

Acta Crystallographica Section C

**Crystal Structure  
Communications**

ISSN 0108-2701

---

## **2,2'-Bi(9,9-di-*n*-propylfluorene)**

**Bernadette Suchod *et al.***

---

### **Electronic paper**

This paper is published electronically. It meets the data-validation criteria for publication in Acta Crystallographica Section C. The submission has been checked by a Section C Co-editor though the text in the 'Comments' section is the responsibility of the authors.

© 2000 International Union of Crystallography • Printed in Great Britain – all rights reserved

2,2'-Bi(9,9-di-*n*-propylfluorene)

Bernadette Suchod,\* Olivier Stéphan and Yann Kervella

Laboratoire de Spectrométrie Physique, Unité Mixte de Recherche (C5588),  
Université Joseph Fourier – Grenoble 1 – CNRS, BP 87 – 38402 Saint Martin  
d'Hères CEDEX, France

Correspondence e-mail: bernadette.suchod@ujf-grenoble.fr

Received 4 May 2000

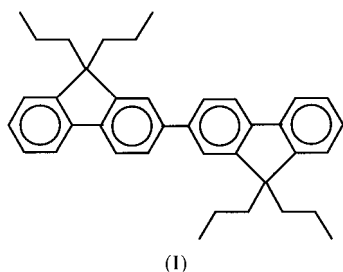
Accepted 23 May 2000

Data validation number: IUC0000148

The central part of the title molecule, C<sub>38</sub>H<sub>42</sub>, is planar, all the rings being in the same plane; the lateral chains (excluding H atoms) are also planar, with each pair almost perpendicular to the ring plane. In the dimer, the two alkyl-substituted fluorene moieties are head-to-foot. The molecule is on a special position of the space group, a centre of symmetry.

## Comment

Oligomers based on fluorene are interesting materials for optoelectronic applications, such as optical limiting, two-photon technology or light-emitting devices (Rheinhardt, 1999). Nevertheless, although polyfluorene-based materials exhibit high luminescent yields, and thermal and oxidative stability, in the solid state, their optical properties are strongly influenced by the degree of organization of the material. As a rule, thin layers of regular poly(alkylfluorene) develop an additional broad band in the yellow part of their luminescent



or electroluminescent spectra attributed to the formation of excimers and/or aggregates (Kläner *et al.*, 1999). One way to suppress these troublesome phenomena is to use a well defined crystalline structure of another dimer of fluorene for which conformational motion is avoided. Recently, we have reported the crystal structure of 2,2'-bi(9,9-dihexylfluorene) (Suchod & Stéphan, 2000). As part of our programme, we present here the structure of another dimer of fluorene, (I), for which the alkyl chains grafted at the 9-position of the fluorene moiety have been shortened from 6 to 3 CH<sub>2</sub> units.

Surprisingly, with *n*-propyl chains the molecular conformation is totally different from that with hexyl ones. Whereas

with the latter, alkyl chains were on the same side of the fluorene ring, with propyl chains the fluorene moieties are head-to-foot. The stacking of the molecules is also very different; the planes of conjugated dimers are parallel but shifted, while in the preceding structure there was a perpendicular arrangement of neighbouring molecules. Nevertheless, in both cases, photoluminescence measurements on crystals clearly indicate that the shift leading to yellow instead of blue light emission is avoided.

## Experimental

The title compound was obtained as described previously (Suchod & Stéphan, 2000) *via* Ni-catalyzed coupling the corresponding of 2-bromofluorene monomeric units.

## Crystal data

C<sub>38</sub>H<sub>42</sub>  
*M<sub>r</sub>* = 498.75  
 Monoclinic, *P*<sub>2</sub><sub>1</sub>/*c*  
*a* = 8.9944 (9) Å  
*b* = 16.257 (2) Å  
*c* = 10.519 (1) Å  
 $\beta$  = 103.08 (1)°  
*V* = 1498.2 (3) Å<sup>3</sup>  
*Z* = 2  
*D<sub>x</sub>* = 1.106 Mg m<sup>-3</sup>

Mo *K*α radiation  
 Cell parameters from 20  
 reflections  
 $\theta$  = 10–12°  
 $\mu$  = 0.062 mm<sup>-1</sup>  
*T* = 293 K  
 Parallelepiped, translucent pale  
 white  
 0.3 × 0.3 × 0.2 mm

## Data collection

Nonius CAD-4 diffractometer  
 $\omega$  scans  
 4655 measured reflections  
 4355 independent reflections  
 3724 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.01  
 $\theta_{\max}$  = 29.96°

*h* = -12 → 12  
*k* = 0 → 22  
*l* = 0 → 14  
 2 standard reflections  
 every 100 reflections  
 intensity decay: 1%

## Refinement

Refinement on *F*  
*R* = 0.076  
*wR* = 0.045  
*S* = 1.183  
 3724 reflections  
 257 parameters  
 All H-atom parameters refined

*w* = 1/(0.1 + 1.4σ<sup>2</sup>)  
 $(\Delta/\sigma)_{\max}$  = 0.027  
 $\Delta\rho_{\max}$  = 0.20 e Å<sup>-3</sup>  
 $\Delta\rho_{\min}$  = -0.18 e Å<sup>-3</sup>  
 Extinction correction: Zachariasen  
 (1967)  
 Extinction coefficient: 0.85 (3)

Data collection: *CAD-4 Software* (Enraf–Nonius, 1998); cell refinement: *CAD-4 Software*; data reduction: *Xtal3.2 SORTRF ADDREF* (Hall *et al.*, 1992); program(s) used to solve structure: *Xtal3.2 GENTAN*; program(s) used to refine structure: *Xtal3.2 CRYLSQ*; molecular graphics: *Xtal3.2 ORTEP*; software used to prepare material for publication: *Xtal3.2 BONDLA CIFIO*.

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

## References

- Enraf–Nonius (1998). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.  
 Hall, S. R., Flack, H. D. & Stewart, J. M. (1992). Editors. *Xtal3.2 Reference Manual*. Universities of Western Australia, Australia, and Maryland, USA.  
 Kläner, G., Lee, J. I., Chan, E., Chen, J. P., Nelson, A., Markiewicz, D., Siemens, R., Scott, J. C. & Miller, R. D. (1999). *Chem. Mater.* **11**, 1800–1805.  
 Rheinhardt, B. A. (1999). *Photonics Sci. News*, **4**, 21–34.  
 Suchod, B. & Stéphan, O. (2000). *Acta Cryst.* **C56**, e92–93.  
 Zachariasen, W. H. (1967). *Acta Cryst.* **23**, 558–564.