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Key indicators

Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.056
 wR factor = 0.169
Data-to-parameter ratio = 13.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

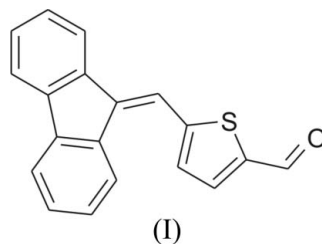
5-(Fluoren-9-ylidenemethyl)thiophene-2-carbaldehyde

The title compound, $\text{C}_{19}\text{H}_{12}\text{OS}$, can be synthesized in good yield (60%) utilizing Vilsmeier–Haack formylation of 2-(9H-fluoren-9-ylidenemethyl)thiophene. The thiophene ring contains one short C–S bond [1.618 (2) Å].

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Comment

The electronic properties of linear π -conjugated systems have acquired a growing importance in many areas of modern chemistry and physics of condensed matter. At the molecular level, linear π -conjugated systems represent the simplest models of molecular wires which, together with their complementary functions such as molecular switches or logic gates, have contributed to the emergence of concepts of molecular electronics and logic (Mullen & Wegner, 1998). Our synthetic research efforts have focused on a set of multi-ring monomer systems based on the thiophene and fluorene ring systems.



In the title compound, (I) (Fig. 1), the S1–C15 bond length of 1.708 (2) Å is in good agreement with similar thiophene compounds in the Cambridge Structural Database (CSD, Version 5.27; Allen, 2002); for example, 5-trimethylsilyl-2,2'-bithienyl-5'-carbaldehyde (Lukevics *et al.*, 2001; CSD refcode CAFNIH). The S1–C18 bond length [1.618 (2) Å], however, is much shorter, possibly as a consequence of the negative inductive effect of the neighbouring formyl group. In the crystal structure, several intermolecular C–H \cdots O contacts are made to O1 (Table 1 and Fig. 2).

Experimental

POCl_3 (5.4 ml, 0.057 mol) was added dropwise to an ice-cold solution containing dry DMF (4.5 ml, 0.057 mol) in dry 1,2-dichloroethane (40 ml). After completion of the addition, the mixture was left to warm to room temperature and stirred for a further 30 min. 2-(9H-Fluoren-9-ylidenemethyl)thiophene (10 g, 0.038 mol, dissolved in 15 ml dry 1,2-dichloroethane) was then added dropwise at room temperature, and the mixture was refluxed for 4 h. After cooling to room temperature, a red precipitate was filtered off, washed with diethyl ether and displaced into 400 ml of 10% aqueous Na_2CO_3 . The

resulting brown–yellow precipitate was filtered off and transferred into a beaker containing 500 ml of boiling diethyl ether. This mixture was refluxed for 10 min, then the organic layer was decanted and evaporated under reduced pressure to obtain a yellow solid (6.6 g, 60%). The crude product was purified by column chromatography using silica gel (Merck 60) with toluene as eluent $R_F = 0.36$ (toluene). Compound (I) was recrystallized from MeOH to obtain yellow plates (m.p. 386–387 K).

Crystal data

$C_{19}H_{12}OS$	$Z = 4$
$M_r = 288.35$	$D_x = 1.489 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 8.146 (2) \text{ \AA}$	$\mu = 0.25 \text{ mm}^{-1}$
$b = 24.075 (5) \text{ \AA}$	$T = 295 \text{ K}$
$c = 6.607 (1) \text{ \AA}$	Plate, yellow
$\beta = 96.93 (3)^\circ$	$0.50 \times 0.22 \times 0.05 \text{ mm}$
$V = 1286.3 (5) \text{ \AA}^3$	

Data collection

Oxford Diffraction Gemini R CCD diffractometer	2724 measured reflections
ω and φ scans	2624 independent reflections
Absorption correction: analytical (Clark & Reid, 1995)	1971 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.987$, $T_{\max} = 1.000$	$R_{\text{int}} = 0.001$
	$\theta_{\max} = 26.4^\circ$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.056$	$w = 1/[\sigma^2(F_o^2) + (0.1192P)^2]$
$wR(F^2) = 0.169$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{\max} < 0.001$
2624 reflections	$\Delta\rho_{\max} = 0.53 \text{ e \AA}^{-3}$
190 parameters	$\Delta\rho_{\min} = -0.23 \text{ e \AA}^{-3}$

Table 1

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C11-H11A\cdots O1^i$	0.93	2.65	3.533 (3)	158
$C14-H14A\cdots O1^i$	0.93	2.67	3.510 (3)	152
$C16-H16A\cdots O1^{ii}$	0.93	2.84	3.351 (3)	115
$C17-H17A\cdots O1^{ii}$	0.93	2.73	3.312 (2)	121

Symmetry codes: (i) $-x + 1, -y + 1, -z + 1$; (ii) $x, y, z - 1$.

H atoms were placed in calculated positions and refined using a riding model, with $C-H = 0.93 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

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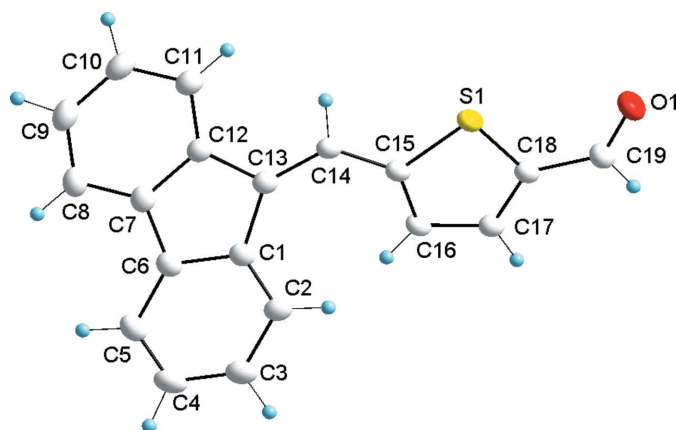


Figure 1

The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 20% probability level for non-H atoms.

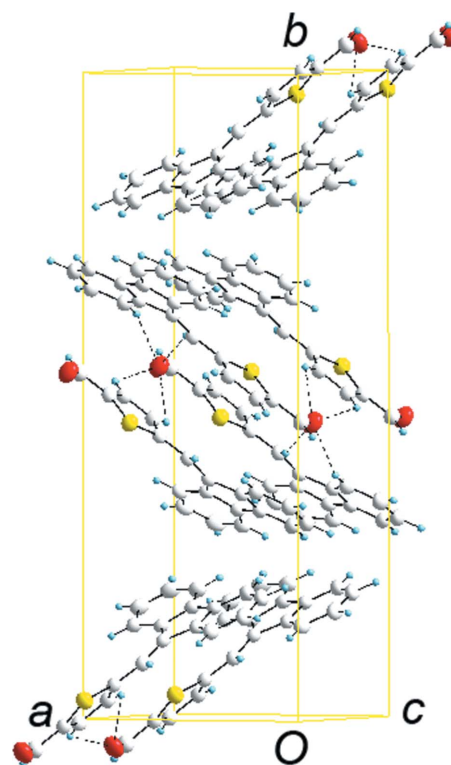


Figure 2

View of the unit cell contents of (I), with $C-H\cdots O$ interactions indicated by dashed lines.

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