# 9-Pentafluorophenylmethylene-9*H*-fluorene

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**Key indicators**

Single-crystal X-ray study
$T = 298$ K
Mean $\sigma$(C–C) = 0.004 Å
*R* factor = 0.045
*wR* factor = 0.113
Data-to-parameter ratio = 11.7

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

The principal structural feature of the title compound, $C_{20}H_9F_5$, is the dihedral angle of 51.22 (5)° between the substituent phenyl ring and the fluorene fragment of the molecule. This results in the close approach of an F atom to the plane of the fluorene fragment, compromising the planarity of the latter. The conformation also permits virtually complete overlap and $\pi$–$\pi$ interaction of the phenyl ring of one molecule with the five-membered ring of the fluorene of another, in infinite chains of head-to-tail molecules.

## Comment

The title compound, (I) (Fig. 1), was synthesized in the context of an investigation into possible syntheses of fullerene species. The bond lengths and angles of (I) are not unusual for a molecule of this type and are, therefore, not discussed in detail here. The only striking feature is the angle of 51.22 (5)° between the least-squares planes, calculated with unit weights for all atoms, of the fluorene fragment (C1–C13) and the substituent phenyl ring (C15–C20). This is brought about primarily by rotation about the C14—C15 bond and is associated with two further effects.



(I)
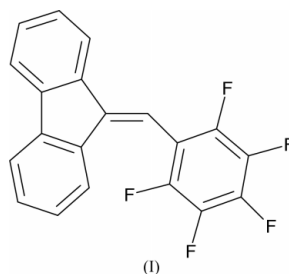
First, within the ring system of the fluorene fragment, the angle between the least-squares planes of the five-membered ring C1/C6/C7/C12/C13 and the six-membered rings C1–C6 and C7–C12 are, respectively, 1.47 (13) and 2.94 (14)°. The displacements of atoms C2, C3, C9, C10 and F1 relative to the plane of the five-membered fluorene ring are, respectively, −0.050 (5), −0.053 (5), −0.1178 (6), −0.1315 (6) and 1.9639 (5) Å. Taking account of the interplanar angles and the magnitudes and signs of the displacements of the atoms relative to the reference plane, the fluorene-ring system is perceived as slightly V-shaped, like the wings of a bird, with the apex of the V directed towards F1; the departure from planarity is greater for the six-membered ring C7–C12, to give F1···C11 and F1···H11 distances of 2.997 (3) and 2.55 Å, respectively. This distortion can be compared with that previously described for 13*H*-dibenzo[*a,g*]fluoren-13-one [Morris *et al.*, 1998; Cambridge Structural Database (Allen, 2002) refcode POVLUH]. The distortion is greater in (I) and

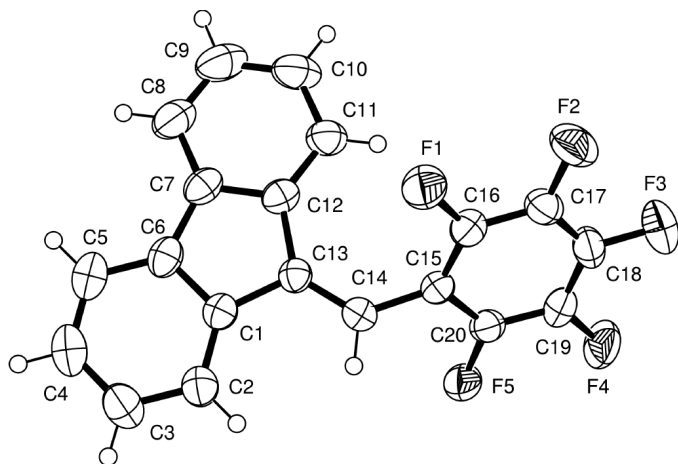DOI: 10.1107/S1600536802023280

**Figure 1**
The molecule of (I), showing the labelling scheme. Non-H atoms are shown as 50% probability ellipsoids and H atoms as spheres of arbitrary radius.
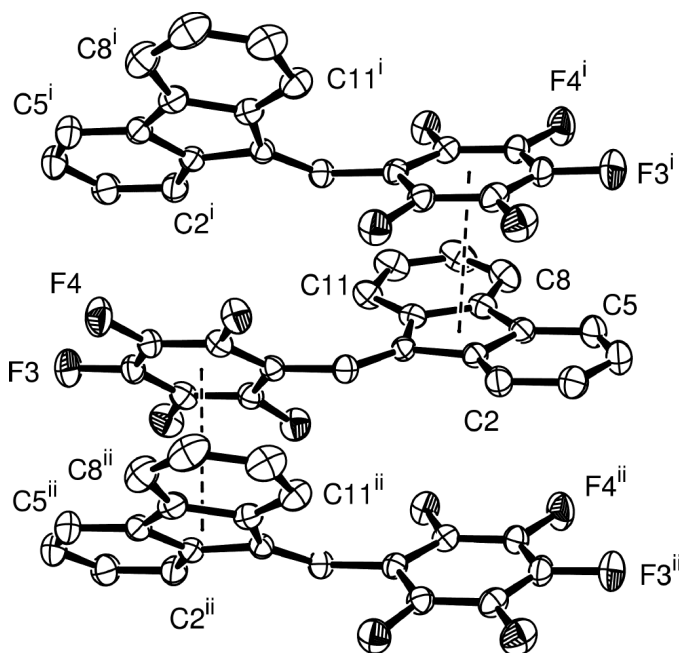


**Figure 2**
A portion of a chain of molecules of (I). Non-H atoms are shown as 30% probability ellipsoids, and the centroids of the overlapping rings are joined by dashed lines. H atoms have been omitted for clarity. [Symmetry codes: (i) $\frac{1}{2} - x$, $\frac{1}{2} + y$, $\frac{1}{2} - z$; (ii) $\frac{1}{2} - x$, $y - \frac{1}{2}$, $\frac{1}{2} - z$].

is brought about by molecular packing (see below), rather than by intramolecular steric effects as it is in the related compound.

Second, the relative orientation of the phenyl substituent and fluorene fragments permits almost complete overlap of and $\pi$–$\pi$ interaction between pairs of molecules arranged head-to-tail and related to one another by the operation of the twofold screw axis, thus creating infinite chains parallel to $b$ (Fig. 2). In this interaction, the dihedral angle between the overlapping rings is 1.02 (13)°. The distance between their centroids and the displacement of each centroid from the plane of the other ring are, respectively, 3.510, 3.454 and

3.453 Å. The overlapping rings are thus very nearly parallel to one another, with a lateral displacement of their centroids of the order of 0.630 Å, and an angle of 10.3° between the average normal to the planes and the line joining their centroids.

## Experimental

*Crystal data*

| | |
|---|---|
| C$_{20}$H$_9$F$_5$ | $D_x$ = 1.524 Mg m$^{-3}$ |
| $M_r$ = 344.27 | Mo $K\alpha$ radiation |
| Monoclinic, $P2_1/n$ | Cell parameters from 14 |
| $a$ = 12.931 (6) Å | reflections |
| $b$ = 7.448 (3) Å | $\theta$ = 8.2–12.3° |
| $c$ = 15.647 (6) Å | $\mu$ = 0.13 mm$^{-1}$ |
| $\beta$ = 95.29 (3)° | $T$ = 298 (2) K |
| $V$ = 1500.5 (11) Å$^3$ | Block, green-yellow |
| $Z$ = 4 | 0.50 × 0.30 × 0.30 mm |

*Data collection*

| | |
|---|---|
| Nicolet $P3$ diffractometer | $\theta_{max}$ = 25.1° |
| $\theta$–2$\theta$ scans | $h$ = 0 → 15 |
| Absorption correction: none | $k$ = 0 → 8 |
| 2772 measured reflections | $l$ = −18 → 18 |
| 2656 independent reflections | 2 standard reflections |
| 1580 reflections with $I > 2\sigma(I)$ | every 50 reflections |
| $R_{int}$ = 0.031 | intensity decay: none |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0485P)^2]$ |
| $R[F^2 > 2\sigma(F^2)]$ = 0.045 | where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2)$ = 0.113 | $(\Delta/\sigma)_{max} < 0.001$ |
| $S$ = 1.01 | $\Delta\rho_{max}$ = 0.19 e Å$^{-3}$ |
| 2656 reflections | $\Delta\rho_{min}$ = −0.18 e Å$^{-3}$ |
| 227 parameters | Extinction correction: *SHELXL*97 |
| H-atom parameters constrained | Extinction coefficient: 0.036 (2) |

H atoms were placed in calculated positions, with C—H = 0.93 Å, and refined as riding, with $U_{iso}$(H) = 1.2$U_{eq}$(C).

Data collection: *P3 Software* (Nicolet, 1980); cell refinement: *P3 Software*; data reduction: *RDNIC* (Howie, 1980); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 1990).

## References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Fletcher, D. A., McMeeking, R. F. & Parkin, D. (1996). *J. Chem. Inf. Comput. Sci.* **36**, 746–749.

Howie, R. A. (1980). *RDNIC*. University of Aberdeen, Scotland.

Morris, D. G., Ryder, K. S & Howie, R. A. (1998). *Acta Cryst.* C**54**, 1542–1544.

Nicolet. (1980). *Nicolet P3/R3 Data Collection Operator's Manual*. Nicolet XRD Corporation, Cupertino, California, USA.

Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.

Spek, A. L. (1990). *Acta Cryst.* A**46**, C-34.