

Supporting Information for:

Synthesis and Properties of Quinoidal Fluorenofluorenes

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Experimental Details

General. ^1H and ^{13}C NMR spectra were recorded in CDCl_3 at room temperature using either a Bruker Avance III HD 500 equipped with a Prodigy multinuclear cryoprobe (^1H : 500 MHz, ^{13}C : 126 MHz) or Bruker Avance III HD 600 MHz (^1H : 600.02 MHz, ^{13}C : 150.89 MHz) NMR spectrometer with Prodigy multinuclear broadband cryoprobe. Chemical shifts (δ) are expressed in ppm relative to the residual non-deuterated solvent (CDCl_3 , ^1H : 7.26 ppm, ^{13}C : 77.16 ppm). UV-Vis spectra were recorded on an HP 8453 UV-Vis spectrometer. THF and toluene were distilled from Na/benzophenone ketyl under nitrogen prior to use. Compounds **9**¹ and **12**² were prepared according to literature procedures. Unless stated otherwise, all solvents and reagents were used as received.

Diphenyl diester 10. Phenylboronic acid (270.7 mg, 2.22 mmol), ditriflate **9** (200 mg, 0.370 mmol), and K_3PO_4 (235.6 mg, 1.11 mmol) were dissolved in dry toluene (25 mL) and the mixture was sparged with N_2 for 1 h. $\text{Pd}(\text{OAc})_2$ (3.3 mg, 0.0148 mmol) and SPhos (12.2 mg, 0.0296 mmol) were then added. After sparging for an additional 20 min the reaction mixture was heated to reflux overnight. After cooling, the mixture was quenched with H_2O and extracted with Et_2O . The organic layer was washed with water and brine solution, and then dried (MgSO_4). The crude reaction mixture was purified via column chromatography on SiO_2 (3:2 hexanes:EtOAc) to yield **10** (123 g, 84 %) as an off-white solid. ^1H NMR (600 MHz, CDCl_3) δ 8.38 (s, 2H), 7.92 (s, 2H), 7.48–7.39 (m, 10H), 3.71 (s, 6H). ^{13}C NMR (126 MHz, CDCl_3) δ 168.90, 140.98, 139.70, 132.60, 131.62, 130.67, 130.31, 128.58, 128.34, 52.38. HRMS (ESI) for $\text{C}_{26}\text{H}_{20}\text{O}_4$ $[\text{M}+\text{H}]^+$: calcd 397.1440, found 397.1448.

Dione 11. A mixture of diester **10** (400 mg, 1.01 mmol), EtOH (96 mL), H_2O (24 mL), and KOH (906 mg) was refluxed overnight. The reaction was concentrated to remove the EtOH and the resulting aqueous mixture was acidified carefully by dropwise addition of concentrated HCl solution. The resulting precipitate was collected, washed with H_2O , and then dried in an oven to give the diacid as a beige solid. The diacid was then stirred in concentrated H_2SO_4 overnight. The reaction mixture was poured over ice and stirred for 5 min. The product was filtered and washed with H_2O , hexanes, and acetone to yield dione **11** (251 mg, 86%) as a bright red solid. Due to

very poor solubility, NMR data for **11** could not be obtained. HRMS (EI+) for C₂₄H₁₂O₂ [M]⁺: calcd 332.0837, found 332.0825.

Fluoreno[3,2-*b*]fluorene 2. An oven dried flask containing THF (15 mL) and mesityl bromide (0.127 mL, 0.831 mmol) was cooled to -78 °C and then *n*-BuLi (0.312 mL, 2.5 M solution, 0.779 mmol) was added slowly. The reaction was stirred for 30 min and then added slowly to a THF solution of dione **11** (59 mg, 0.104 mmol) under N₂ at -78 °C. After warming the solution to room temperature overnight, the reaction was quenched with saturated NH₄Cl solution, and extracted with CH₂Cl₂. The organic phase was washed with water and then brine solution. The organic layer was dried (MgSO₄) and the volatiles removed to give a crude yellow solid that was used without further purification.

Under N₂ the crude diol (~50 mg, ~0.174 mmol) and SnCl₂ (185 mg, 0.699 mmol) were dissolved in toluene (20 mL). Immediately 10 drops of trifluoroacetic acid (TFA) were added and the solution became a deep blue color. Upon completion (ca. 2-4 h), the mixture was passed through a SiO₂ plug eluting with 1:1 hexanes:CH₂Cl₂. The solution was concentrated to dryness then dissolved in minimal CH₂Cl₂ and layered with CH₃CN and cooled in the freezer. The precipitated product was filtered to yield **2** (17 mg, 30%) as a dark blue-purple solid. ¹H NMR (500 MHz, CDCl₃) δ 7.56 (d, *J* = 6.8 Hz, 2H), 7.38 (s, 2H), 7.13–7.09 (m, 2H), 7.09–7.06 (m, 2H), 7.02 (s, 4H), 6.95 (s, 2H), 6.86 (d, *J* = 7.0 Hz, 2H), 2.39 (s, 6H), 2.12 (s, 12H). ¹³C NMR (151 MHz, CDCl₃) δ 143.97, 137.64, 137.41, 137.40, 137.00, 134.90, 131.69, 130.42, 128.37, 128.08, 127.64, 126.70, 124.92, 122.08, 120.76, 21.35, 20.46. UV-Vis (CH₂Cl₂) λ_{max} (ε) 342 (20,860), 561 sh (8820), 600 (11,640) nm. HRMS (EI+) for C₄₂H₃₄ [M]⁺: calcd 538.2661, found 538.2677. Note: the poor solubility of **2** hindered the acquisition of good NMR spectra, as the poor solubility has the side effect of greatly exaggerating impurities present in the CDCl₃ of H-grease impurities present in the samples from our Schlenk line.

Diphenyl 13. To a mixture of phenylboronic acid (6.01 g, 44.3 mmol), dibromide **12**² (5.00 g, 15.9 mmol), Pd(dppf)Cl₂ (229 mg, 0.39 mmol), and K₂CO₃ (6.02 g, 60.8 mmol) in a 350 mL heavy-walled flask was added dry toluene (60 mL). After degassing the mixture with N₂ for 30 min, the reaction was sealed and heated to reflux overnight. After cooling to r.t. the reaction was

filtered to remove solid impurities and the filter cake was washed with CH₂Cl₂. The filtrate was concentrated under reduced pressure and recrystallized from toluene to yield **13** (3.12 g, 63%) as fine white needles. ¹H NMR (600 MHz, CDCl₃) δ 7.52 (t, *J* = 7.4 Hz, 4H), 7.45 (t, *J* = 7.4 Hz, 2H), 7.35 (d, *J* = 8.6 Hz, 2H), 7.32–7.30 (m, 4H), 7.27 (d, *J* = 8.6 Hz, 2H), 2.20 (s, 6H). ¹³C NMR (151 MHz, CDCl₃) δ 140.24, 138.11, 132.12, 131.51, 130.33, 128.60, 128.52, 127.08, 125.60, 20.73. HRMS (ESI) for C₂₄H₂₀ [M+H]⁺: calcd 309.1643, found 309.1647.

Dione 14. Diphenyl **13** (0.503 g, 1.6 mmol), KOH (0.972 g, 17.3 mmol), and pyridine (15 mL) were heated to reflux. Once the mixture was at reflux, KMnO₄ (3 g, 19 mmol) and water (8.7 mL) were added portionwise over 4 h. After refluxing overnight, the reaction mixture was cooled and then filtered through a celite plug with a hot solution of 10% aqueous KOH. The filtrate was acidified with concentrated HCl upon which a precipitate formed. Filtration yielded the mono-acid side product as an off-white solid. Further acidification of this filtrate yielded the crude diacid as a white flaky solid, which was subsequently dissolved in concentrated H₂SO₄ (10 mL) and stirred overnight. The reaction was quenched by pouring over ice to give a bright red precipitate. The solid was filtered and washed with acetone to yield dione **14** (248 mg, 54%). ¹H NMR (500 MHz, CDCl₃) δ 8.57 (d, *J* = 8.4 Hz, 2H), 8.10 (d, *J* = 7.5 Hz, 2H), 7.92 (d, *J* = 8.4 Hz, 2H), 7.79–7.73 (m, 2H), 7.64–7.57 (m, 2H), 7.40 (d, *J* = 7.3 Hz, 2H). Due to poor solubility, ¹³C NMR data of **14** could not be obtained. HRMS (EI+) for C₂₄H₁₂O₂ [M]⁺: calcd 332.0837, found 332.0831.

Fluoreno[4,3-*c*]fluorene 8. To an oven-dried flask containing dione **14** (150 mg, 0.45 mmol) dissolved in THF under N₂ was added mesitylmagnesium bromide (4 mL, 1.0 M solution, 4 mmol) was added at 0 °C. The reaction solution was stirred overnight and transitioned from a dark reddish-brown color to a turquoise color. The reaction was quenched with saturated NH₄Cl solution, extracted with CH₂Cl₂, and the organic phase was washed with water and then brine solution. The organic layer was dried (MgSO₄) and the volatiles removed. The resulting crude solid was used without further purification.

Under N₂ the crude diol was dissolved in degassed toluene (20 mL) and anhydrous SnCl₂ (809 mg, 4.3 mmol) was added. The reaction was stirred for 16 h at room temperature at which

time the solution had turned a deep purple color. The reaction solution was evaporated and the crude product was purified on a silica gel plug eluting with 4:1 hexanes:CH₂Cl₂. The crude product was recrystallized by layering CH₃CN over a saturated solution in CHCl₃. The solid was collected by filtration to yield **8** (128 mg, 47%) as dark blue crystal. ¹H NMR (600 MHz, CDCl₃) δ 7.85 (d, *J* = 7.6 Hz, 2H), 7.57 (d, *J* = 9.4 Hz, 2H), 7.11 (t, *J* = 7.5 Hz, 2H), 7.04 (t, *J* = 7.3 Hz, 2H), 7.00 (s, 4H), 6.80 (d, *J* = 7.3 Hz, 2H), 6.70 (d, *J* = 9.3 Hz, 2H), 2.38 (s, 6H), 2.13 (s, 12H). ¹³C NMR (151 MHz, CDCl₃) δ 144.00, 143.84, 138.09, 137.68, 137.26, 136.99, 134.15, 132.92, 130.12, 128.35, 127.88, 126.92, 125.41, 124.99, 122.47, 122.12, 21.34, 20.41. UV-Vis (CH₂Cl₂) λ_{max} (ε) 331 (34,160), 554 sh (14,950), 594 (19,480), 637 (14,970) nm. HRMS (ESI) for C₄₂H₃₄ [M+H]⁺: calcd 539.2736, found 539.2739.

X-ray Crystallographic Data

General. Diffraction intensities for **8** were collected at 173 K on a Bruker Apex2 CCD diffractometer using a *Incoatec* Cu $I\mu S$ source, $\text{CuK}\alpha$ radiation, 1.54178 Å. Space group was determined based on intensity statistics. Absorption correction was applied by SADABS.³ Structure was solved by direct methods and Fourier techniques and refined on F^2 using full matrix least-squares procedures. All non-H atoms were refined with anisotropic thermal parameters. H atoms were treated in calculated positions in a rigid group model. All calculations were performed by the SHELXL-2014/7 packages.⁴

Crystallographic Data for 8: $\text{C}_{42}\text{H}_{34}$, $M = 538.69$, $0.09 \times 0.08 \times 0.06$ mm, $T = 173(2)$ K, Triclinic, space group $P-1$, $a = 7.1561(6)$ Å, $b = 8.0619(6)$ Å, $c = 12.8650(10)$ Å, $\alpha = 87.837(4)^\circ$, $\beta = 88.161(4)^\circ$, $\gamma = 75.494(4)^\circ$, $V = 717.84(10)$ Å³, $Z = 1$, $Z' = 0.5$, $D_c = 1.246$ Mg m⁻³, $\mu(\text{Cu}) = 0.529$ mm⁻¹, $F(000) = 286$, $2\theta_{\text{max}} = 133.00^\circ$, 8275 reflections, 2481 independent reflections [$R_{\text{int}} = 0.0454$], $R_1 = 0.0621$, $wR_2 = 0.1733$ and $\text{GOF} = 1.065$ for 2481 reflections (190 parameters) with $I > 2\sigma(I)$, $R_1 = 0.0677$, $wR_2 = 0.1778$ and $\text{GOF} = 1.065$ for all reflections, max/min residual electron density $+0.459/-0.442$ eÅ⁻³.

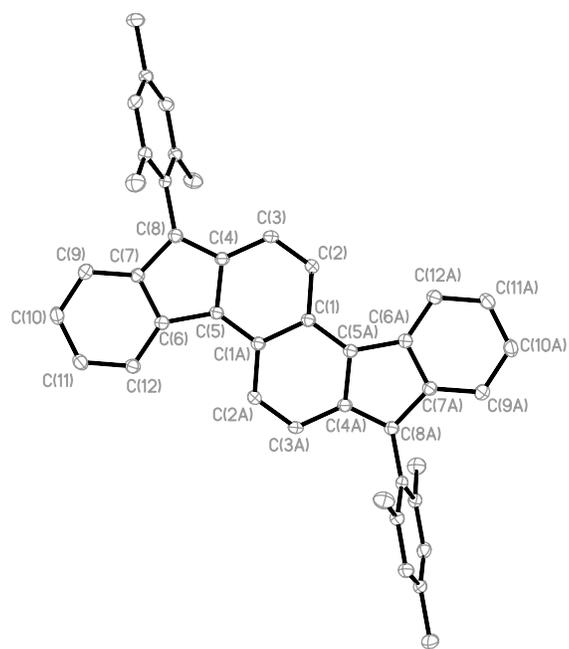


Figure S1. Molecular structure and atom labeling for fluoreno[4,3-*c*]fluorene **8**; ellipsoids at the 50% probability level.

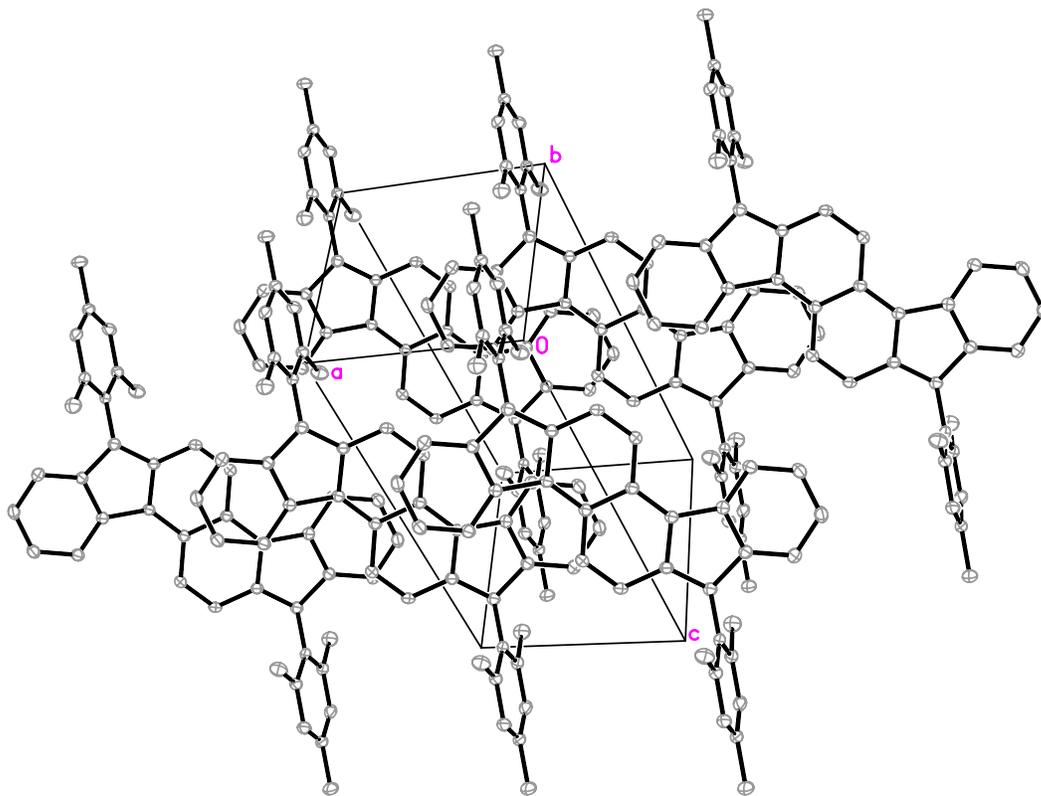


Figure S2. Molecular packing of fluoreno[4,3-*c*]fluorene **8**.

Computational Details

All calculations related were performed using Gaussian 09.⁵ Geometries and TD-DFT calculations were optimized using RB3LYP/6-31++G(d,p) level of theory and the structures were verified as global minima by the absence of imaginary frequencies. All NICS-XY scans were carried out with the Aroma package⁶ with the B3LYP/6-311+G* level of theory following the established procedures as a singlet in either the open or closed shell regime as stated in the plot. Biradical character index values were calculated using an unrestricted long range corrected method with a range separating parameter μ of 0.33 bohr⁻¹ similar to that used by the Nakano group for calculating the biradical character of indenofluorenes.⁷

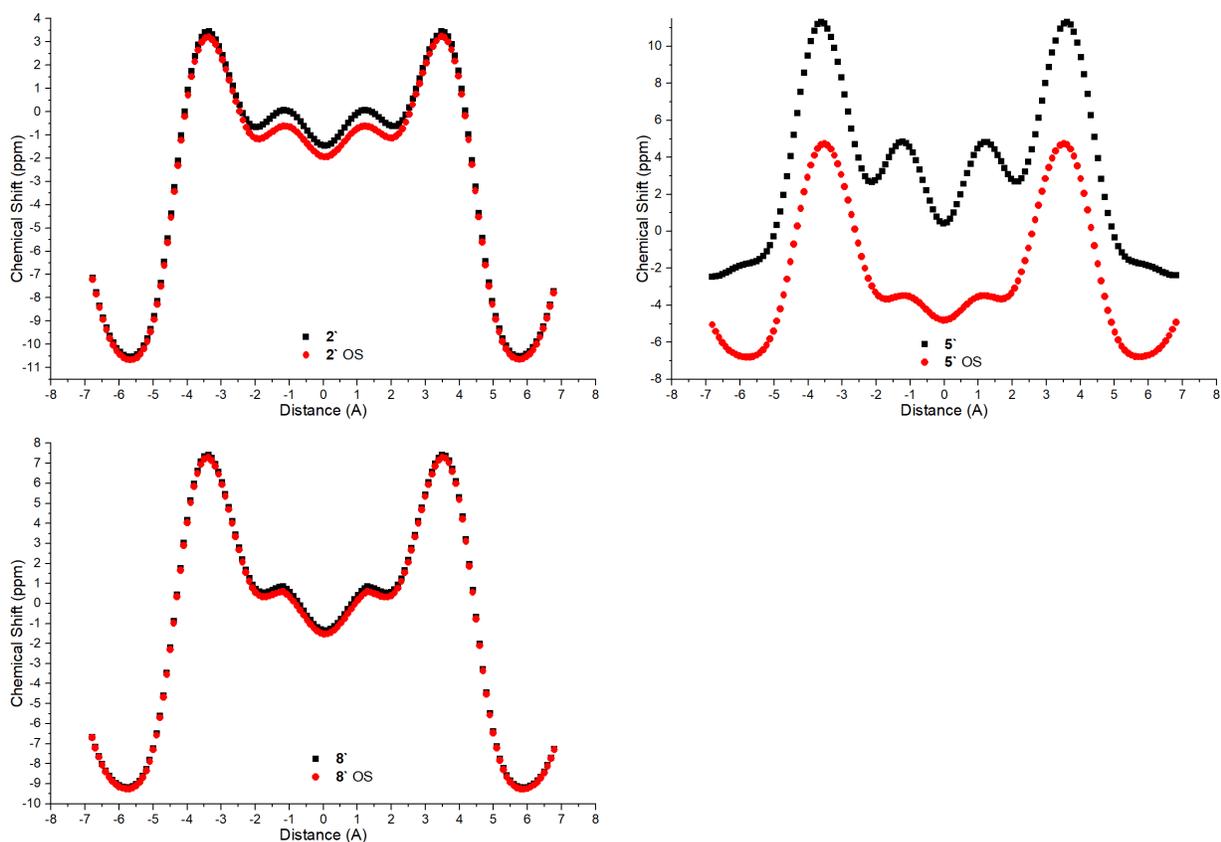


Figure S3. Comparison of the NICS-XY scans of the open and closed shell structures for fluorenofluorene isomers 2', 5', and 8'.

Calculated Geometries

Γ

Zero-point correction=	0.251575 (Hartree/Particle)
Thermal correction to Energy=	0.264910
Thermal correction to Enthalpy=	0.265854
Thermal correction to Gibbs Free Energy=	0.212308
Sum of electronic and zero-point Energies=	-769.141567
Sum of electronic and thermal Energies=	-769.128233
Sum of electronic and thermal Enthalpies=	-769.127288
Sum of electronic and thermal Free Energies=	-769.180834

H	-2.43941	3.46846	0.
H	2.34832	4.94205	0.
H	2.43941	-3.46846	0.
H	-2.34832	-4.94205	0.
H	1.85782	-5.8825	0.
H	-0.50516	-6.61454	0.
H	0.50516	6.61454	0.
H	-1.85782	5.8825	0.
H	2.42643	-0.74692	0.
H	-2.42643	0.74692	0.
C	0.37194	-1.36626	0.
C	1.38063	-0.44883	0.
C	1.03666	0.94686	0.
C	-0.37194	1.36626	0.
C	-1.38063	0.44883	0.
C	-1.03666	-0.94686	0.
C	1.83487	2.07039	0.
C	0.99155	3.25502	0.
C	-0.37194	2.83469	0.
C	0.37194	-2.83469	0.
C	-1.83487	-2.07039	0.
C	-0.99155	-3.25502	0.
C	-1.39683	3.77515	0.
C	1.31193	4.61521	0.
C	1.39683	-3.77515	0.
C	-1.31193	-4.61521	0.
C	1.06593	-5.13921	0.
C	-0.27243	-5.55371	0.
C	0.27243	5.55371	0.
C	-1.06593	5.13921	0.
H	2.91968	2.08058	0.
H	-2.91968	-2.08058	0.

2'

Zero-point correction=	0.297931 (Hartree/Particle)
Thermal correction to Energy=	0.313994
Thermal correction to Enthalpy=	0.314938
Thermal correction to Gibbs Free Energy=	0.254485
Sum of electronic and zero-point Energies=	-922.737573
Sum of electronic and thermal Energies=	-922.721510
Sum of electronic and thermal Enthalpies=	-922.720566
Sum of electronic and thermal Free Energies=	-922.781018

C	-1.7309	-1.86858	0.
C	-2.46988	-0.60267	0.
C	-1.7539	0.62373	0.
C	-0.36975	0.63339	0.
C	0.36976	-0.6334	0.
C	-0.36975	-1.87376	0.
C	0.36976	1.87376	0.
C	1.73091	1.86857	0.
C	2.46989	0.60267	0.
C	1.75391	-0.62373	0.
C	2.72993	2.93887	0.
C	4.01528	2.312	0.
C	3.82893	0.87735	0.
C	-2.72994	-2.93887	0.
C	-4.01528	-2.31199	0.
C	-3.82892	-0.87734	0.
C	-2.62251	-4.32709	0.
C	-3.79325	-5.09751	0.
C	-5.05672	-4.4855	0.
C	-5.17858	-3.0934	0.
C	2.6225	4.32709	0.
C	3.79323	5.09752	0.
C	5.05671	4.48551	0.
C	5.17858	3.09341	0.
H	-2.29666	1.56648	0.
H	0.19296	-2.80484	0.
H	-0.19296	2.80483	0.
H	2.29666	-1.56648	0.
H	4.62811	0.14461	0.
H	-4.6281	-0.14461	0.
H	-1.65073	-4.81359	0.
H	-3.72245	-6.18124	0.
H	-5.95005	-5.10328	0.

H	-6.15983	-2.62657	0.
H	1.65072	4.81358	0.
H	3.72243	6.18124	0.
H	5.95004	5.1033	0.
H	6.15984	2.62659	0.

5'

Zero-point correction=	0.297026 (Hartree/Particle)
Thermal correction to Energy=	0.313139
Thermal correction to Enthalpy=	0.314083
Thermal correction to Gibbs Free Energy=	0.253581
Sum of electronic and zero-point Energies=	-922.724625
Sum of electronic and thermal Energies=	-922.708512
Sum of electronic and thermal Enthalpies=	-922.707567
Sum of electronic and thermal Free Energies=	-922.768070

C	2.43509	-1.26102	0.
C	2.43427	0.19625	0.
C	1.23944	0.89124	0.
C	0.	0.20425	0.
C	-0.00017	-1.24923	0.
C	1.22698	-1.95349	0.
C	-1.23952	0.89145	0.
C	-2.43433	0.19662	0.
C	-2.43534	-1.26073	0.
C	-1.22722	-1.95334	0.
C	-3.81453	0.61	0.
C	-4.6281	-0.58692	0.
C	-3.77839	-1.71837	0.
C	3.77794	-1.71905	0.
C	4.62805	-0.5878	0.
C	3.81456	0.60948	0.
C	-4.42848	1.87175	0.
C	-5.81686	1.94771	0.
C	-6.6189	0.77726	0.
C	-6.04078	-0.47985	0.
C	6.04074	-0.48095	0.
C	6.61915	0.77599	0.
C	5.81734	1.94663	0.
C	4.42898	1.87103	0.
H	1.23019	1.9794	0.

H	1.21179	-3.04155	0.
H	-1.23002	1.97961	0.
H	-1.2122	-3.04139	0.
H	-4.09665	-2.75433	0.
H	4.09576	-2.75515	0.
H	-3.83191	2.77998	0.
H	-6.30091	2.92012	0.
H	-7.70041	0.87631	0.
H	-6.65792	-1.37423	0.
H	6.65766	-1.37548	0.
H	7.70068	0.87477	0.
H	6.30155	2.91896	0.
H	3.83275	2.7795	0.

8`

Zero-point correction=	0.297946 (Hartree/Particle)
Thermal correction to Energy=	0.314284
Thermal correction to Enthalpy=	0.315228
Thermal correction to Gibbs Free Energy=	0.253709
Sum of electronic and zero-point Energies=	-922.727065
Sum of electronic and thermal Energies=	-922.710728
Sum of electronic and thermal Enthalpies=	-922.709783
Sum of electronic and thermal Free Energies=	-922.771303

C	-2.46518	0.74896	0.
C	-1.66871	1.93717	0.
C	-0.21186	1.84626	0.
C	0.41918	0.61128	0.
C	-0.41918	-0.61128	0.
C	-1.85981	-0.46798	0.
C	1.85981	0.46798	0.
C	2.46518	-0.74896	0.
C	1.66871	-1.93717	0.
C	0.21186	-1.84626	0.
C	2.05271	-3.26025	0.
C	0.86689	-4.0911	0.
C	-0.28592	-3.24179	0.
C	-2.05271	3.26025	0.
C	-0.86689	4.0911	0.
C	0.28592	3.24179	0.
C	-0.74292	5.48093	0.

C	0.53696	6.04946	0.
C	1.66871	5.23022	0.
C	1.55093	3.82957	0.
C	0.74292	-5.48093	0.
C	-0.53696	-6.04946	0.
C	-1.66871	-5.23022	0.
C	-1.55093	-3.82957	0.
H	-3.54887	0.82873	0.
H	-2.4685	-1.35977	0.
H	2.4685	1.35977	0.
H	3.54887	-0.82873	0.
H	3.07285	-3.62769	0.
H	-3.07285	3.62769	0.
H	-1.62727	6.11254	0.
H	0.65034	7.12956	0.
H	2.65833	5.67755	0.
H	2.45938	3.2406	0.
H	1.62727	-6.11254	0.
H	-0.65034	-7.12956	0.
H	-2.65833	-5.67755	0.
H	-2.45938	-3.2406	0.

Table S1. TD-DFT calculated transitions for model fluorenofluorenes **2'** and **8'**.

FF 2'			
Excited state 1	HOMO-1 to LUMO	647.41 nm	Oscillator strength f = 0
Excited state 2	HOMO-2 to LUMO	606.55 nm	Oscillator strength f = 0.6830
	HOMO to LUMO		
Excited state 3	HOMO to LUMO+1	466.36 nm	Oscillator strength f = 0.0000
Excited state 4	HOMO to LUMO+3	410.18 nm	Oscillator strength f = 0.0000
	HOMO-2 to LUMO		
Excited state 5	HOMO-3 to LUMO	404.68 nm	Oscillator strength f = 0.0296
FF 8'			
Excited state 1	HOMO-1 to LUMO	765.20 nm	Oscillator strength f = 0
Excited state 2	HOMO-2 to LUMO	631.05 nm	Oscillator strength f = 0.3892
	HOMO to LUMO		
	HOMO-1 to LUMO+1		
Excited state 3	HOMO-2 to LUMO	486.65 nm	Oscillator strength f = 0.2611
	HOMO to LUMO		
	HOMO-1 to LUMO+1		

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