

A flip-disorder in the structure of 3-[2-(anthracen-9-yl)ethenyl]thiophene

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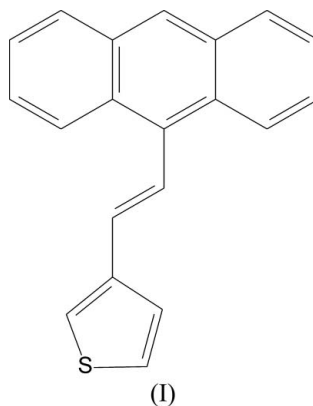
Key indicators

Single-crystal X-ray study
T = 100 K
Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$
Disorder in main residue
R factor = 0.060
wR factor = 0.110
Data-to-parameter ratio = 13.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the crystal structure of the title compound, $\text{C}_{20}\text{H}_{14}\text{S}$, the thiophene rings are disordered; such a flip-type disorder is typical for simple, monosubstituted thiophene derivatives. Two planar fragments, the thiophene and the anthracene units, are almost perpendicular in order to relieve the $\text{H}\cdots\text{H}$ steric strains. The crystal packing is determined by van der Waals interactions, π - π stacking between the anthracene fragments, and some weak $\text{C}-\text{H}\cdots\text{S}$ and $\text{C}-\text{H}\cdots\pi$ short directional contacts.

Comment

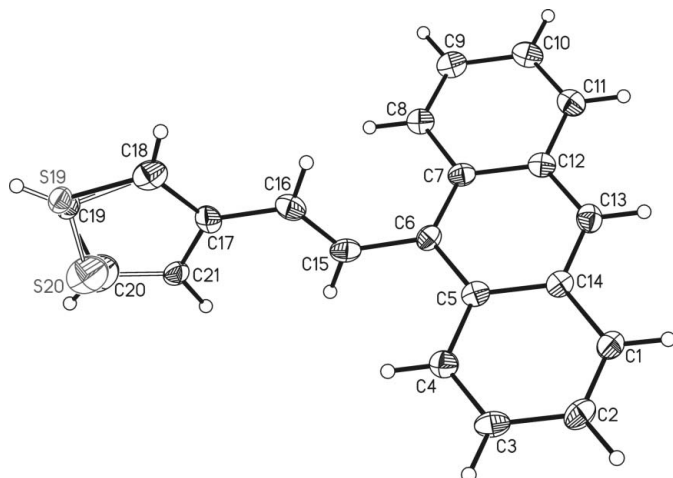
Since their discovery, conjugated polymers and oligomers (Shirakawa *et al.*, 1977) have been investigated extensively for use in, for example, solar cells or light-emitting diodes. Oligo- and polythiophenes have good chemical stability in both the oxidized and reduced states; in particular, 3-styryl-substituted thiophenes have been studied intensively due to their unique electronic and optical properties (*e.g.* Collis *et al.*, 2003; Grant *et al.*, 2005; Wagner & Officer, 2005).



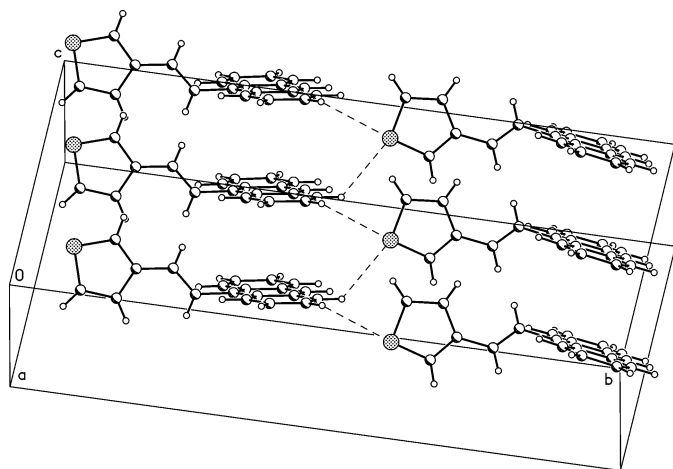
In the crystal structure of (I), a flip-disorder of the thiophene ring is observed (Fig. 1). There are two positions of the thiophene ring, rotated by *ca* 180°. These two orientations are not equivalent; the site-occupation factors refined to 0.689 (3) and 0.311 (3). A disorder of this kind is often observed in the structures of simple thiophene derivatives with one substituent, for example in a family of thiophene-3-carboxamides (Howell *et al.*, 2005) or in 3-thienylacrylonitriles (Sonar *et al.*, 2004, 2005*a,b*).

Both the thiophene and the anthracene units are almost planar; the maximum deviations from the least-squares planes are 0.011 (9) Å for atom C17 from the thiophene ring, and 0.034 (2) Å for atom C8 from the whole anthracene fragment. In the latter, the dihedral angle between the terminal rings is as small as 1.4 (1)°. The dihedral angle between the anthra-

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**Figure 1**

The molecular structure of (I) (Siemens, 1989). Displacement ellipsoids are drawn at the 50% probability level. H atoms are depicted as small spheres of arbitrary radii. The minor occupancy component of the thiophene ring is depicted with hollow bonds.

**Figure 2**

The stacking of molecules, showing some of the C—H...S contacts (dashed lines) connecting the stacks.

cene and thiophene planes is $72.6(3)^\circ$. The whole vinylthiophene group is twisted with respect to the naphthalene fragment, as shown by a comparison of torsion angles, for instance $C4A-C5-C11-C12 = 114.7(3)^\circ$ and $C11-C12-C15-C16 = -7.5(4)^\circ$. This conformation is probably a result of the steric stress between vinylic atoms H11 and H12, and naphthalene atoms H4 and H6, respectively. As a result of the twist, these H...H distances are comparable with the H...H distances between the vinylic and the thiophene ring H atoms (the shortest distances are $H4 \cdots H11 = 2.49 \text{ \AA}$ and $H16 \cdots H11 = 2.33 \text{ \AA}$).

In the crystal structure, there are columns of molecules aligned perpendicular to the anthracene rings (approximately along the [101] direction). There is a partial stack between neighboring rings (Fig. 2). The distance between the centroids of these rings is 3.59 \AA ; taking into account the offset, the distance between the planes is around 3.45 \AA , which might

suggest reasonable stacking interactions between the π -electron systems. There are also some weak specific interactions that also can play a role in the crystal structure, namely C—H...S and C—H... π directional contacts (Table 1).

Experimental

The title compound was synthesized according to a literature procedure (Collis *et al.*, 2001) and the details will be published elsewhere.

Crystal data

$C_{20}H_{14}S$	$Z = 4$
$M_r = 286.37$	$D_x = 1.329 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 5.4991(9) \text{ \AA}$	$\mu = 0.22 \text{ mm}^{-1}$
$b = 23.968(4) \text{ \AA}$	$T = 100(1) \text{ K}$
$c = 10.9768(18) \text{ \AA}$	Block, colorless
$\beta = 98.478(14)^\circ$	$0.3 \times 0.07 \times 0.05 \text{ mm}$
$V = 1431.0(4) \text{ \AA}^3$	

Data collection

Kuma KM-4-CCD four-circle diffractometer	2710 independent reflections
ω scans	1419 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{\text{int}} = 0.074$
6934 measured reflections	$\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.060$	$w = 1/[\sigma^2(F_o^2) + (0.04P)^2]$
$wR(F^2) = 0.110$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.99$	$(\Delta/\sigma)_{\text{max}} = 0.001$
2710 reflections	$\Delta\rho_{\text{max}} = 0.31 \text{ e \AA}^{-3}$
197 parameters	$\Delta\rho_{\text{min}} = -0.32 \text{ e \AA}^{-3}$

Table 1

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

Cg1 denotes the centroid of the thiophene ring, and Cg4 the centroid of the terminal (C8) ring of the anthracene fragment.

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$C2-H2 \cdots S13^i$	0.95	3.02	3.742 (6)	134
$C8-H8 \cdots S13^{ii}$	0.95	2.94	3.841 (5)	159
$C2-H2 \cdots S17^{iii}$	0.95	3.11	3.963 (16)	151
$C14-H14 \cdots Cg4^{ii}$	0.95	2.86	3.632	140
$C8-H8 \cdots Cg1^{iv}$	0.95	2.88	3.589	132

Symmetry codes: (i) $-x + 1, y + \frac{1}{2}, -z + \frac{3}{2}$; (ii) $x - 1, -y + \frac{1}{2}, z - \frac{1}{2}$; (iii) $x + 1, -y + \frac{1}{2}, z + \frac{1}{2}$; (iv) $x, -y + \frac{1}{2}, z + \frac{1}{2}$.

The flip-type disorder means that in their alternative positions, the different types of atoms (in this case sulfur and carbon) occupy positions that are close to each other, which influences their U^{ij} values. The alternative positions of S and C atoms were constrained to have the same U^{ij} components. H atoms were positioned geometrically (C—H = 0.95 \AA) and refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier atom})$.

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: *Stereochemical Workstation Operation Manual* (Siemens, 1989); software used to prepare material for publication: *SHELXL97*.

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