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3,3′-Didecyl-5,5′-bis(4-phenylquinolin-2-yl)-2,2′-bithienyl

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The structure of the title compound, $C_{58}H_{64}N_2S_2$, is primarily dictated by intermolecular van der Waals interactions of the didecyl chains attached to the bithiophene backbone. These interactions result in torsional strain on the aromatic plane, which disrupts conjugation.

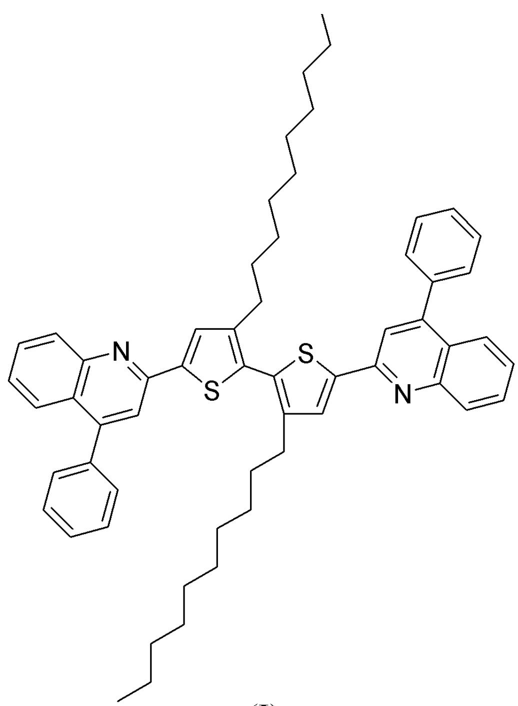
Key indicators

Single-crystal X-ray study
T = 130 K
Mean σ(C–C) = 0.007 Å
Disorder in main residue
R factor = 0.067
wR factor = 0.151
Data-to-parameter ratio = 14.2

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

Comment

The title compound, (I), is an important model for correlating structure–property relationships of chromophores incorporated into polymeric backbones with the single-crystal counterpart (Tonzola *et al.*, 2003). The addition of increasingly longer alkyl chains results in improved solubility of the monomeric units and resulting polymer in organic solvents, as well as modifying the nature of intermolecular interactions. Previous structures of related oligophenylquinolines (Shetty *et al.*, 1999) show strong π stacking; however, this crystal structure clearly illustrates that once these chains reach a critical length, the van der Waals forces between these chains not only disrupt the π stacking, but also introduce torsional strain. In the structure presented here, the linked thiophenes are twisted by 44.9 (3)°. This distortion of the aromatic plane certainly impacts the ground-state electronic band structure of the molecule in the crystalline state.



(I)

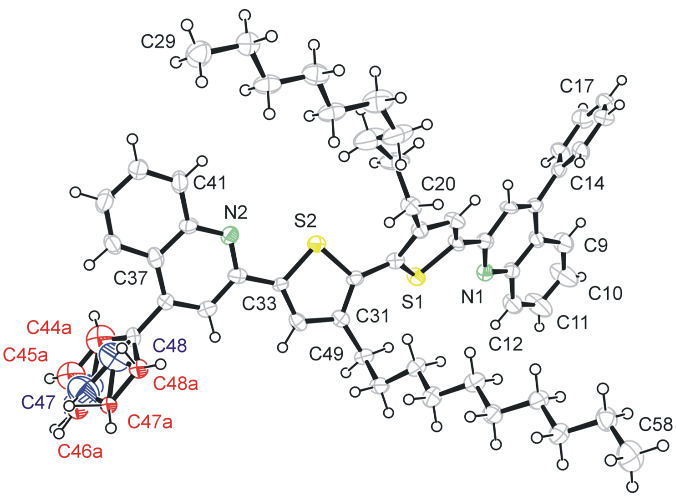


Figure 1
View of the molecule, showing the atom-labeling scheme for atoms discussed in the text, and illustrating the twist of the thiophene rings. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size. The disordered phenyl ring is illustrated in blue and red.

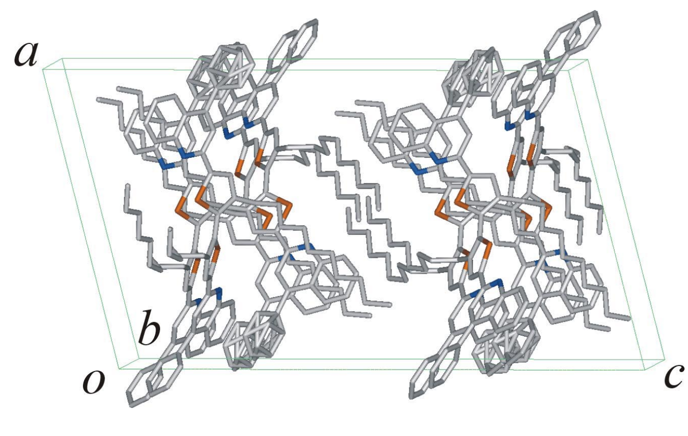


Figure 2
Molecular packing diagram of (I), illustrating van der Waals interactions between alkyl chains. H atoms have been omitted for clarity.

Experimental

The title compound was prepared according to the procedure reported by Tonzola *et al.* (2004). Crystals were grown at 273 (2) K [m.p. 295 (2) K].

Crystal data

$C_{58}H_{64}N_2S_2$	$D_x = 1.185$ Mg m^{-3}
$M_r = 853.23$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 102 reflections
$a = 17.4640$ (9) Å	$\theta = 2.4$–$24.4°$
$b = 9.4710$ (5) Å	$\mu = 0.15$ mm^{-1}
$c = 29.8230$ (19) Å	$T = 130$ (2) K
$\beta = 104.153$ (2)°	Needle, yellow
$V = 4783.0$ (5) Å^3	0.48 × 0.12 × 0.02 mm
$Z = 4$	

Data collection

Nonius KappaCCD diffractometer	8601 independent reflections
φ scans	2806 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*HKL*2000; Otwinowski & Minor, 1997)	$R_{int} = 0.153$
$T_{min} = 0.932$, $T_{max} = 0.996$	$\theta_{max} = 25.7°$
71 973 measured reflections	$h = -21 \rightarrow 21$
	$k = -11 \rightarrow 10$
	$l = -36 \rightarrow 36$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.067$	$w = 1/[\sigma^2(F_o^2)]$
$wR(F^2) = 0.151$	$(\Delta/\sigma)_{max} = 0.010$
$S = 0.86$	$\Delta\rho_{max} = 0.50$ e Å^{-3}
8601 reflections	$\Delta\rho_{min} = -0.35$ e Å^{-3}
607 parameters	

To alleviate problems associated with sample absorption and twinning, a sample was chosen that exhibited well resolved diffraction patterns. Unfortunately, the small sample size resulted in a large R_{int} value, despite using the longest exposure time possible. Indicators of the low melting point of the sample are the disordered phenyl ring (C44–C48) and the excessive thermal motion within one quinoline ring (C9–C12), which are manifested in unusually large displacement parameters. All H atoms were initially located in a difference Fourier map and were refined with a riding model. model. H atoms were placed in geometrically idealised positions and constrained to ride on their parent atoms, with C—H distances in the range 0.95–1.00 Å. U_{iso}(H) values were set at $1.2U_{eq}$ of the parent atom for CH groups and $1.5U_{eq}$ of the parent atom for methyl groups.

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL*2000 (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *maXus* (Mackay *et al.*, 1998); software used to prepare material for publication: *SHELXL*97 (Sheldrick, 1997).

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