Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

2,2′-Bi(9,9-dihexylfluorene)

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Received 14 January 2000
Accepted 24 January 2000

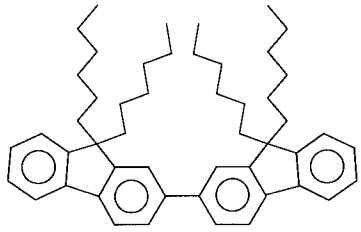
Data validation number: IUC0000024

The central part of the title molecule, $C_{50}H_{66}$, is planar, all the rings being in the same plane; the lateral chains are also planar (excluding H atoms), almost perpendicular to the ring plane and grafted on the same side of the molecule. The molecule has nearly a mirror plane, perpendicular to the central C—C bond, instead of the centre of symmetry expected. The orientation of the plane of the rings is approximately 45° from the unit-cell *b* axis, so that neighbouring molecules are essentially perpendicular.

Comment

Conducting polymers based on fluorene repeat units are well known to exhibit attractive luminescent properties allowing for instance the synthesis of blue light electroluminescent devices (Kraft *et al.*, 1998; Stéphan & Vial, 1999). The corresponding polyfluorenes exhibit good thermal and chemical stability, high solubility and good solid-state fluorescence quantum yields. Nevertheless, in the solid state, the formation of film aggregates leads to altered spectrocopic properties (Klarner *et al.*, 1998; Stéphan & Vial, 1999). As a result, although the luminescence from isolated chain, such as in dilute solution, is blue, in the solid state, a broad and unstructured red-shifted band emission is observed due to the excimer emission. One way to avoid this excimer emission, which is an important problem, may be to investigate the use of oligomeric polyfluorene segments for which a well defined crystallization may occur. We report here the structure of the shortest oligomer which can be derived from fluorene, *i.e.* the dimer, (I).

The main result concerning the molecular conformation is that the hexyl chains grafted at the 9 positions are on the same side of the rings, which is uncommon if compared to conducting polymers such as polypyrroles or polythiophenes in which the repeat units are head to foot (Handbook of Conducting Polymers, 1998). We note that one of the chains has a high thermal motion (U_{eq} for C119 = 0.19 Å^2), the three others being normal. This can be explained by the environment, C119 having only one neighbour at less than 4.0 Å, while the others have four or five such neighbours. We tried to refine the structure from low-temperature (193 K) data but, although the displacement parameters are of course globally smaller, *U*(C119) remains much higher than the others and the refinement is not better than the room-temperature one.



(I)

The stacking of the molecules is such that ring planes are perpendicular in neighbouring molecules; there is no π-stacking between the planar conjugated fluorene segments. This result is in agreement with the photoluminescence measurements on dimer crystals, for which the shift leading to yellow instead of blue light is not observed.

Experimental

The title compound was obtained via Ni-catalyzed coupling of 2-bromo-9,9-dihexylfluorene monomeric units. The hexyl chains are grafted in order to allow a high solubility in common organic solvents.

Crystal data

$C_{50}H_{66}$	D_x = 1.043 Mg m^{-3}
M_r = 667.08	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 20 reflections
a = 15.975 (2) Å	θ = 10–12°
b = 15.773 (2) Å	μ = 0.058 mm^{-1}
c = 17.142 (2) Å	T = 293 K
β = 100.51 (1)°	Parallelepiped, translucent white
V = 4246.9 (7) Å^3	0.3 × 0.3 × 0.2 mm
Z = 4	

Data collection

Enraf–Nonius CAD-4 diffractometer	θ_{max} = 24.98°
ω scans	$h = -18 \rightarrow 18$
7842 measured reflections	$k = -5 \rightarrow 18$
7460 independent reflections	$l = -4 \rightarrow 20$
4526 reflections with $I_{net} > 0.54\sigma(I_{net})$	2 standard reflections every 100 reflections intensity decay: 1%
R_{int} = 0.017	

Refinement

Refinement on F	$w = 1/(0.1 + 1.4\sigma^2)$
R = 0.100	$(\Delta/\sigma)_{max}$ = 0.003
wR = 0.039	$\Delta\rho_{max}$ = 0.35 e Å^{-3}
S = 1.511	$\Delta\rho_{min}$ = −0.41 e Å^{-3}
4526 reflections	Extinction correction: Zachariasen (1967)
452 parameters	Extinction coefficient: 0.72 (3)
H-atom parameters not refined	

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *Xtal*3.2 *SORTRF ADDREF* (Hall *et al.*, 1992); program(s) used to solve structure: *Xtal*3.2 *GENTAN*; program(s) used to refine structure: *Xtal*3.2 *CRYLSQ*; molecular graphics: *Xtal*3.2 *ORTEP*; software used to prepare material for publication: *Xtal*3.2 *BONDLA CIFIO*.

The authors thank M. T. Averbuch and A. Durif for the data collection.

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