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2′,7′-Di-1-naphthylspiro[cyclopropane-1,9′-fluorene]

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.036
wR factor = 0.094
Data-to-parameter ratio = 9.2

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

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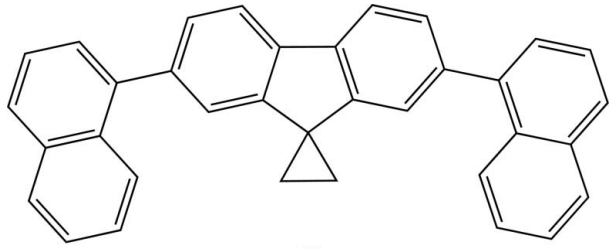
In the title compound, $C_{35}H_{24}$, the fluorene ring system is essentially planar and makes a dihedral angle of 90.02 (2)° with the plane of the cyclopropane ring. The dihedral angles between the fluorene ring system and the naphthalene ring systems are 52.26 (3) and 57.55 (3)°, and π–π stacking occurs between nearly parallel naphthalene ring systems.

Comment

Spirobifluorene derivatives have attracted much attention due to their potential utility in organic light-emitting diodes (Muller *et al.*, 2003). Spiro-linked molecules exhibit greater morphological stability and more intense fluorescence compared to the corresponding non-spiro-linked compounds. These enhanced properties occur without a significant change in their absorption and fluorescence spectra (Yu *et al.*, 2000). Meanwhile, steric factors can lead to an enhanced rigidity at the spiro center, thereby preventing rotation of the adjacent aryl groups, which reduces close packing and intermolecular interaction between chromophores in the solid state (Lee *et al.*, 2005). As part of an investigation on spirobifluorene derivatives (Wang *et al.*, 2006), the crystal structure of the title compound, (I), is presented here.



(I)

The molecular structure of (I) is shown in Fig. 1. The fluorene ring system is essentially planar, and makes a dihedral angle of 90.02 (2)° with the plane of the cyclopropane ring. The dihedral angles between the fluorene ring and naphthalene ring systems are 52.26 (3) (containing atom C16) and 57.55 (3)° (containing atom C26). The C10—C11 bond of the cyclopropane is significantly shorter than the C9—C10 and C9—C11 bonds (Table 1).

π–π Stacking is observed between the nearly parallel naphthalen systeme rings. The centroid-to-centroid separation between the C21-benzene and C21^{i}-benzene rings is 3.7769 (17) Å [dihedral angle= 6.39 (4)°], and the centroid-to-centroid separation between the C31-benzene and C31^{ii}-benzene rings is 3.7288 (18) Å [dihedral angle = 4.31 (10)°] [symmetry codes: (i) $\frac{3}{2} - x$, y, $-\frac{1}{2} + z$; (ii) $\frac{3}{2} - x$, y, $\frac{1}{2} + z$].

Experimental

Compound (I) was prepared by a method similar to that reported previously (Wang *et al.*, 2006). The crude products were purified by column chromatography (silica gel) using *n*-hexane/dichloromethane (5:1 *v*/*v*) as eluant. Compound (I) was obtained as a pale-yellow solid in 80% yield. Single crystals of (I) were obtained by slow evaporation of a hexane–dichloromethane (5:1 *v*/*v*) solution at room temperature.

Crystal data

$C_{35}H_{24}$
M_r = 444.54
Orthorhombic, $Pca2_1$
a = 17.355 (4) Å
b = 18.225 (4) Å
c = 7.4532 (18) Å
V = 2357.4 (9) Å^3
Z = 4
D_x = 1.253 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 296 (2) K
Block, colorless
0.24 × 0.20 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: none
21945 measured reflections
2914 independent reflections
2338 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.094
S = 1.04
2914 reflections
317 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.06P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0121 (14)

Table 1
Selected bond lengths (Å).

C9—C10	1.521 (3)	C10—C11	1.479 (3)
C9—C11	1.511 (3)		

H atoms were placed in calculated positions, with C—H = 0.93 (aromatic) or 0.97 Å (methylene), and refined as riding, U_{iso}(H) = 1.2U_{eq}(C). In the absence of significant anomalous scattering effects, Friedel pairs were averaged.

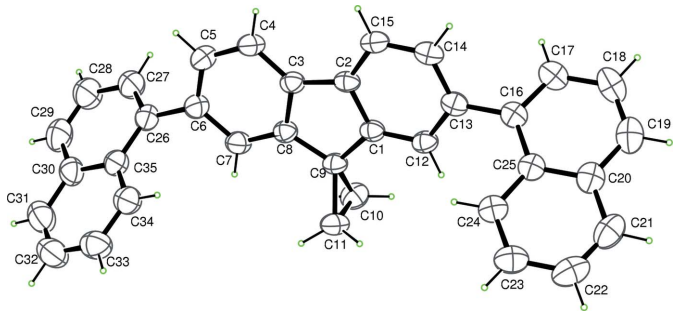


Figure 1
The molecular structure of (I), shown with 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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