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ISSN 2414-3146

9,9-Diethyl-7-ethynyl-*N*,*N*-diphenyl-9*H*-fluoren-2-amine

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Received 3 December 2016
Accepted 16 December 2016

Edited by J. Simpson, University of Otago, New Zealand

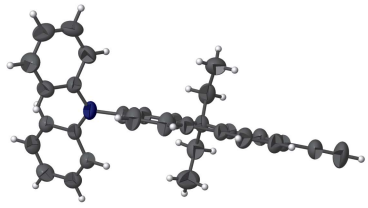
Keywords: fluorene; phenyl rings; intermolecular C–H···π(ring) contacts; crystal structure.

CCDC reference: 1523351

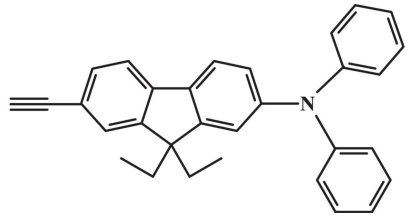
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{31}H_{27}N$, the fluorene unit is approximately planar (r.m.s deviation = 0.0255 Å). The dihedral angles between the fluorene fused ring system and two phenyl rings are 88.37 (5) and 66.31 (6)°. Weak intermolecular C—H···π(ring) interactions help to stabilize the crystal structure.

3D view



Chemical scheme



Structure description

Materials with enhanced two-photon absorption (TPA) properties have attracted considerable research interest in recent years due to their potential applications in photonics and optoelectronics. Optical limiting, two-photon microscopy, upconverted lasing, three-dimensional microfabrication and optical data storage constitute other important applications of TPA materials (Fitilis *et al.*, 2007). Fluorene-based materials, such as terfluorenes, oligofluorenes, and polyfluorenes have emerged as promising candidates for OLEDs due to their high photoluminescence (PL) and electroluminescence (EL) efficiencies, good thermal stability and color tunability across the full visible range (Omer *et al.*, 2009). Diphenylaminofluorene-based organic dyes with acetylene/vinyl linkages have been explored as potential candidates for applications in dye-sensitized solar cells, organic light-emitting diodes and non-linear optics, see: Singh *et al.* (2012); Thomas *et al.* (2012); Rogers *et al.* (2007). The structures of several compounds related to the title compound have been determined, see for example: Belfield *et al.* (1999); Liu *et al.* (2012); Liao *et al.* (2010); Shelton *et al.* (2013).

The title compound, 9,9-diethyl-7-ethynyl-*N*,*N*-diphenyl-9*H*-fluoren-2-amine was synthesized by a two-step protocol involving the Sonogashira coupling of 2-methylbut-3-yn-2-ol with the corresponding aryl bromide and the base-catalysed cleavage of the resulting functionalized but-3-yn-2-ol. In view of the potential importance of this material in the applications mentioned previously, the crystal structure determination was carried

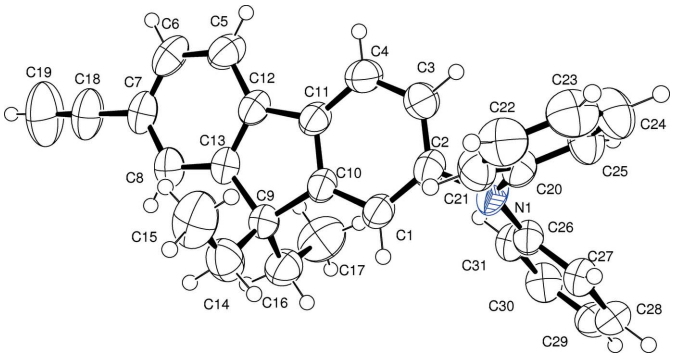


Figure 1
The molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

out and the results are presented here. The molecular structure of the title compound is shown in Fig. 1. The fluorene moiety is almost planar with maximum deviation of 0.0447 (15) Å for C2 and a root mean square deviation of 0.0255 Å from the best-fit plane through all 13 non-hydrogen atoms. The fluorene fused ring system (C1–C13) makes dihedral angles of 88.37 (5) and 66.31 (6)°, respectively, with the phenyl rings (C20–C25) and (C26–C31). The dihedral angle between the phenyl rings is 61.28 (7)°. The sum of the bond angles around N1 (359.86°) indicates that the N1 atom exhibits sp^2 hybridization. The widening of the exocyclic angles C4—C11—C12 [131.22 (19)°] and C11—C12—C5 [130.6 (2)°] that deviate significantly from the expected value of 120°, might be due to the repulsion between H4 at C4 and H5 at C5 (H4···H5 = 2.692 Å). The torsion angle C8—C7—C18—C19 [−148 (10)°] indicates that the ethynyl group is in a (−)anticlinal (−*ac*) orientation with with respect to the (C5–C8/C13/C12) ring of the fluorene ring system. The ethyl substituents on the five-membered ring of the fluorene moiety are in (−)synclinal (−*sc*) which is evident from the torsion angles C10—C9—C16—C17 = −51.9 (2)° and C13—C9—C14—C15 = −51.7 (2)°. While no classical hydrogen bonds are present, two weak intermolecular C—H···π interactions contribute to the stability of the crystal packing (Table 1, Fig2. 2 and 3).

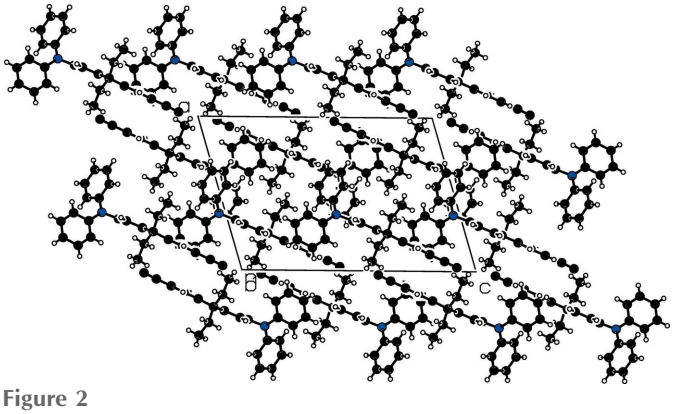


Figure 2
Crystal packing of the title compound viewed along the *b* axis.

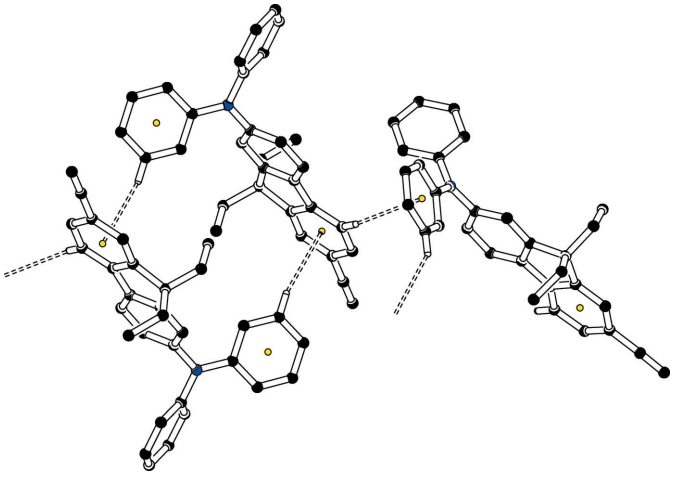


Figure 3
Part of the crystal packing of the title compound, showing the C—H···π interactions

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

*Cg*1 is the centroid of the C26–C31 phenyl ring and *Cg*2 is the centroid of the C5–C8/C13/C12 phenyl ring of the fluorene moiety.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···*Cg*1^{i}	0.93	2.76	3.508 (3)	138
C30—H30···*Cg*2^{ii}	0.93	2.94	3.764 (2)	149

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{31}H_{27}N$
M_r	413.54
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, *b*, *c* (Å)	12.7365 (7), 10.5803 (9), 18.6662 (11)
β (°)	106.531 (3)
V (Å^3)	2411.4 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Crystal size (mm)	0.40 × 0.30 × 0.20
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.974, 0.987
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17899, 5915, 2979
R_{int}	0.039
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.669
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.055, 0.181, 0.98
No. of reflections	5915
No. of parameters	290
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.16

Computer programs: *APEX2*, *SAINT* and *XPREP* (Bruker, 2008), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

Synthesis and crystallization

A mixture of 7-bromo-9,9-diethyl-*N*,*N*-diphenyl-9*H*-fluoren-2-amine (5.0 g, 10.68 mmol), 2-methylbut-3-yn-2-ol (1.07 g,12.8 mmol), $Pd(PPh_3)_2Cl_2$ (75 mg, 0.11 mmol), PPh_3 (56 mg, 0.21 mmol), and CuI (21 mg, 0.11 mmol) were mixed in triethylamine (100 ml) under a nitrogen atmosphere. The resulting mixture was heated and stirred at 373 K for 24 h. After completion of the reaction, the mixture was poured into water and extracted with ethyl acetate. The organic extract was washed with brine solution and dried over Na_2SO_4. Finally, the solvent was removed under vacuum to yield a yellow residue, which was purified by column chromatography as a yellow liquid (5.2 g, 55%), that underwent a further cleavage reaction on treatment with KOH (in toluene to produce the title acetylene as a yellow solid. Yield 71%; m.p. 393–395 K.

^{1}H NMR (500 MHz, $CDCl_3$) δ 0.35 (*t*, *J* = 7.5 Hz, 6 H), 1.95–1.87 (*m*, 4 H), 3.12 (*s*, 1 H), 7.05–7.01 (*m*, 3 H), 7.09 (*d*, *J* = 2.0 Hz, 1 H), 7.13–7.11 (*m*, 4 H), 7.28–7.25 (*m*, 4 H), 7.42 (*d*, *J* = 1.0 Hz, 1 H), 7.46 (*dd*, *J* = 6.5, 1.5 Hz, 1 H), 7.57–7.55 (*m*, 2 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.7, 149.9, 147.9, 147.8, 142.2, 135.7, 131.3, 126.5, 123.5, 122.7, 120.8, 119.3, 119.0, 118.9, 84.8, 56.1, 32.6, 8.5. HRMS calculated for $C_{31}H_{27}N$ [M^+] *m*/*z* 413.2138 found 413.2123.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. One low angle reflection affected by the beamstop was omitted from the final refinement cycles.

Acknowledgements

The authors thank the Sophisticated Analytical Instrument Facility, IIT Madras, Chennai, for the single-crystal X-ray data collection.

References

Belfield, K. D., Hagan, D. J., Van Stryland, E. W., Schafer, K. J. & Negres, R. A. (1999). *Org. Lett.* **1**, 1575–1578.
Bruker (2008). *APEX2*, *SAINT*, *XPREP* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Fitilis, I., Fakis, M., Polyzos, I., Giannetas, V., Persephonis, P., Vellis, P. & Mikroyannidis, J. (2007). *Chem. Phys. Lett.* **447**, 300–304.
Liao, C., Yarnell, J. E., Glusac, K. D. & Schanze, K. S. (2010). *J. Phys. Chem. B*, **114**, 14763–14771.
Liu, R., Zhou, D., Azenkeng, A., Li, Z., Li, Y., Glusac, K. D. & Sun, W. (2012). *Chem. Eur. J.* **18**, 11440–11448.
Omer, K. M., Ku, S. Y., Wong, K.-T. & Bard, A. J. (2009). *J. Am. Chem. Soc.* **131**, 10733–10741.
Rogers, J. E., Slagle, J. E., Krein, D. M., Burke, A. R., Hall, B. C., Fratini, A., McLean, D. G., Fleitz, P. A., Cooper, T. M., Drobizhev, M., Makarov, S. N., Rebane, A., Kim, K. Y., Farley, R. & Schanze, K. S. (2007). *Inorg. Chem.* **46**, 6483–6494.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Shelton, A. H., Price, R. S., Brokmann, L., Dettlaff, B. & Schanze, K. S. (2013). *Appl. Mater. Interfaces*, **5**, 7867–7874.
Singh, P., Baheti, A., Thomas, K. R. J., Lee, C.-P. & Ho, K.-C. (2012). *Dyes Pigments*, **95**, 523–533.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Thomas, K. R. J., Kapoor, N., Bolisetty, M. N. K. P., Jou, J.-H., Chen, Y.-L. & Jou, Y.-C. (2012). *J. Org. Chem.* **77**, 3921–3932.

full crystallographic data

IUCrData (2016). **1**, x162006 [https://doi.org/10.1107/S241431461602006X]

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Crystal data

$C_{31}H_{27}N$
M_r = 413.54
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 12.7365 (7) Å
b = 10.5803 (9) Å
c = 18.6662 (11) Å
β = 106.531 (3)°
V = 2411.4 (3) Å^3
Z = 4
$F(000)$ = 880
D_x = 1.139 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5915 reflections
θ = 2.3–28.4°
μ = 0.07 mm^{-1}
T = 296 K
Block, yellow
0.40 × 0.30 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2008)
T_{min} = 0.974, T_{max} = 0.987
17899 measured reflections
5915 independent reflections
2979 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 28.4°, θ_{min} = 2.3°
h = −16→16
k = −11→13
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.181
S = 0.98
5915 reflections
290 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0937P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: SHELXL, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0103 (17)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C21	0.55085 (16)	0.2135 (2)	1.03753 (10)	0.0643 (6)
H21	0.5508	0.1528	1.0735	0.077*
C22	0.64185 (16)	0.2875 (3)	1.04460 (12)	0.0740 (7)
H22	0.7034	0.2756	1.0851	0.089*
C23	0.64316 (17)	0.3774 (3)	0.99344 (14)	0.0766 (7)
H23	0.7051	0.4271	0.9988	0.092*
C24	0.55307 (17)	0.3948 (2)	0.93396 (12)	0.0768 (7)
H24	0.5537	0.4568	0.8988	0.092*
C25	0.46098 (16)	0.3210 (2)	0.92554 (10)	0.0644 (6)
H25	0.3998	0.3336	0.8848	0.077*
C20	0.45945 (14)	0.2291 (2)	0.97722 (9)	0.0505 (5)
C27	0.36126 (15)	0.0663 (2)	0.84942 (10)	0.0546 (5)
H27	0.4332	0.0919	0.8560	0.066*
C28	0.30536 (17)	0.0053 (2)	0.78493 (10)	0.0608 (5)
H28	0.3400	−0.0094	0.7481	0.073*
C29	0.19913 (17)	−0.0347 (2)	0.77381 (11)	0.0640 (6)
H29	0.1618	−0.0752	0.7297	0.077*
C30	0.14928 (16)	−0.0136 (2)	0.82890 (11)	0.0642 (6)
H30	0.0781	−0.0419	0.8225	0.077*
C31	0.20344 (14)	0.0488 (2)	0.89339 (10)	0.0562 (5)
H31	0.1680	0.0637	0.9298	0.067*
C26	0.31065 (14)	0.08984 (19)	0.90484 (9)	0.0474 (4)
C2	0.32513 (15)	0.1446 (2)	1.03489 (9)	0.0538 (5)
C1	0.31211 (14)	0.0285 (2)	1.06600 (9)	0.0514 (5)
H1	0.3327	−0.0457	1.0470	0.062*
C10	0.26812 (14)	0.02479 (19)	1.12564 (9)	0.0477 (5)
C11	0.23914 (14)	0.1362 (2)	1.15521 (9)	0.0518 (5)
C4	0.25459 (17)	0.2518 (2)	1.12523 (11)	0.0687 (6)
H4	0.2365	0.3264	1.1452	0.082*
C3	0.29750 (17)	0.2546 (2)	1.06483 (11)	0.0682 (6)
H3	0.3078	0.3320	1.0442	0.082*
C9	0.24326 (14)	−0.0910 (2)	1.16669 (9)	0.0520 (5)
C16	0.16364 (17)	−0.1821 (2)	1.11368 (11)	0.0719 (6)
H16A	0.2013	−0.2211	1.0810	0.086*
H16B	0.1441	−0.2487	1.1432	0.086*

C17	0.06195 (19)	−0.1228 (3)	1.06713 (14)	0.0999 (9)
H17A	0.0173	−0.1857	1.0356	0.150*
H17B	0.0800	−0.0579	1.0367	0.150*
H17C	0.0225	−0.0863	1.0988	0.150*
C14	0.34677 (18)	−0.1643 (3)	1.20693 (12)	0.0773 (7)
H14A	0.3255	−0.2375	1.2308	0.093*
H14B	0.3807	−0.1949	1.1698	0.093*
C15	0.43024 (18)	−0.0919 (3)	1.26448 (13)	0.0985 (9)
H15A	0.4917	−0.1455	1.2866	0.148*
H15B	0.3986	−0.0630	1.3025	0.148*
H15C	0.4541	−0.0205	1.2415	0.148*
C13	0.19257 (14)	−0.0270 (2)	1.22260 (9)	0.0509 (5)
C8	0.15084 (14)	−0.0827 (2)	1.27558 (10)	0.0600 (5)
H8	0.1502	−0.1702	1.2800	0.072*
C7	0.10976 (15)	−0.0069 (3)	1.32245 (10)	0.0622 (6)
C6	0.11196 (16)	0.1229 (3)	1.31574 (10)	0.0693 (7)
H6	0.0859	0.1729	1.3479	0.083*
C5	0.15192 (16)	0.1802 (2)	1.26230 (10)	0.0660 (6)
H5	0.1517	0.2677	1.2576	0.079*
C12	0.19252 (14)	0.1035 (2)	1.21568 (9)	0.0518 (5)
C18	0.06541 (18)	−0.0628 (3)	1.37757 (12)	0.0861 (8)
C19	0.0276 (3)	−0.1050 (4)	1.42180 (17)	0.1355 (14)
H19	−0.0028	−0.1390	1.4573	0.163*
N1	0.36621 (12)	0.15140 (17)	0.97122 (7)	0.0590 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C21	0.0670 (12)	0.0672 (16)	0.0527 (11)	0.0011 (11)	0.0077 (9)	0.0075 (10)
C22	0.0524 (12)	0.0841 (19)	0.0727 (13)	0.0025 (12)	−0.0028 (10)	−0.0065 (13)
C23	0.0582 (13)	0.0771 (19)	0.0940 (16)	−0.0180 (12)	0.0205 (12)	−0.0110 (14)
C24	0.0750 (15)	0.0739 (18)	0.0801 (14)	−0.0177 (12)	0.0196 (12)	0.0172 (13)
C25	0.0574 (11)	0.0753 (16)	0.0556 (11)	−0.0088 (11)	0.0083 (9)	0.0125 (11)
C20	0.0503 (10)	0.0575 (14)	0.0459 (9)	−0.0052 (9)	0.0173 (8)	−0.0029 (9)
C27	0.0548 (10)	0.0615 (14)	0.0500 (10)	−0.0019 (9)	0.0188 (8)	0.0014 (9)
C28	0.0759 (13)	0.0580 (14)	0.0529 (10)	0.0068 (11)	0.0257 (10)	−0.0049 (10)
C29	0.0744 (13)	0.0572 (15)	0.0549 (11)	−0.0053 (11)	0.0094 (10)	−0.0105 (10)
C30	0.0560 (11)	0.0712 (16)	0.0619 (12)	−0.0090 (10)	0.0108 (10)	0.0009 (11)
C31	0.0530 (11)	0.0673 (15)	0.0501 (10)	−0.0038 (9)	0.0174 (8)	0.0016 (9)
C26	0.0512 (10)	0.0503 (12)	0.0418 (8)	−0.0019 (8)	0.0150 (7)	0.0035 (8)
C2	0.0601 (11)	0.0611 (14)	0.0441 (9)	−0.0130 (9)	0.0211 (8)	−0.0031 (9)
C1	0.0587 (11)	0.0550 (13)	0.0443 (9)	−0.0039 (9)	0.0206 (8)	−0.0038 (9)
C10	0.0529 (10)	0.0531 (13)	0.0386 (8)	−0.0046 (9)	0.0154 (7)	−0.0011 (8)
C11	0.0606 (11)	0.0532 (14)	0.0462 (9)	−0.0104 (9)	0.0226 (8)	−0.0066 (9)
C4	0.0982 (16)	0.0506 (15)	0.0712 (13)	−0.0120 (12)	0.0465 (12)	−0.0089 (11)
C3	0.0951 (15)	0.0522 (14)	0.0692 (12)	−0.0147 (11)	0.0427 (12)	0.0003 (11)
C9	0.0597 (11)	0.0541 (13)	0.0463 (9)	0.0010 (9)	0.0214 (8)	0.0038 (9)
C16	0.0879 (15)	0.0630 (16)	0.0703 (13)	−0.0146 (12)	0.0315 (12)	−0.0076 (11)

C17	0.0784 (17)	0.120 (3)	0.0949 (17)	−0.0123 (16)	0.0142 (14)	−0.0243 (17)
C14	0.0819 (15)	0.0798 (19)	0.0796 (14)	0.0173 (13)	0.0384 (12)	0.0197 (13)
C15	0.0623 (14)	0.149 (3)	0.0800 (15)	0.0118 (16)	0.0137 (12)	0.0062 (17)
C13	0.0496 (10)	0.0641 (15)	0.0393 (9)	−0.0024 (9)	0.0132 (8)	0.0036 (9)
C8	0.0587 (11)	0.0731 (16)	0.0501 (10)	0.0004 (10)	0.0182 (9)	0.0124 (10)
C7	0.0539 (11)	0.0919 (19)	0.0427 (10)	−0.0035 (11)	0.0168 (8)	0.0059 (11)
C6	0.0666 (13)	0.098 (2)	0.0517 (11)	−0.0093 (12)	0.0304 (10)	−0.0158 (12)
C5	0.0758 (13)	0.0680 (16)	0.0626 (12)	−0.0131 (11)	0.0332 (10)	−0.0150 (11)
C12	0.0541 (10)	0.0615 (15)	0.0430 (9)	−0.0090 (9)	0.0187 (8)	−0.0064 (9)
C18	0.0724 (14)	0.135 (3)	0.0576 (12)	0.0028 (14)	0.0290 (11)	0.0205 (14)
C19	0.124 (2)	0.203 (4)	0.101 (2)	0.006 (2)	0.0660 (19)	0.058 (2)
N1	0.0655 (10)	0.0740 (13)	0.0426 (8)	−0.0238 (9)	0.0235 (7)	−0.0060 (8)

Geometric parameters (Å, º)

C21—C22	1.373 (3)	C11—C12	1.459 (2)
C21—C20	1.380 (2)	C4—C3	1.386 (3)
C21—H21	0.9300	C4—H4	0.9300
C22—C23	1.351 (3)	C3—H3	0.9300
C22—H22	0.9300	C9—C14	1.529 (3)
C23—C24	1.363 (3)	C9—C13	1.532 (2)
C23—H23	0.9300	C9—C16	1.538 (3)
C24—C25	1.380 (3)	C16—C17	1.478 (3)
C24—H24	0.9300	C16—H16A	0.9700
C25—C20	1.374 (3)	C16—H16B	0.9700
C25—H25	0.9300	C17—H17A	0.9600
C20—N1	1.422 (2)	C17—H17B	0.9600
C27—C28	1.373 (3)	C17—H17C	0.9600
C27—C26	1.388 (2)	C14—C15	1.490 (3)
C27—H27	0.9300	C14—H14A	0.9700
C28—C29	1.376 (3)	C14—H14B	0.9700
C28—H28	0.9300	C15—H15A	0.9600
C29—C30	1.372 (3)	C15—H15B	0.9600
C29—H29	0.9300	C15—H15C	0.9600
C30—C31	1.374 (3)	C13—C8	1.381 (2)
C30—H30	0.9300	C13—C12	1.387 (3)
C31—C26	1.390 (2)	C8—C7	1.394 (3)
C31—H31	0.9300	C8—H8	0.9300
C26—N1	1.400 (2)	C7—C6	1.380 (3)
C2—C3	1.380 (3)	C7—C18	1.434 (3)
C2—C1	1.389 (3)	C6—C5	1.382 (3)
C2—N1	1.430 (2)	C6—H6	0.9300
C1—C10	1.382 (2)	C5—C12	1.392 (3)
C1—H1	0.9300	C5—H5	0.9300
C10—C11	1.395 (3)	C18—C19	1.158 (3)
C10—C9	1.525 (3)	C19—H19	0.9300
C11—C4	1.383 (3)		

C22—C21—C20	120.2 (2)	C10—C9—C14	112.37 (15)
C22—C21—H21	119.9	C10—C9—C13	100.07 (16)
C20—C21—H21	119.9	C14—C9—C13	111.15 (14)
C23—C22—C21	120.86 (19)	C10—C9—C16	111.90 (14)
C23—C22—H22	119.6	C14—C9—C16	108.49 (19)
C21—C22—H22	119.6	C13—C9—C16	112.75 (15)
C22—C23—C24	119.6 (2)	C17—C16—C9	114.8 (2)
C22—C23—H23	120.2	C17—C16—H16A	108.6
C24—C23—H23	120.2	C9—C16—H16A	108.6
C23—C24—C25	120.5 (2)	C17—C16—H16B	108.6
C23—C24—H24	119.7	C9—C16—H16B	108.6
C25—C24—H24	119.7	H16A—C16—H16B	107.5
C20—C25—C24	120.11 (18)	C16—C17—H17A	109.5
C20—C25—H25	119.9	C16—C17—H17B	109.5
C24—C25—H25	119.9	H17A—C17—H17B	109.5
C25—C20—C21	118.68 (18)	C16—C17—H17C	109.5
C25—C20—N1	122.16 (16)	H17A—C17—H17C	109.5
C21—C20—N1	119.15 (18)	H17B—C17—H17C	109.5
C28—C27—C26	120.19 (17)	C15—C14—C9	115.6 (2)
C28—C27—H27	119.9	C15—C14—H14A	108.4
C26—C27—H27	119.9	C9—C14—H14A	108.4
C27—C28—C29	121.27 (18)	C15—C14—H14B	108.4
C27—C28—H28	119.4	C9—C14—H14B	108.4
C29—C28—H28	119.4	H14A—C14—H14B	107.4
C30—C29—C28	118.83 (18)	C14—C15—H15A	109.5
C30—C29—H29	120.6	C14—C15—H15B	109.5
C28—C29—H29	120.6	H15A—C15—H15B	109.5
C29—C30—C31	120.71 (18)	C14—C15—H15C	109.5
C29—C30—H30	119.6	H15A—C15—H15C	109.5
C31—C30—H30	119.6	H15B—C15—H15C	109.5
C30—C31—C26	120.73 (18)	C8—C13—C12	120.10 (18)
C30—C31—H31	119.6	C8—C13—C9	128.4 (2)
C26—C31—H31	119.6	C12—C13—C9	111.46 (15)
C27—C26—C31	118.25 (16)	C13—C8—C7	119.6 (2)
C27—C26—N1	121.20 (15)	C13—C8—H8	120.2
C31—C26—N1	120.55 (15)	C7—C8—H8	120.2
C3—C2—C1	120.17 (17)	C6—C7—C8	119.62 (19)
C3—C2—N1	119.33 (19)	C6—C7—C18	119.8 (2)
C1—C2—N1	120.50 (18)	C8—C7—C18	120.6 (2)
C10—C1—C2	119.07 (19)	C7—C6—C5	121.5 (2)
C10—C1—H1	120.5	C7—C6—H6	119.2
C2—C1—H1	120.5	C5—C6—H6	119.2
C1—C10—C11	120.56 (18)	C6—C5—C12	118.3 (2)
C1—C10—C9	128.10 (18)	C6—C5—H5	120.9
C11—C10—C9	111.33 (15)	C12—C5—H5	120.9
C4—C11—C10	120.23 (17)	C13—C12—C5	120.81 (18)
C4—C11—C12	131.22 (19)	C13—C12—C11	108.57 (16)
C10—C11—C12	108.53 (17)	C5—C12—C11	130.6 (2)

C11—C4—C3	118.9 (2)	C19—C18—C7	178.1 (3)
C11—C4—H4	120.6	C18—C19—H19	180.0
C3—C4—H4	120.6	C26—N1—C20	122.60 (14)
C2—C3—C4	121.1 (2)	C26—N1—C2	119.97 (14)
C2—C3—H3	119.5	C20—N1—C2	117.29 (14)
C4—C3—H3	119.5		

C20—C21—C22—C23	0.8 (4)	C13—C9—C14—C15	−51.7 (2)
C21—C22—C23—C24	−0.1 (4)	C16—C9—C14—C15	−176.18 (18)
C22—C23—C24—C25	−0.3 (4)	C10—C9—C13—C8	178.72 (17)
C23—C24—C25—C20	−0.1 (4)	C14—C9—C13—C8	−62.4 (2)
C24—C25—C20—C21	0.8 (3)	C16—C9—C13—C8	59.7 (2)
C24—C25—C20—N1	179.5 (2)	C10—C9—C13—C12	−1.77 (17)
C22—C21—C20—C25	−1.1 (3)	C14—C9—C13—C12	117.12 (19)
C22—C21—C20—N1	−179.93 (19)	C16—C9—C13—C12	−120.81 (18)
C26—C27—C28—C29	−0.5 (3)	C12—C13—C8—C7	−0.6 (2)
C27—C28—C29—C30	−0.6 (3)	C9—C13—C8—C7	178.83 (16)
C28—C29—C30—C31	1.5 (3)	C13—C8—C7—C6	−0.5 (3)
C29—C30—C31—C26	−1.2 (3)	C13—C8—C7—C18	179.61 (17)
C28—C27—C26—C31	0.8 (3)	C8—C7—C6—C5	1.4 (3)
C28—C27—C26—N1	179.70 (19)	C18—C7—C6—C5	−178.63 (18)
C30—C31—C26—C27	0.1 (3)	C7—C6—C5—C12	−1.3 (3)
C30—C31—C26—N1	−178.85 (18)	C8—C13—C12—C5	0.8 (3)
C3—C2—C1—C10	2.0 (3)	C9—C13—C12—C5	−178.76 (15)
N1—C2—C1—C10	−177.44 (15)	C8—C13—C12—C11	−179.06 (14)
C2—C1—C10—C11	−1.2 (3)	C9—C13—C12—C11	1.39 (19)
C2—C1—C10—C9	177.93 (16)	C6—C5—C12—C13	0.2 (3)
C1—C10—C11—C4	−0.3 (3)	C6—C5—C12—C11	179.97 (17)
C9—C10—C11—C4	−179.56 (17)	C4—C11—C12—C13	178.18 (19)
C1—C10—C11—C12	178.43 (15)	C10—C11—C12—C13	−0.3 (2)
C9—C10—C11—C12	−0.87 (19)	C4—C11—C12—C5	−1.7 (3)
C10—C11—C4—C3	1.0 (3)	C10—C11—C12—C5	179.85 (18)
C12—C11—C4—C3	−177.32 (17)	C6—C7—C18—C19	32 (10)
C1—C2—C3—C4	−1.2 (3)	C8—C7—C18—C19	−148 (10)
N1—C2—C3—C4	178.21 (16)	C27—C26—N1—C20	21.4 (3)
C11—C4—C3—C2	−0.3 (3)	C31—C26—N1—C20	−159.70 (19)
C1—C10—C9—C14	64.3 (2)	C27—C26—N1—C2	−163.01 (19)
C11—C10—C9—C14	−116.43 (18)	C31—C26—N1—C2	15.9 (3)
C1—C10—C9—C13	−177.68 (16)	C25—C20—N1—C26	48.3 (3)
C11—C10—C9—C13	1.56 (17)	C21—C20—N1—C26	−132.9 (2)
C1—C10—C9—C16	−58.0 (2)	C25—C20—N1—C2	−127.4 (2)
C11—C10—C9—C16	121.22 (17)	C21—C20—N1—C2	51.4 (3)
C10—C9—C16—C17	−51.9 (2)	C3—C2—N1—C26	−120.5 (2)
C14—C9—C16—C17	−176.40 (18)	C1—C2—N1—C26	58.9 (2)
C13—C9—C16—C17	60.0 (2)	C3—C2—N1—C20	55.3 (2)
C10—C9—C14—C15	59.6 (2)	C1—C2—N1—C20	−125.3 (2)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C26–C31 phenyl ring and Cg2 is the centroid of the C5–C8/C13/C12 phenyl ring of the fluorene moiety.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···*Cg*1^{i}	0.93	2.76	3.508 (3)	138
C30—H30···*Cg*2^{ii}	0.93	2.94	3.764 (2)	149

Symmetry codes: (i) *x*, −*y*−1/2, *z*−1/2; (ii) −*x*, −*y*, −*z*.