\mu = 0.39 \text{ mm}^{-1}$
$\beta = 99.375 (3)^\circ$	$T = 293 (2) \text{ K}$
$V = 1545.4 (5) \text{ \AA}^3$	Block, yellow
$Z = 4$	$0.46 \times 0.24 \times 0.18 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer	3378 independent reflections
φ and ω scans	2107 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.031$
$T_{\text{min}} = 0.841$, $T_{\text{max}} = 0.933$	$\theta_{\text{max}} = 28.0^\circ$
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 $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.244$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.94 \text{ e \AA}^{-3}$
3378 reflections	$\Delta\rho_{\text{min}} = -0.37 \text{ e \AA}^{-3}$
208 parameters	
H-atom parameters constrained	

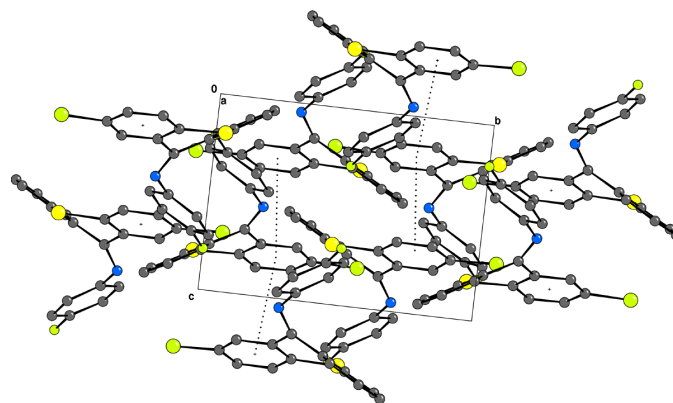


Figure 2
Packing diagram of (I), indicating the aromatic π – π interactions by dashed lines. H atoms have been omitted for clarity.

Table 1

Selected geometric parameters (Å, °).

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–H = 0.93–0.97 Å, and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. 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).

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