

Badia Jerdioui,^a Ahmed Jorti,^a
Zoubida Chami,^a Abdelrhani
Elachqar,^a Mohammed
Zenkouar,^a Brahim El Bali^a and
Michael Bolte^{b*}

^aUFR de Physicochimie Moléculaire,
Département de Chimie, Faculté des Sciences
Dhar Mehraz, Université Sidi Mohamed Ben
Abdellah, 30000 Fès, Morocco, and ^bInstitut für
Organische Chemie, J.-W.-Goethe-Universität
Frankfurt, Marie-Curie-Straße 11, 60439
Frankfurt/Main, Germany

Correspondence e-mail:
bolte@chemie.uni-frankfurt.de

Key indicators

Single-crystal X-ray study
 $T = 173\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
Disorder in main residue
 R factor = 0.046
 wR factor = 0.109
Data-to-parameter ratio = 15.7

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

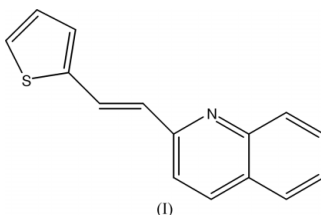
trans-1-(2-Quinolylyl)-2-(2-thienyl)ethylene

The title compound, $\text{C}_{15}\text{H}_{11}\text{NS}$, contains a thiophene ring and a quinoline moiety connected by an ethylene bridge, which shows a *trans* configuration. The thiophene ring is disordered over two sites by rotation about the exocyclic C—C bond.

Received 9 May 2003
Accepted 13 May 2003
Online 17 June 2003

Comment

Many synthetic antimalarial products, such as chloroquinine (Joule *et al.*, 1995, and references therein), possess a skeleton based on the quinolenic moiety. Most of these products are active in biological processes (Zouhiri *et al.*, 2000). Moreover, bichromophores containing two or more quinoline molecules linked by hydrocarbon chains are known to be active chelating agents for metal ions (Wong & Wong, 1996). Bichromophores containing the quinoline nucleus (Radhakrishnan *et al.*, 1995; Wang & Ho, 1997) or naphthalene (Arai & Tokumaru, 1993) exhibit the same behaviour as those containing pyridine (Favaro *et al.*, 1973) or benzene derivatives (Létard *et al.*, 1993; Lewis & Yang, 1997). Furthermore, the photophysical aspect of styrylquinoline derivatives is still attracting the attention of many researchers (Arai *et al.*, 1994).



As a result of the acidic nature of methyl H atoms in the 2-position of pyridine and quinoline, we have adapted the condensation reaction of 2-picoline with benzaldehyde, based on the conventional synthetic method reported in the literature (Wang & Ho, 1997). This process results in quinolenic olefins, by condensation of 2-methylquinoline with different kinds of aldehydes. All products obtained by this reaction have a *trans* configuration. We did check this result by our numerous other spectroscopic investigations, mainly IR, mass and NMR (^1H and ^{13}C); in particular, by a study of the chemical shifts of the ethyl protons by ^1H NMR, as well as by IR absorption bands of the deformations out of the plane of the ethylenic double bond. We found the same conformation when we studied the crystal structure of *trans*-1-(2-quinolylyl)-2-(2-thienyl)ethylene and *trans*-bis(4-quinolylyl)ethylene (Jerdioui *et al.*, 1999). We describe here the synthesis and X-ray crystal structure analysis of the title compound, (I). The crystallographic results are in agreement with the spectroscopic investigations, in particular the molecular conformation. The present study will allow us to understand more

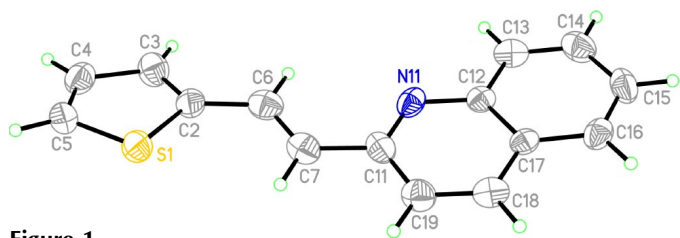


Figure 1

A perspective view of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Only the main conformation is shown.

deeply the influence of the thienyl group on the behaviour of this derivative, in both its ground and excited states.

The thiophene ring and the quinoline moiety are nearly coplanar, the dihedral angle between them being $13.4 (1)^\circ$. The ethylenic double bond is in the *trans*-configuration.

Experimental

2 g (13.9 mmol) of 2-methylquinoline and 2.6 ml of anhydrous acetic acid were mixed in a 100 ml flask equipped with a reflux condenser. After heating to 333 K, 17 mmol of thionaldehyde were added. The mixture was then heated at 393 K for 2 h, the course of the reaction being followed by thin-layer chromatography. After cooling to room temperature, the solution was neutralized with CaCO_3 . The extraction was effected with dichloromethane. Evaporation of the solvent produced a yellow solid, which was then recrystallized from a mixture of equimolar hexane/dichloromethane, to yield yellowish crystals in the form of plates.

Crystal data

$\text{C}_{15}\text{H}_{11}\text{NS}$	Mo $K\alpha$ radiation
$M_r = 237.31$	Cell parameters from 512 reflections
Orthorhombic, $P2_12_12_1$	$\theta = 1-20^\circ$
$a = 6.0100 (12) \text{ \AA}$	$\mu = 0.25 \text{ mm}^{-1}$
$b = 7.8502 (16) \text{ \AA}$	$T = 173 \text{ K}$
$c = 25.258 (5) \text{ \AA}$	Plate, yellow
$V = 1191.7 (4) \text{ \AA}^3$	$0.41 \times 0.26 \times 0.06 \text{ mm}$
$Z = 4$	
$D_x = 1.323 \text{ Mg m}^{-3}$	

Data collection

Siemens CCD three-circle diffractometer	2438 independent reflections
ω scans	1882 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.047$
$T_{\text{min}} = 0.891$, $T_{\text{max}} = 0.976$	$\theta_{\text{max}} = 27.2^\circ$
9574 measured reflections	$h = -7 \rightarrow 7$
	$k = -9 \rightarrow 9$
	$l = -30 \rightarrow 31$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0462P)^2 + 0.4035P]$
$R[F^2 > 2\sigma(F^2)] = 0.046$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.109$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.41 \text{ e \AA}^{-3}$
2438 reflections	$\Delta\rho_{\text{min}} = -0.20 \text{ e \AA}^{-3}$
155 parameters	Absolute structure: Flack (1983),
H-atom parameters constrained	962 Friedel pairs
	Flack parameter = 0.07 (15)

Table 1

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

C2—C6	1.465 (4)	C11—N11	1.335 (3)
C6—C7	1.312 (4)	N11—C12	1.375 (3)
C7—C11	1.478 (4)		
C7—C6—C2	124.3 (3)	C11—N11—C12	117.3 (2)
C6—C7—C11	124.4 (3)		
C2—C6—C7—C11	$-176.4 (3)$		

The thiophene ring is disordered. The resolution of the data did not allow the two distinct positions for the S and C atoms to be distinguished. Only one peak was found for each atom in the difference map. Thus, a C and an S atom were refined sharing the same position and the same displacement parameters, simply refining the site-occupation factor of the respective C and S atoms in order to determine the ratio of the different orientations; this turned out to be 0.820 (3):0.180 (3). All H atoms except those of the disordered atoms were located by difference Fourier synthesis and refined with fixed individual displacement parameters [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$], using a riding model with $\text{C—H} = 0.95 \text{ \AA}$.

Data collection: SMART (Siemens, 1995); cell refinement: SMART; data reduction: SAINT (Siemens, 1995); program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: XP (Sheldrick, 1991); software used to prepare material for publication: SHELXL97.

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