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2,7-Dibromo-9,9-bis(4-hydroxyphenyl)-9*H*-fluorene

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Key indicators

Single-crystal X-ray study
T = 193 K
Mean σ(C–C) = 0.004 Å
R factor = 0.037
wR factor = 0.091
Data-to-parameter ratio = 16.0

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

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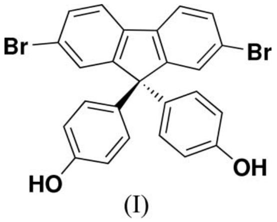
In the solid state, the title compound, $C_{25}H_{16}Br_2O_2$, shows significant deviations of the fluorene ring system from planarity. A layered hydrogen-bonded structure is formed that may serve as a model for the solid-state structure of phenol-functionalized polyfluorene.

Comment

The fluorescent conjugated polymer polyfluorene and its derivatives are currently being investigated as chemical and biochemical sensory materials. Phosphonate- (Zhou, Qian *et al.*, 2005), phenol- (Zhou, Cheng *et al.*, 2005), imidazole- (Zhou *et al.*, 2004) and sulfonate-functionalized (Huang *et al.*, 2005) polyfluorene have shown sensitivity toward Fe^{3+}, F^-, Cu^{2+}, and avidin respectively. In order to better understand the potential sensing ability of phenol-functionalized polyfluorene we have determined the solid-state structure of the previously synthesized (Lindgren *et al.*, 2005) title compound, (I).



(I)

The structure of (I) is shown in Fig. 1. Rather than being approximately flat, the fluorene unit shows an observable bend. The largest deviations from the least-squares plane for the 13 fluorene carbons are observed for C10 [0.181 (3) Å] and C3 [0.179 (2) Å]; the dihedral angle between the fluorene benzene rings is 12.95 (16)°. The most significant non-bonded intermolecular contacts would be between neighboring Br atoms [Br1···Br2$(-x, \frac{1}{2}+y, \frac{1}{2}-z)$ = 3.7162 (7) Å]; we suggest that this is the driving force for the fluorene bending.

Fig. 2 shows the crystal packing of compound (I), viewed down the *b* axis, showing the network of hydrogen bonds within and between layers. We believe that such hydrogen bonding would also be a strong driving force in ordering the corresponding polymer, and may allow selective intercalation of ionic species of suitable size. In addition, such ordering may alter the electronic and hence photoluminescent properties of the polymers made up of this repeat unit.

Experimental

The title compound was prepared according to a previously published procedure (Lindgren *et al.*, 2005). To obtain suitable single crystals, the colorless solid was crystallized from a toluene–ethyl acetate solution (10:1).

Crystal data

$C_{25}H_{16}Br_2O_2$
$M_r = 508.20$
Monoclinic, $P2_1/c$
$a = 9.1346\ (14)$ Å
$b = 12.926\ (2)$ Å
$c = 17.772\ (3)$ Å
$\beta = 102.004\ (2)^\circ$
$V = 2052.5\ (6)$ Å^3
$Z = 4$
$D_x = 1.645$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 3.97$ mm^{-1}
$T = 193\ (2)$ K
Prism, colorless
$0.77 \times 0.28 \times 0.25$ mm

Data collection

Bruker SMART 1000 CCD area-detector/PLATFORM diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
$T_{\min} = 0.168$, $T_{\max} = 0.371$
11022 measured reflections
4227 independent reflections
3244 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.043$
$\theta_{\max} = 26.4^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.091$
$S = 1.02$
4227 reflections
265 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0282P)^2 + 1.7675P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.54$ e Å^{-3}
$\Delta\rho_{\min} = -0.63$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0037 (4)

Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1—H1$O\cdots$O2$^{\rm i}$	0.84	1.98	2.819 (3)	173
O2—H2$O\cdots$O1$^{\rm ii}$	0.84	1.90	2.707 (3)	161

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

H atoms were placed in idealized positions (C—H = 0.95 and O—H = 0.84 Å) and were assigned isotropic displacement parameters 1.2 (for C—H) or 1.5 (for O—H) times $U_{\rm eq}$ of their parent atoms.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *DIRDIF96* (Beurskens *et al.*, 1996); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2003); software used to prepare material for publication: *SHELXTL*.

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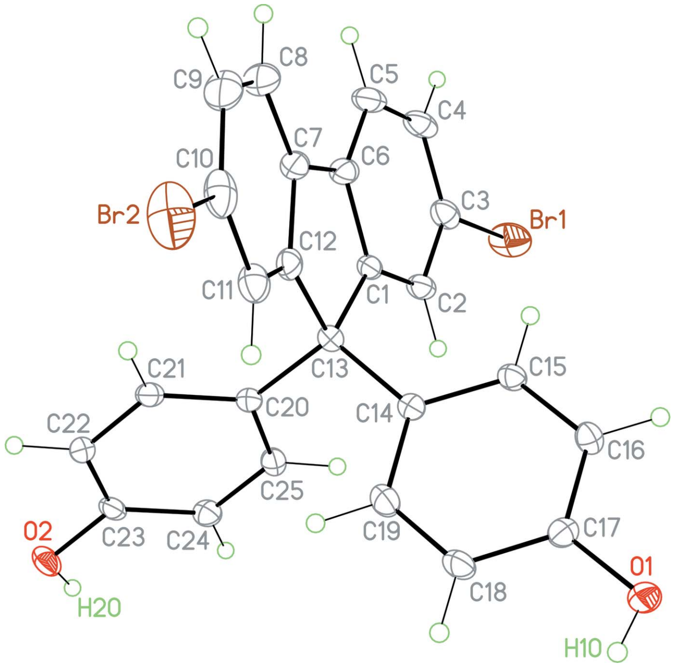

Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented by spheres of an arbitrary radius.

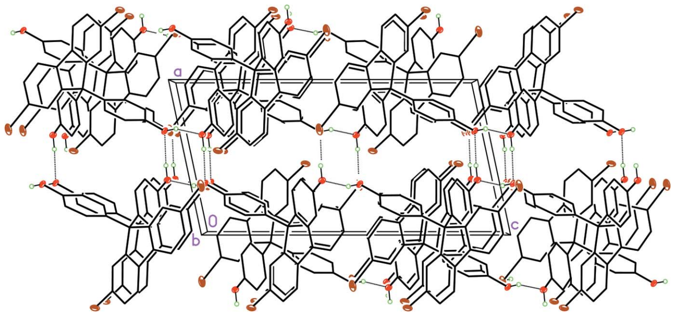

Figure 2
Illustration of the crystal packing (view direction is parallel to the crystallographic *b* axis). Dashed lines indicate hydrogen bonds.

References

Beurskens, P. T., Beurskens, G., Bosman, W. P., de Gelder, R., Garcia Granda, S., Gould, R. O., Israel, R. & Smits, J. M. M. (1996). *DIRDIF96*. University of Nijmegen, The Netherlands.

Bruker (2001). *SMART*. Version 5.054. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (2003). *SADABS* (Version 2.10), *SAINT* (Version 7.06A) and *SHELXTL* (Version 6.14). Bruker AXS Inc., Madison, Wisconsin, USA.

Huang, F., Wang, X., Wang, D., Yang, W. & Cao, Y. (2005). *Polymer*, **46**, 12010–12015.

Lindgren, L. J., Wang, X., Inganäs, O. & Andersson, M. R. (2005). *Synth. Met.* **154**, 97–100.

Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.

Zhou, G., Cheng, Y., Wang, L., Jing, X. & Wang, F. (2005). *Macromolecules*, **38**, 2148–2153.

Zhou, G., Qian, G., Ma, L., Cheng, Y., Xie, Z., Wang, L., Jing, X. & Wang, F. (2005). *Macromolecules*, **38**, 5416–5424.

Zhou, X., Yan, J. & Pei, J. (2004). *Macromolecules*, **37**, 7078–7070.

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