Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Theoretical investigation of the broad one-photon absorption line-shape of a flexible symmetric carbazole derivative

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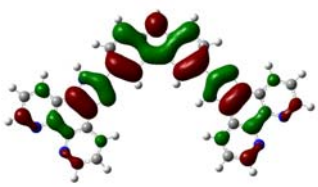
* Corresponding authors: fabrizio.santoro@iccom.cnr.it, linnakth@gmail.com, xianzhao@sdu.edu.cn

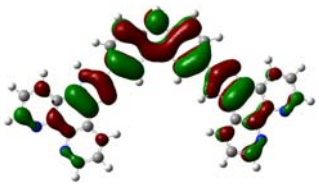


HOMO_ R=H (Cs)

LUMO+2_ R=H (Cs)

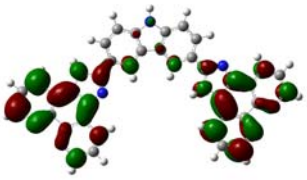
LUMO+3_ R=H (Cs)

LUMO+4_ R=H (Cs)

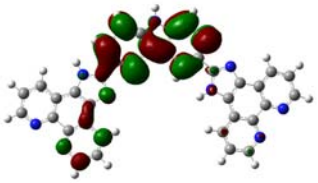


HOMO_ R=H (C1)

LUMO+2_ R=H (C1)



LUMO+3_ R=H (C1)



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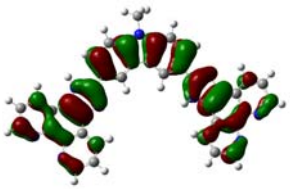
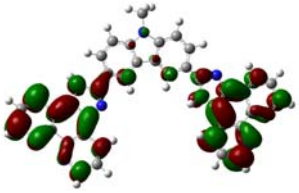
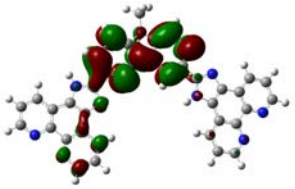


HOMO-1_ R=CH_3

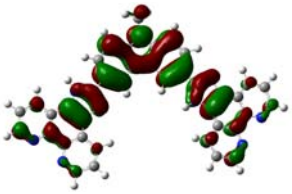
LUMO+2_ R= CH_3



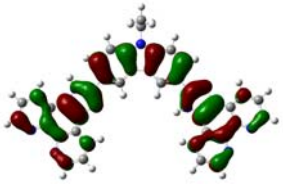
LUMO+3_ R= CH_3



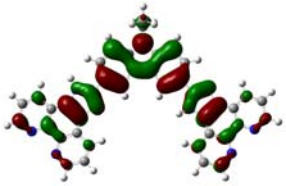
LUMO+4_ R= CH_3



HOMO_ R=CH_3

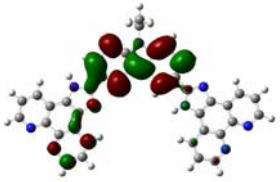


HOMO-1_ R= C_2H_5



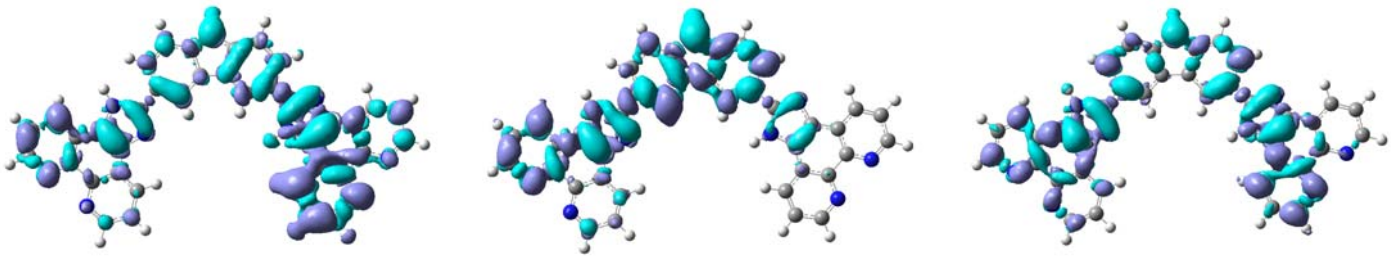
HOMO_ R= C_2H_5

LUMO+2_ R= C_2H_5

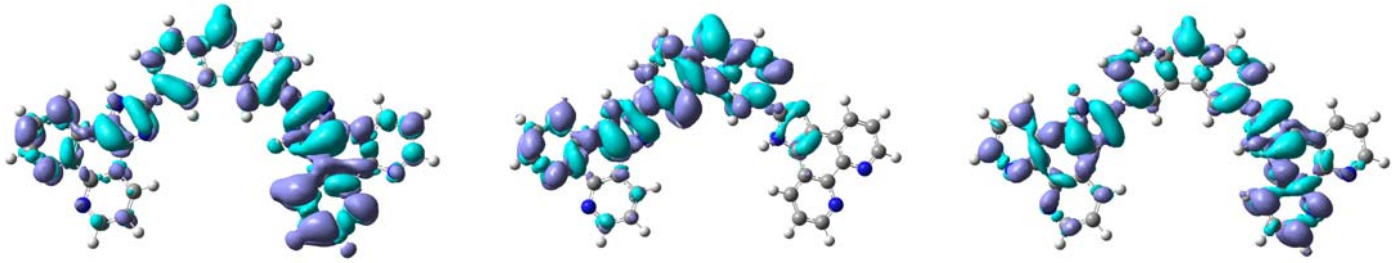


LUMO+4_ R= C_2H_5

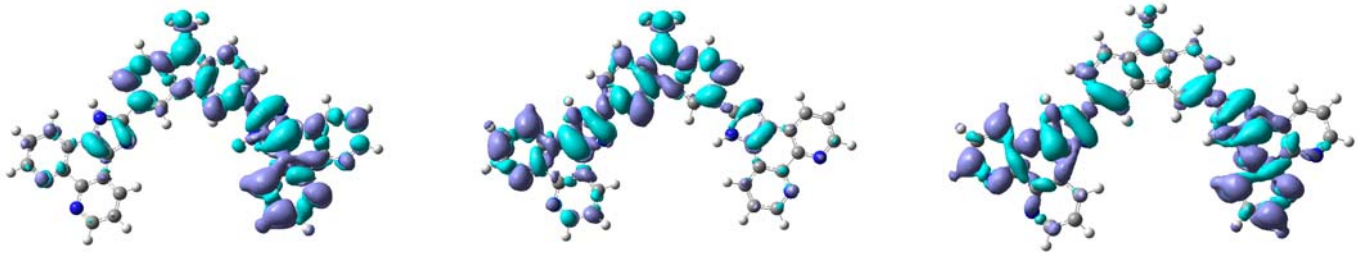
Fig. S1 *R-POCP. T*he corresponding molecular orbitals of derivatives with R changing from H to C_2H_5



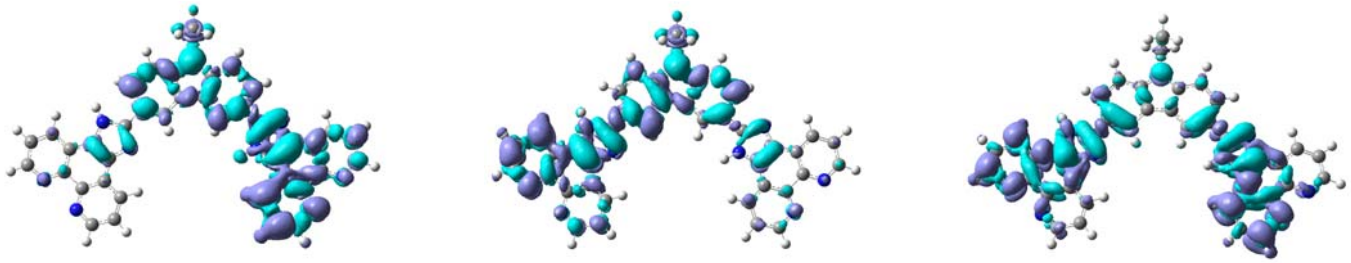
Cube_S_3_ R=H (Cs) | Cube_S_4_ R=H (Cs) | Cube_ S_5_ R=H (Cs)



Cube _S_3_ R=H (C_1) | Cube _S_4_ R=H (C_1) | Cube_ S_5_ R=H (C_1)



Cube _S_3_ R=CH_3 | Cube _S_4_ R=CH_3 | Cube_S_5_ R=CH_3



Cube _S_3_ R= C_2H_5 | Cube _S_4_ R= C_2H_5 | Cube_ S_5_ R= C_2H_5

Fig. S2 *R-POCP. Difference between the electronic densities of S_3-S_5 and ground state of R=H, CH_3 and* C_2H_5

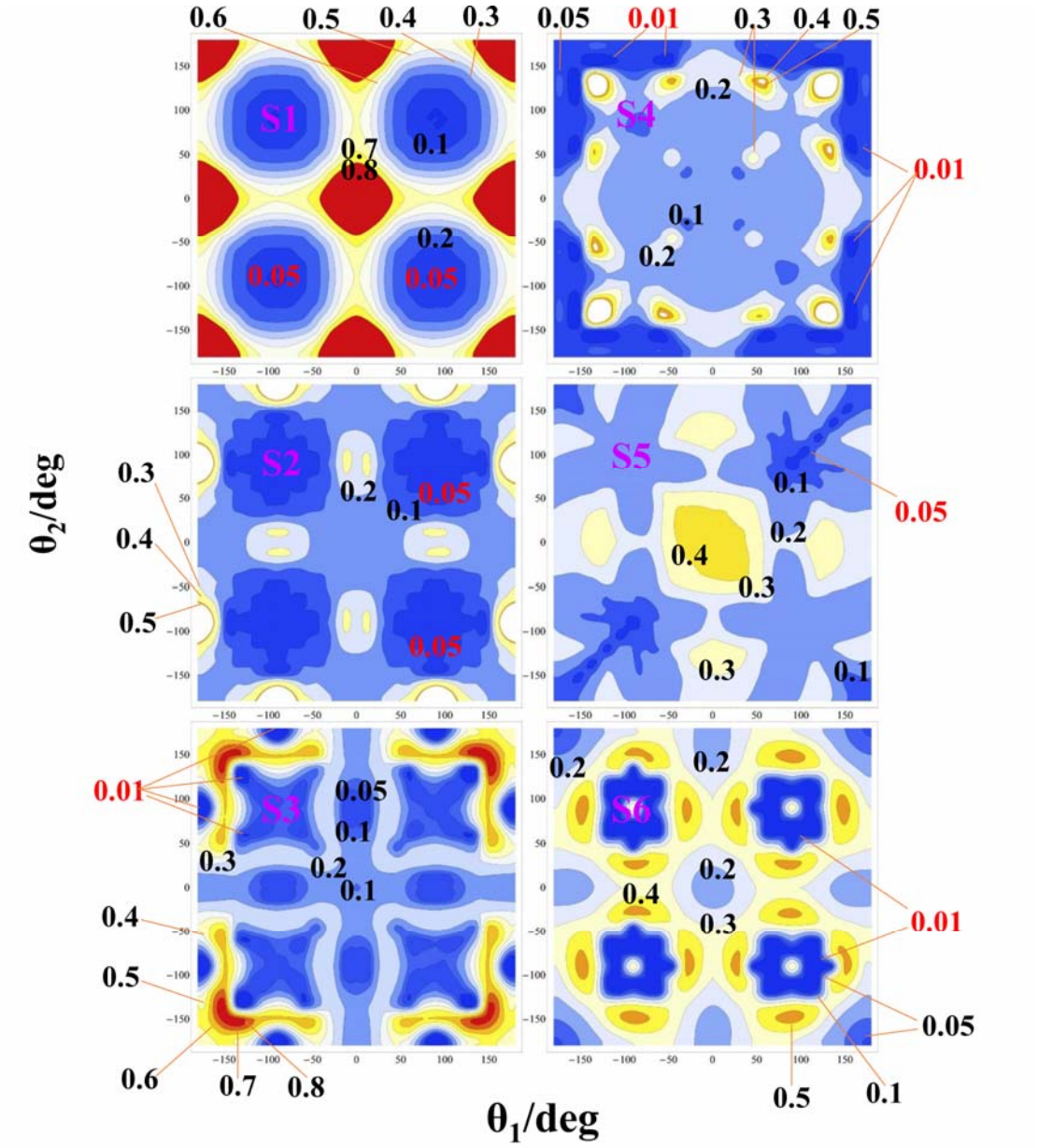


Fig. S3 *H-POCP. ES relaxed scan as a function of the dihedral angles θ_1 and θ_2, the oscillator strengths of the minima structure of each excited states are highlighted in red*

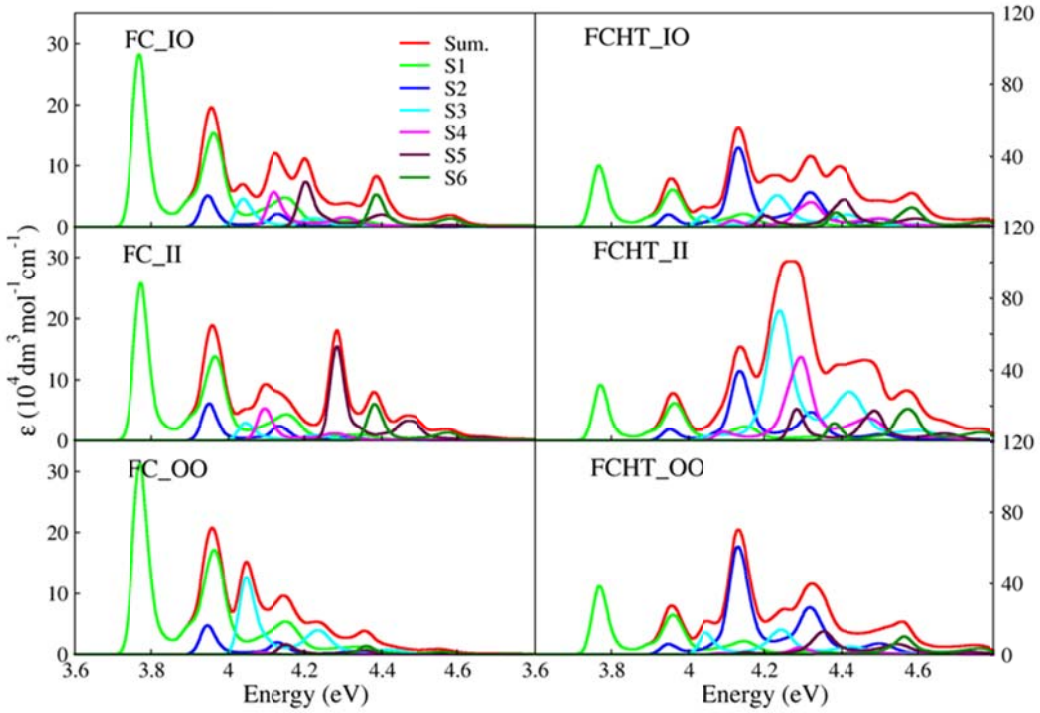


Fig. S4 *H-POCP. Vibronic spectra computed with the TD approach at 0K for the first six excited electronic states of H-POCP excited states considering only the 196 fast* ***r*** *coordinates. Spectra convoluted with a Gaussian with HWHM=0.02eV.*

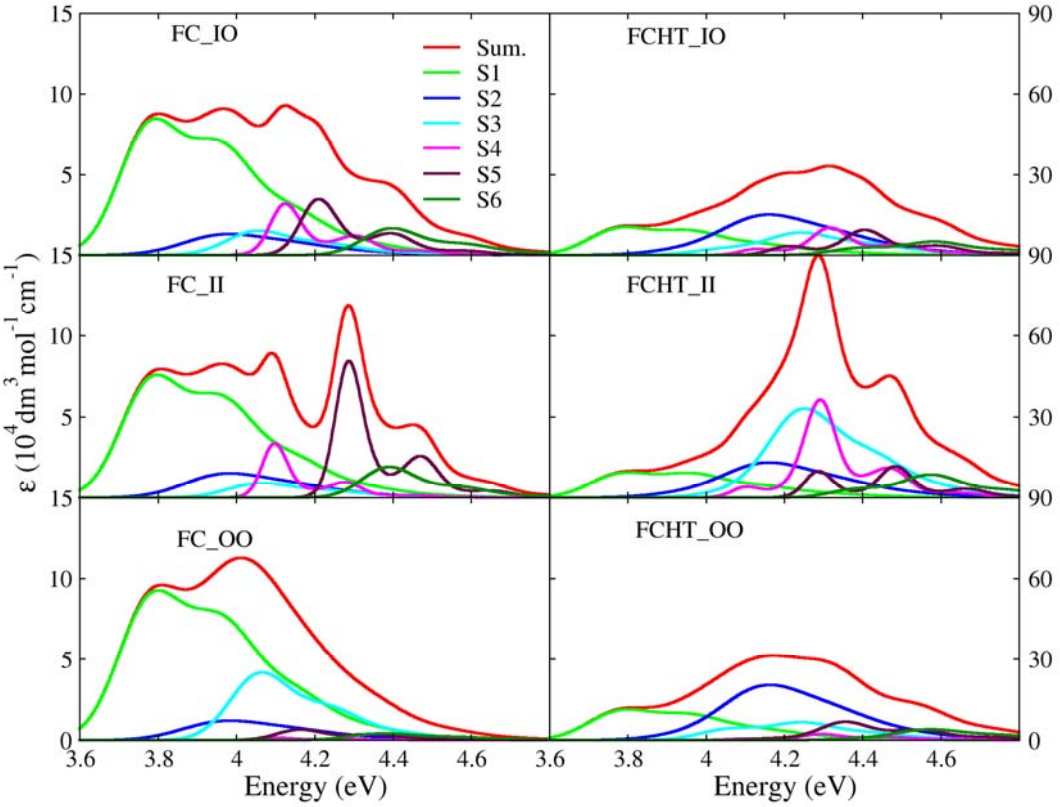


Fig. S5 *H-POCP. Vibronic spectra computed with the TD approach at 300K for the first six excited electronic states of H-POCP excited states considering only the 196 fast* ***r*** *coordinates. Spectra convoluted with a Gaussian representing the solvent inhomogeneous broadening specific for each state of each conformer and reported in Table 2*

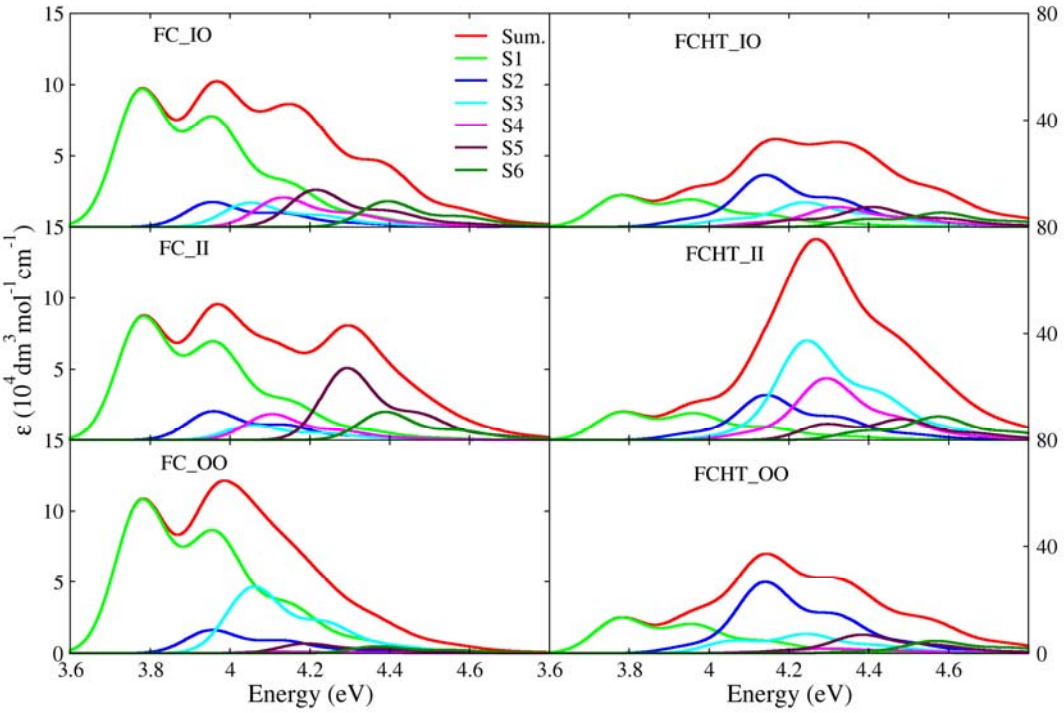


Fig. S6 *H-POCP. Vibronic spectra computed with the TD approach at 300K for the first six excited electronic states of H-POCP excited states considering only the 196 fast* ***r*** *coordinates. Spectra convoluted with a Gaussian averaged solvent inhomogeneous broadening with HWHM of 0.07eV*

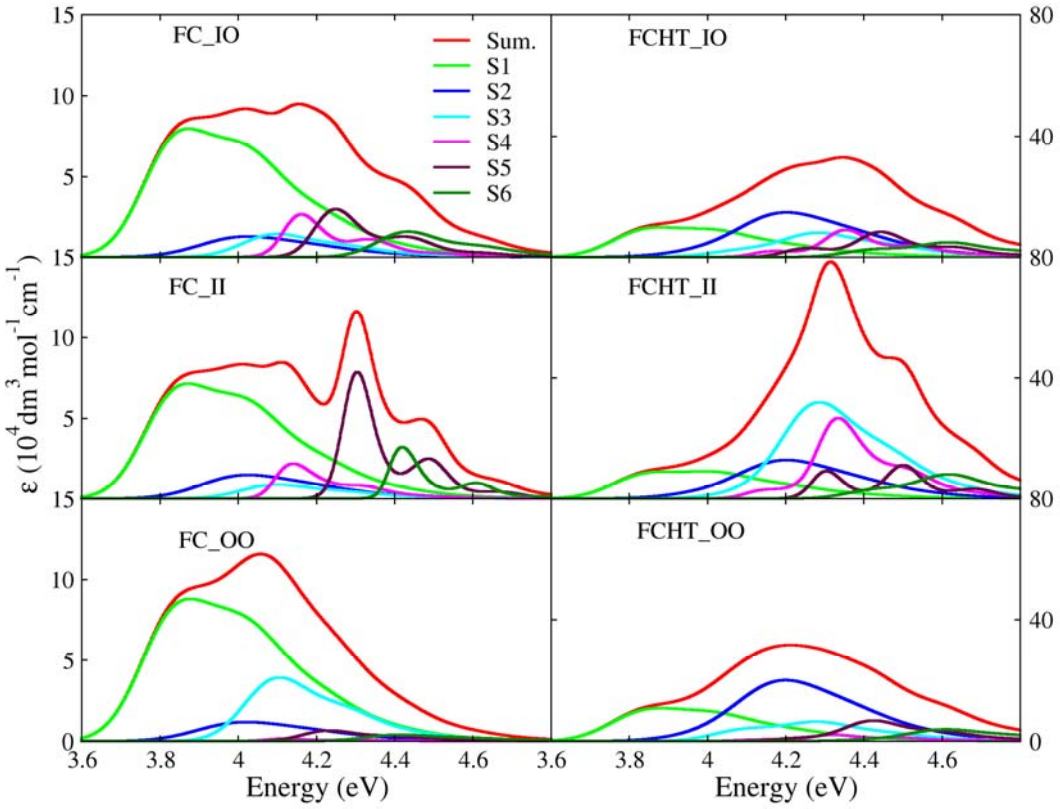


Fig. S7 *H-POCP. FC and FCHT spectra obtained convoluting 196*FC/FCHT* spectra with torsional broadening of six excited states of three conformers of H-POCP, calculated at 300K. Spectra convoluted with a Gaussian representing the solvent inhomogeneous broadening specific for each state of each conformer and reported in Table 2*

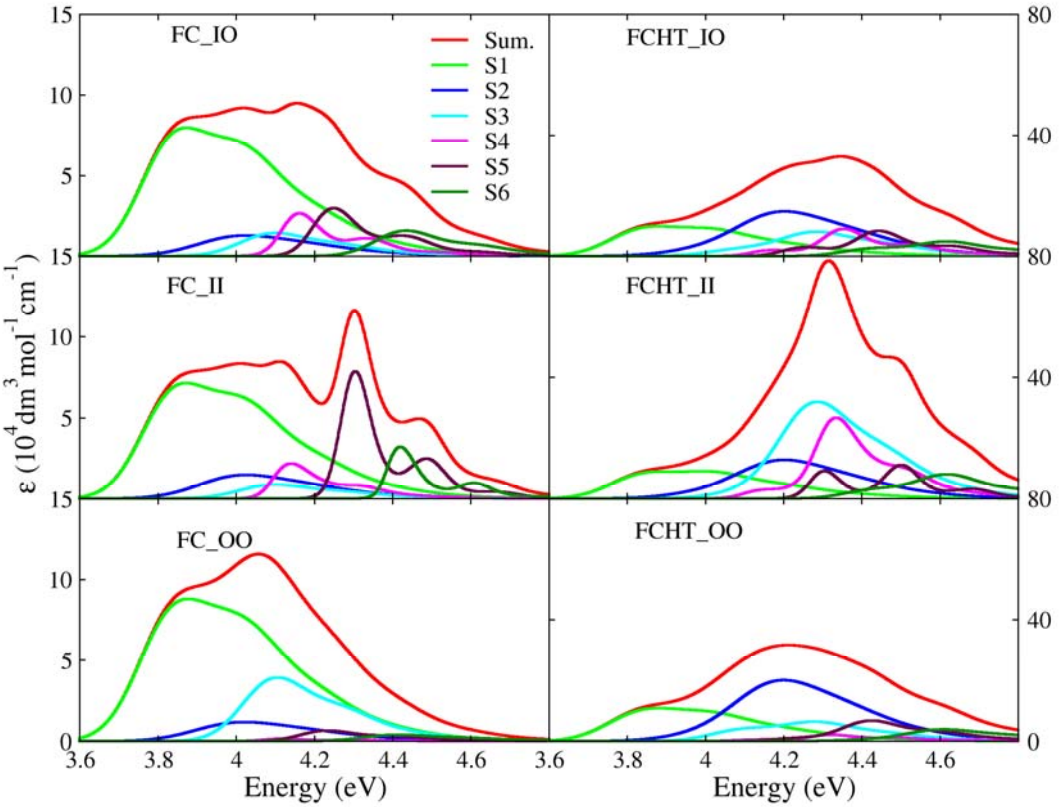


Fig. S8 *H-POCP. FC and FCHT spectra obtained convoluting 196*FC/FCHT* spectra with torsional broadening of S_1-S_6 of three conformers of H-POCP at 300K, convoluted with an averaged solvent broadening with HWHM of 0.07eV*

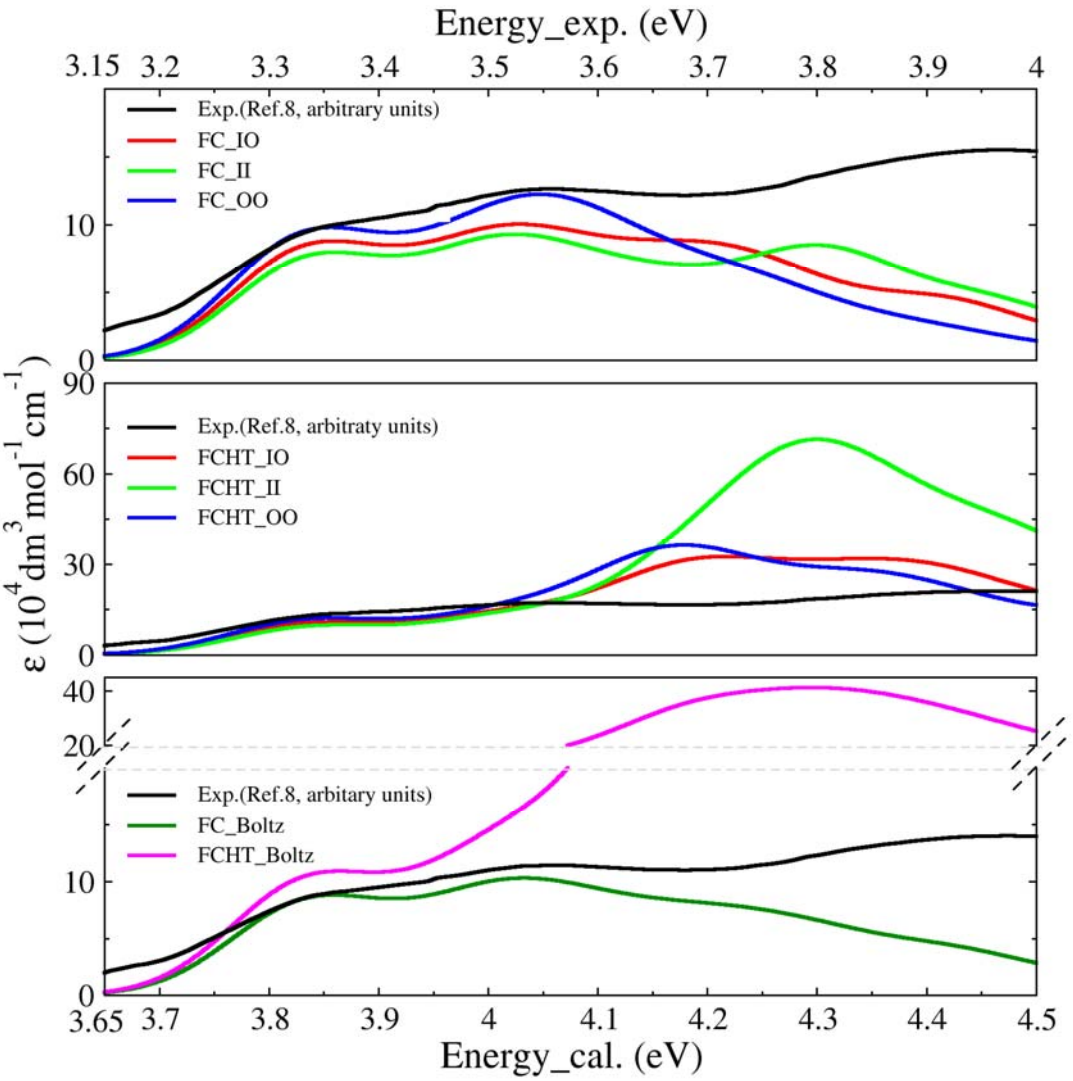


Fig. S9 *H-POCP. Comparison of the experimental spectrum of POCP with the total FC and FCHT spectra computed for H-POCP by convoluting the histograms of the torsional broadening with the vibronic spectra at 300K, convoluted with an averaged solvent broadening with HWHM of 0.07eV*

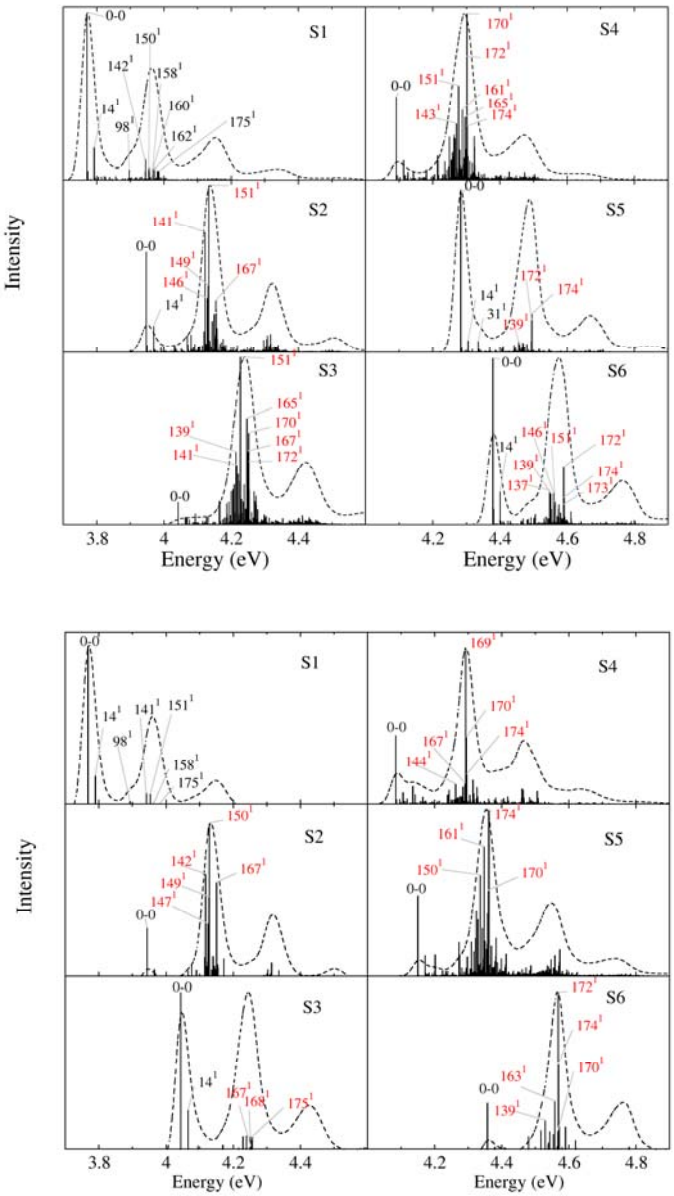
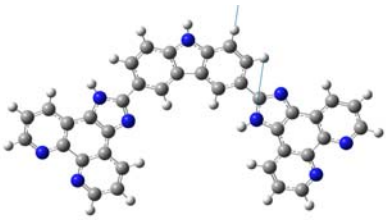
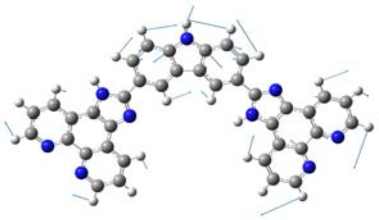
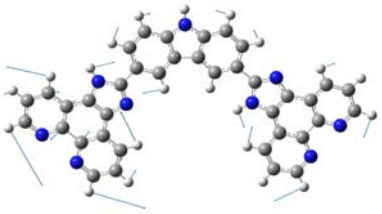
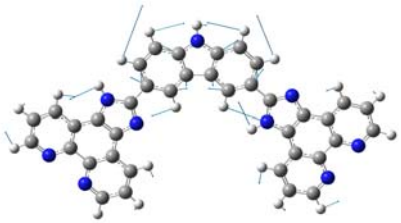
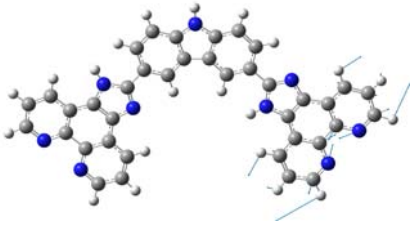
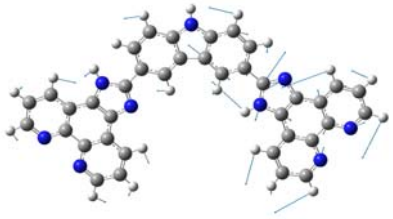
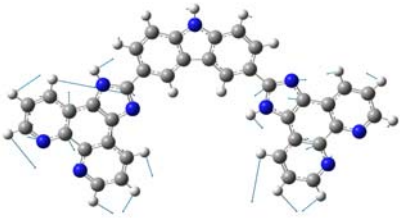
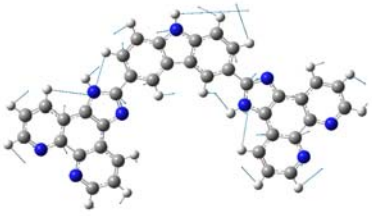
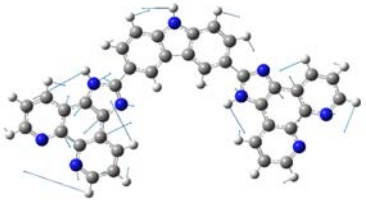
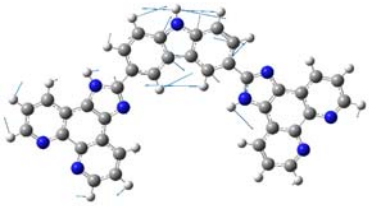
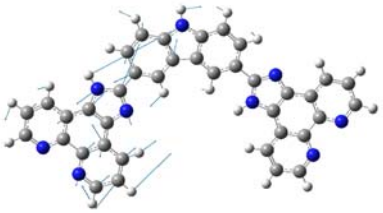
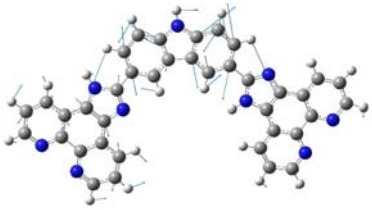
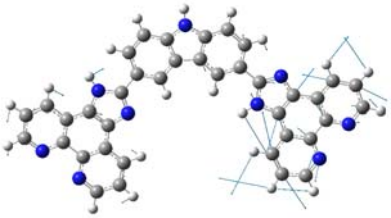
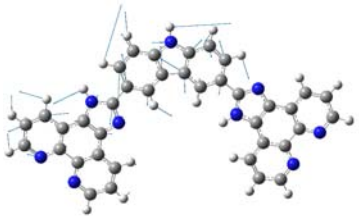
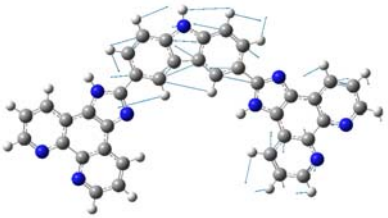
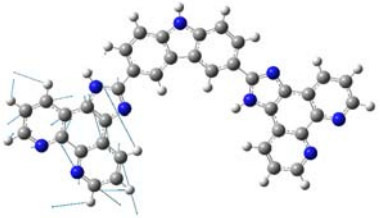
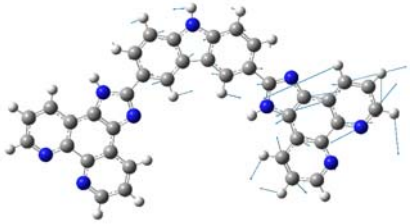


Fig. S10 *H-POCP. Assignments of the main stick bands of the FCHT spectra of the S_1-S_6 excited electronic states of conformers II (top) and OO (bottom). Vibrational contributions are labelled as "n^x", where x indicates the quanta deposited on the excited-state normal mode n. Modes contributing most to HT are highlighted in red. Spectra are convoluted with a Gaussian spectral shape function with a HWHM of 0.02 eV. The convergence of the TI calculations for all the conformers, measured as the percentage of the recovered total intensity is always above 99 % for FC spectra and above 97.9% for FC+HT spectra*

 mode 14 (142.23 cm^{-1})	 mode 98 (1000.61 cm^{-1})	 mode 137 (1352.39 cm^{-1})
 mode 138 (1354.38 cm^{-1})	 mode 140 (1380.5 cm^{-1})	 mode 141 (1389.80 cm^{-1})
 mode 146 (1450.25 cm^{-1})	 mode 148 (1459.57 cm^{-1})	 mode 149 (1461.82 cm^{-1})
 mode 151 (1538.02 cm^{-1})	 mode 158 (1538.02 cm^{-1})	 mode 164 (1617.33 cm^{-1})
 mode 168 (1662.10 cm^{-1})	 mode 170 (1671.31 cm^{-1})	 mode 171 (1678.30 cm^{-1})
 mode 172 (1696.00 cm^{-1})	 mode 173 (1699.54 cm^{-1})	 mode 174 (1699.54 cm^{-1})

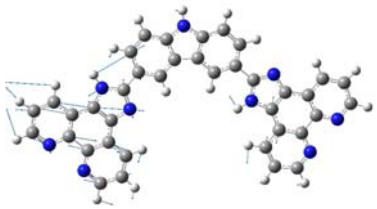
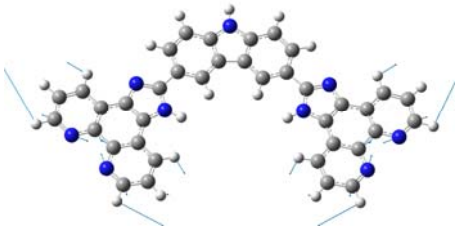
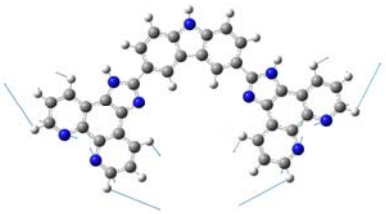
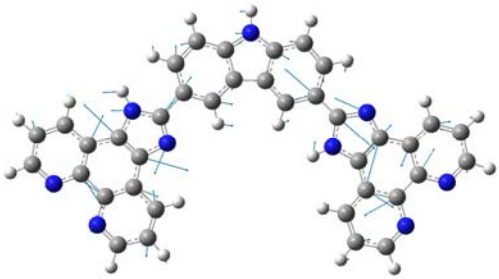
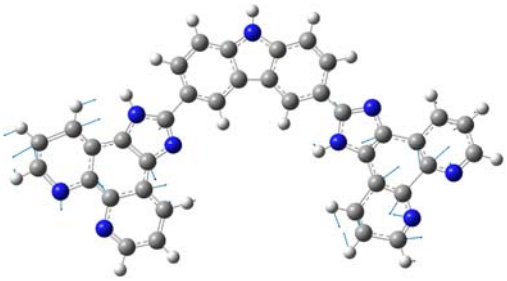
		
mode 175 (1706.23 cm^{-1})	mode 142 (II, 1389.62cm^{-1})	mode 142 (OO, 1389.44cm^{-1})

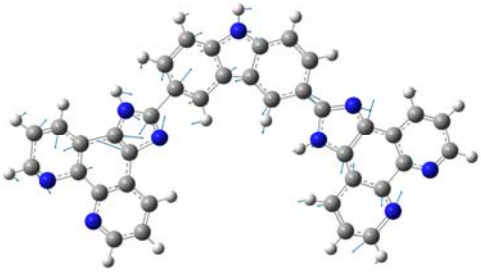
Fig. S11 *H-POCP. Selected vibrational modes in Figure11, calculated for the ground electronic state at the CAMB3LYP/PCM/6-31G(d,p) level in DMF of IO conformer, frequencies are reported in parenthesis*



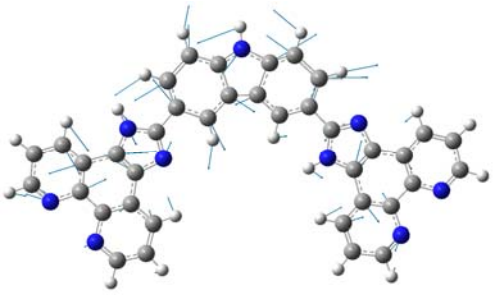
mode 1 (IO_S_1, 1846i)



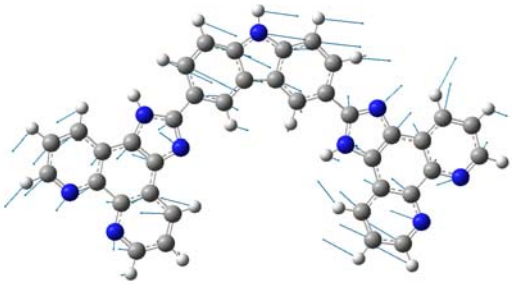
mode 1 (IO_S_2, 1051i)



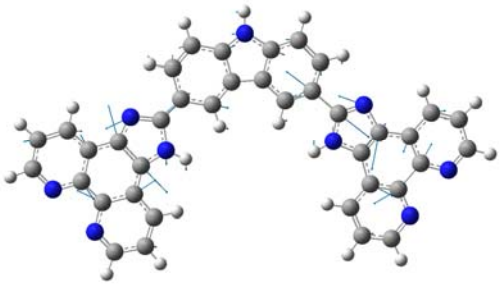
mode 1 (IO_S_3, 1119i)



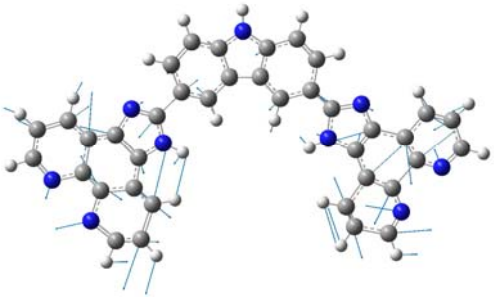
mode 1 (IO_S_4, 671i)



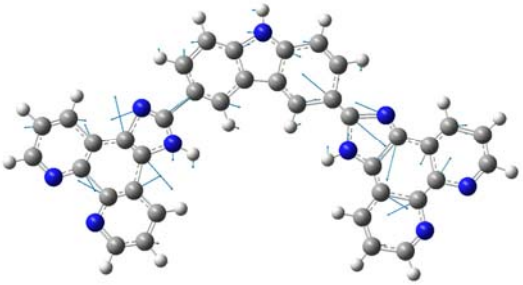
mode 1 (IO_S_6, 48i)



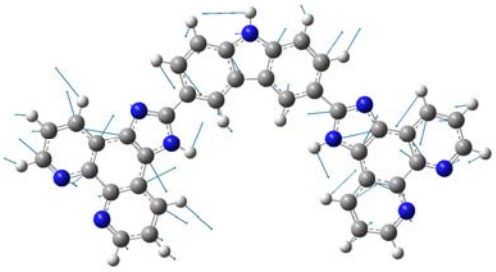
mode 1 (II_S_1, 1985i)



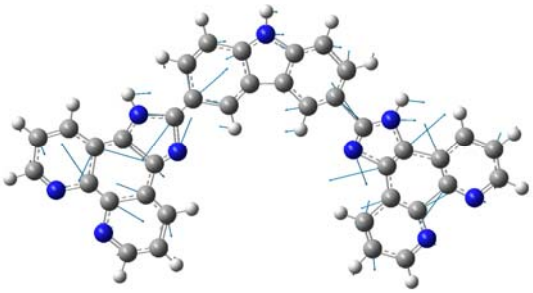
mode 1 (II_S_2, 941i)



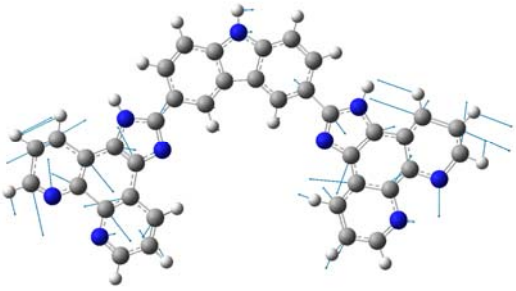
mode 1 (II_S_3, 3513i)



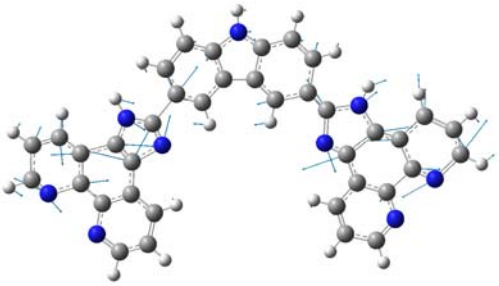
mode 1 (II_S_5, 454i)



mode 1 (OO_S_1, 1840i)



mode 1 (OO_S_2, 960i)



mode 1 (OO_S_3, 1260i)

Fig. S12 *H-POCP. Selected vibrational modes highlighted in Table 3, calculated for the excited state at the ground state geometry at the CAMB3LYP/PCM/6-31G(d,p) level in DMF, frequencies are reported in parenthesis*

Table S1: *R-POCP. N3-C5-C6-C7 (θ_1, degree) and N4-C8-C9-C10 (θ_2, degree) dihedral angles (See labels in Figure 1), oscillator strengths ($\delta_{OPA,}$ au), as well as transition energies (reported in parenthesis,eV) for the first ten excited states of carbazole analogues with R varying from H to C_8H_{17}, optimized at CAM-B3LYP/6-31G (d,p), in DMF.*

R	θ_1	θ_2	S_1	S_2	S_3	S_4	S_5	S_6	S_7	S_8	S_9	S_{10}
H_Cs	-180	0	1.24 (3.92)	0.17 (4.05)	0.16 (4.13)	0.19 (4.21)	0.23 (4.29)	0.15 (4.47)	0.57 (4.64)	0.00 (4.65)	0.00 (4.65)	0.62 (4.69)
H_C_1	-167.3	166.9	1.16 (3.95)	0.15 (4.06)	0.19 (4.15)	0.19 (4.22)	0.23 (4.30)	0.18 (4.48)	0.59 (4.65)	0.00 (4.65)	0.00 (4.65)	0.64 (4.72)
CH_3	-167.3	167.0	1.23 (3.92)	0.16 (4.05)	0.04 (4.12)	0.22 (4.17)	0.33 (4.28)	0.11 (4.46)	0.67 (4.64)	0.00 (4.65)	0.00 (4.65)	0.68 (4.69)
C_2H_5	-167.9	168.4	1.24 (3.91)	0.17 (4.05)	0.03 (4.11)	0.22 (4.16)	0.35 (4.28)	0.11 (4.46)	0.66 (4.63)	0.00 (4.65)	0.00 (4.65)	0.7 (4.69)
$C_2H_{5\_planar}$ [a]	180	180	1.29 (3.89)	0.19 (4.04)	0.02 (4.10)	0.19 (4.15)	0.36 (4.27)	0.10 (4.45)	0.08 (4.62)	0.00 (4.65)	0.00 (4.65)	0.68 (4.67)
C_3H_7	-169.3	169.8	1.25 (3.91)	0.18 (4.05)	0.02 (4.11)	0.22 (4.16)	0.36 (4.27)	0.1 (4.45)	0.66 (4.62)	0.00 (4.65)	0.00 (4.65)	0.71 (4.68)
C_4H_9	-171.4	172.0	1.27 (3.90)	0.18 (4.04)	0.02 (4.11)	0.21 (4.16)	0.36 (4.27)	0.1 (4.45)	0.65 (4.62)	0.00 (4.65)	0.00 (4.65)	0.71 (4.67)
C_5H_{11}	-172.5	173.5	1.27 (3.90)	0.19 (4.04)	0.02 (4.10)	0.20 (4.15)	0.37 (4.27)	0.1 (4.45)	0.65 (4.62)	0.00 (4.65)	0.00 (4.65)	0.71 (4.67)
C_6H_{13}	-166.2	-177.63	1.25 (3.90)	0.18 (4.05)	0.02 (4.11)	0.22 (4.16)	0.39 (4.27)	0.09 (4.45)	0.67 (4.63)	0.00 (4.65)	0.00 (4.65)	0.72 (4.68)
C_7H_{15}	-166.6	-176.3	1.25 (3.90)	0.18 (4.05)	0.02 (4.11)	0.22 (4.16)	0.39 (4.27)	0.09 (4.45)	0.67 (4.62)	0.00 (4.65)	0.00 (4.65)	0.73 (4.68)
C_8H_{17}	-164.3	-174.8	1.24 (3.91)	0.18 (4.05)	0.02 (4.11)	0.23 (4.16)	0.39 (4.28)	0.09 (4.45)	0.68 (4.63)	0.00 (4.65)	0.00 (4.65)	0.73 (4.68)
$C_8H_{17\_inter}$ [b]	-162.3	-161.7	1.16 (3.95)	0.16 (4.06)	0.03 (4.12)	0.27 (4.18)	0.35 (4.29)	0.11 (4.47)	0.68 (4.64)	0.00 (4.65)	0.00 (4.65)	0.75 (4.71)

a: *is a planar Transition State of C_2H_5 with a planar geometry*

b:*is optimized with a conformation whose tail of the octane interacts with the pi rings*

Table S2: *R-POCP. Transition natures of the redistributed state S_3-S_5 with R changing from H to C_2H_5, the corresponding transition Coefficient and energies (in eV) reported in parenthesis*

States	R=H (IO, Cs)	R=H (C_1)	R=CH_3	R=C_2H_5
S_3	H^{a}→L^{b}+2 (0.47,4.13 eV)	H→L+2 (0.47, 4.15 eV)	H→L+2(0.40, 4.12 eV)	H→L+2 (0.38, 4.11 eV) H→L+4 (0.31, 4.11 eV)
S_4	H→L+4(0.43,4.21 eV)	H→L+4(0.45, 4.22 eV)	H→L+4(0.46, 4.17 eV)	H→L+4 (0.44, 4.16 eV)
S_5	H→L+3 (0.35,4.30 eV) H→L+4(0.34, 4.30 eV)	H→L+3 (0.36, 4.30 eV) H→L+4 (0.34, 4.30 eV)	H-1→L+2 (-0.36, 4.28 eV) H→L+3 (0.42, 4.28 eV)	H-1→L+2 (0.37, 4.28 eV) H→L+4 (0.42, 4.28 eV)

a*: the highest occupied molecular orbital (HOMO);*

b*: the lowest unoccupied molecular orbital (LUMO)*

Table S3: *Et-POCP. Excitation energies E_{gf} (eV), oscillator strengths δ_{OPA} (au) for one-photon absorption, and dominating transition nature for the first 10 lowest excited states of Et-POCP in DMF obtained at CAMB3LYP/6-31G(d,p) level at the geometry optimized at CAMB3LYP/6-31G(d,p) level*

State	E_{gf}	δ_{OPA}	Transition	Coefficient
S_1	3.91	1.24	H→L	0.50
S_2	4.05	0.17	H-1→L	0.41
			H→L+1	0.44
S_3	4.11	0.03	H-1→L+2	0.31
			H→L+4	0.38
S_4	4.16	0.22	H→L+4	0.44
S_5	4.28	0.35	H-1→+2	-0.37
			H→L+3	0.42
S_6	4.46	0.11	H-1→L+3	0.31
			H→L+5	0.43
S_7	4.63	0.66	H-1→L+4	0.48
S_8	4.65	0.00	H-1→L+5	0.42
			H→L+6	-0.35
S_9	4.65	0.00	H-7→L	0.38
			H-7→L+1	0.45
S_{10}	4.69	0.70	H-→L+5	0.38
			H→L+6	0.44

Table S4: *H-POCP. Excitation energies E_{gf} (eV) with the symmetric reported in parenthesis, oscillator strength δ_{OPA} (au) and square of transition dipole moments (μ^2) of the first ten excited states, obtained at CAM-B3LYP/6-31G(d,p) level in DMF for the three conformers of H-POCP*

Ev	II	IO	OO
S_1	3.93 (B2)	3.92 (A')	3.92 (B2)
S_2	4.05 (A1)	4.05 (A')	4.05 (A1)
S_3	4.14 (B2)	4.13 (A')	4.14 (B2)
S_4	4.17 (A1)	4.21 (A')	4.20(A1)
S_5	4.36 (A1)	4.29 (A')	4.27 (A1)
S_6	4.45 (B2)	4.47 (A')	4.45 (B2)
S_7	4.62 (B2)	4.64 (A')	4.65 (A2)
S_8	4.65 (A2)	4.65 (A')	4.65 (B1)
S_9	4.65 (B1)	4.65 (A')	4.68 (B2)
S_{10}	4.69 (A1)	4.69 (A')	4.69 (A1)
δ_{OPA}	II	IO	OO
S_1	1.11	1.24	1.38
S_2	0.20	0.17	0.16
S_3	0.098	0.16	0.43
S_4	0.15	0.19	0.013
S_5	0.42	0.23	0.062
S_6	0.16	0.16	0.045
S_7	0.72	0.57	0
S_8	0	0	0
S_9	0	0	0.48
S_{10}	0.62	0.62	0.62
μ^2	II	IO	OO
S_1	11.51	12.91	14.39
S_2	1.96	1.72	1.60
S_3	0.97	1.55	4.23
S_4	1.48	1.81	0.13
S_5	3.89	2.21	0.60
S_6	1.48	1.42	0.41
S_7	6.37	5.03	0
S_8	0	0	0
S_9	0	0	4.22
S_{10}	5.45	5.39	5.37

Table S5: *H-POCP. Vertical and adiabatic excitation energies E (hartree), solvent reorganization energy λ (eV), as well as oscillator strength δ_{OPA} (au) for the first six excited states, computed with the state-specific (SS) implementation of PCM at CAM-B3LYP/6-31G(d,p) level in DMF for three carbazole analogue IO, II, OO*

States	ES (neq)	ES (eq)	λ (eV)	δ_{OPA} (neq)	δ_{OPA} (eq)
		IO			
S_1	-1952.46908693	-1952.48350591	0.3924	0.9009	0.3146
S_2	-1952.46832654	-1952.48351043	0.4132	0.0849	0.3145
S_3	-1952.46142711	-1952.46492751	0.0953	0.2648	0.3745
S_4	-1952.45625271	-1952.45695783	0.0192	0.1494	0.1382
S_5	-1952.45437828	-1952.45552028	0.0311	0.1432	0.1106
S_6	-1952.45187698	-1952.45496845	0.0841	0.1302	0.1705
		II			
S_1	-1952.46880593	-1952.47271717	0.1064	0.8406	0.6872
S_2	-1952.46809242	-1952.47428660	0.1686	0.0731	0.0559
S_3	-1952.46121259	-1952.46505528	0.1046	0.1939	0.2362
S_4	-1952.45688896	-1952.45735588	0.0127	0.0891	0.094
S_5	-1952.45179985	-1952.45251043	0.0193	0.2492	0.2289
S_6	-1952.45132097	-1952.45415209	0.0770	0.1346	0.2215
		OO			
S_1	-1952.46880593	-1952.47271717	0.1064	0.9524	0.7270
S_2	-1952.46809242	-1952.47428660	0.1686	0.0891	0.0863
S_3	-1952.46121259	-1952.46505528	0.1046	0.5509	0.6844
S_4	-1952.45688896	-1952.45735588	0.0127	0.0103	0.0164
S_5	-1952.45179985	-1952.45251043	0.0193	0.0423	0.0345
S_6	-1952.45132097	-1952.45415209	0.0770	0.0689	0.0857

Table S6: *H-POCP. Transition dipole derivatives (for transitions $S_0 \rightarrow S_k$, k=1-6, in atomic units) along the normal modes that result in a large HT contribution to the spectrum intensity. The frequency associated to the normal mode is given in parenthesis. The modes correspond to the diagonalization of the final state (from VH calculations).*

k (freq, cm^{-1})	$(\frac{\partial \mu_x^{if}}{\partial Q_k})$	$(\frac{\partial \mu_y^{if}}{\partial Q_k})$	$(\frac{\partial \mu_z^{if}}{\partial Q_k})$	Module
		IO_$S_0 \rightarrow S_1$		
1 (1846i)	1.2361	-0.9781	0.0000	1.5763
		IO_$S_0 \rightarrow S_2$		
1 (1051i)	-1.9556	-2.0237	0.0000	2.8142
175 (2435)	-1.6903	-2.0294	0.0000	2.6411
		IO_$S_0 \rightarrow S_3$		
1 (1119i)	0.3867	-2.2515	0.0000	2.2844
175 (2507)	1.0456	-0.3812	0.0000	1.1130
174 (1943)	-0.3147	-0.9521	0.0000	1.0027
		IO_$S_0 \rightarrow S_4$		
1(671i)	-1.8511	1.0042	0.0000	2.1059
175 (2196)	-1.3048	-0.3255	0.0000	1.3448
		IO_$S_0 \rightarrow S_5$		
174 (2154)	-0.6653	-1.1123	0.0000	1.2960
175 (2383)	-0.0352	0.8184	0.0000	0.8192
91 (941)	-0.0687	-0.6537	0.0000	0.6573
28 (366)	-0.0230	-0.6307	0.0000	0.6311
76 (812)	0.0263	0.6275	0.0003	0.6280
		IO_$S_0 \rightarrow S_6$		
1 (48i)	3.1751	-1.0153	-0.0001	3.3335
28 (352)	1.2542	-0.3209	0.0000	1.2947
46 (513)	0.8336	-0.2616	0.0000	0.8737
175 (2067)	-0.7453	0.4473	0.0000	0.8692
5 (49)	-0.7622	0.2610	0.0000	0.8057
20 (238)	-0.6101	0.1922	0.0000	0.6396
12 (103)	0.6002	-0.1668	0.0000	0.6229
39 (454)	0.4853	-0.1947	0.0000	0.5229
		II_$S_0 \rightarrow S_1$		
1 (1985i)	0.0000	0.0000	1.7589	1.7589
		II_$S_0 \rightarrow S_2$		
175 (2594)	0.0000	-2.4845	0.0000	2.4845
1 (941i)	0.0000	-2.1305	0.0000	2.1305
		II_$S_0 \rightarrow S_3$		
1 (3513i)	0.0000	0.0000	-3.5275	3.5275
174 (2023)	0.0000	1.1031	0.0000	1.1031
175 (2356)	0.0000	0.0000	- 1.0653	1.0653

		II_S_0→S_4		
196 (4145)	0.0000	2.3829		2.3829
28 (358)	0.0000	0.0000	- 1.0774	1.0774
46 (506)	0.0001	0.0000	- 0.9222	0.9222
21(241)	0.0000	0.0000	- 0.8346	0.8346
51 (575)	0.0001	0.0000	0.7785	0.7785
74 (776)	0.0001	0.0000	0.5476	0.5476
		II_S_0→S_5		
1 (454i)	0.0000	-2.4557	0.0000	2.4557
174 (1900)	0.0000	-0.9572	0.0000	0.9572
47(532)	0.0000	-0.9144	0.0000	0.9144
69 (746)	0.0000	-0.6605	0.0000	0.6605
		II_S_0→S_6		
24 (294)	0.0000	1.7346	0.0000	1.7346
175 (2227)	0.0000	-1.3373	0.0000	1.3373
21 (243)	- 0.9630	0.0000	0.0001	0.9630
51 (563)	- 0.8931	0.0000	0.0001	0.8931
47 (523)	- 0.8248	0.0000	0.0000	0.8248
54 (580)	0.0000	-0.0002	- 0.7990	0.7990
23 (271)	0.0000	- 0.7601	0.0000	0.7601
13 (152)	0.0000	0.0000	0.7001	0.7001
67 (726)	0.0001	0.0000	0.6392	0.6392
48 (548)	0.0000	-0.0001	0.5851	0.5851
63 (713)	0.0000	0.0000	0.5380	0.5380
		OO_S_0→S_1		
1 (1840i)	0.0000	0.0000	-1.4515	1.4515
58 (646)	0.0000	0.6109	0.0000	0.6109
75 (779)	0.0000	0.5765	0.0000	0.5765
87 (878)	0.0000	0.5723	0.0000	0.5723
61 (659)	0.0000	0.5246	0.0000	0.5246
		OO_S_0→S_2		
1(960i)	0.0000	3.6808	0.0000	3.6808
175 (2048)	0.0000	-3.0225	0.0000	3.0225
45 (501)	0.0000	0.6720	0.0000	0.6720
		OO_S_0→S_3		
1 (1260i)	0.0000	0.0000	1.0889	1.0889
174 (2030)	0.0000	-1.0358	0.0000	1.0358
175 (2479)	0.0000	-0.1729	0.0000	0.1729
		OO_S_0→S_4		
175 (1844)	0.0000	1.0564	0.0000	1.0564
		OO_S_0→S_5		
175 (2554)	0.0000	-1.7001	0.0000	1.7001
		OO_S_0→S_6		
5	0.0000	-0.0001	3.2694	3.2694

28	0.0000	0.0000	1.6389	1.6389
4	0.0000	0.0000	- 0.9528	0.9528
45	0.0000	0.0000	- 0.8080	0.8080
175	0.0000	0.0000	0.7695	0.7695
38	0.0000	0.0000	- 0.7670	0.7670
21	0.0000	-0.0001	- 0.7520	0.7520
42	0.0000	0.0000	0.6046	0.6046

Note: due to strong Duschinsky mixings, it is not always possible to establish a one-to-one correspondence between these excited-state modes and the ground-state modes shown in Fig. 11.

Table S7: *H-POCP. Projection over the transition dipole moments of the transition dipole derivatives (for transitions $S_0 \rightarrow S_k$, k=1-6) along the normal modes that result in a large HT contribution to the spectrum intensity for II and OO. The frequency associated to the normal mode in given in parenthesis. For each transition the modes correspond to the diagonalization of the final state Hessian. (highlighted the terms that are connected with the couplings indicated in Table 3, in blue for the state above, and in red with the state below)*

Projection on (II)						
K (freq, cm^{-1})	$\mu_{S0\text{-}S1}$	$\mu_{S0\text{-}S2}$	$\mu_{S0\text{-}S3}$	$\mu_{S0\text{-}S4}$	$\mu_{S0\text{-}S5}$	$\mu_{S0\text{-}S6}$
			$S_0 \rightarrow S_1$			
1_1 (1985i)	0.00	**1.00**	0.00	1.00	1.00	0.00
			$S_0 \rightarrow S_2$			
175_2 (2594)	***-1.00***	0.00	-1.00	0.00	0.00	-1.00
1_2 (941i)	-1.00	0.00	**-1.00**	0.00	0.00	-1.00
			$S_0 \rightarrow S_3$			
1_3 (3513i)	0.00	1.00	0.00	**1.00**	1.00	0.00
174_3 (2023)	1.00	0.00	1.00	0.00	0.00	1.00
175_3 (2356)	0.00	***-1.00***	0.00	-1.00	-1.00	0.00
			$S_0 \rightarrow S_4$			
196_4 (4145)	-1.00	0.00	***-1.00***	0.00	0.00	-1.00
28_4 (358)	0.00	-1.00	0.00	-1.00	-1.00	0.00
46_4 (506)	0.00	1.00	0.00	1.00	1.00	0.00
			$S_0 \rightarrow S_5$			
1_5 (454i)	-1.00	0.00	-1.00	0.00	0.00	**-1.00**
174_5 (1900)	1.00	0.00	1.00	0.00	0.00	1.00
47_5 (532)	1.00	0.00	1.00	0.00	0.00	1.00
			$S_0 \rightarrow S_6$			
24_6 (294)	-1.00	0.00	-1.00	0.00	0.00	-1.00
175_6 (2226)	0.00	1.00	0.00	1.00	***1.00***	0.00
21_6 (243)	1.00	0.00	1.00	0.00	0.00	1.00
Projection on (OO)						
K (freq, cm^{-1})	$\mu_{S0\text{-}S1}$	$\mu_{S0\text{-}S2}$	$\mu_{S0\text{-}S3}$	$\mu_{S0\text{-}S4}$	$\mu_{S0\text{-}S5}$	$\mu_{S0\text{-}S6}$
			$S_0 \rightarrow S_1$			
1_1 (1840i)	0.00	**-1.00**	0.00	1.00	-1.00	0.00

			$S_0 \rightarrow S_2$			
1_2 (960i)	-1.00	0.00	**-1.00**	0.00	0.00	-1.00
175_2 (2407)	***1.00***	0.00	1.00	0.00	0.00	1.00
			$S_0 \rightarrow S_3$			
1_3 (1260i)	0.00	-1.00	0.00	1.00	**-1.00**	0.00
174_3 (2030)	1.00	0.00	1.00	0.00	0.00	1.00
175_3 (2479)	0.00	***-1.00***	0.00	1.00	-1.00	0.00
			$S_0 \rightarrow S_4$			
175_4 (1844)	-1.00	0.00	-1.00	0.00	0.00	-1.00
			$S_0 \rightarrow S_5$			
175_5 (2554)	1.00	0.00	***1.00***	0.00	0.00	1.00
			$S_0 \rightarrow S_6$			
5_6 (83)	-1.00	0.00	-1.00	0.00	0.00	-1.00
28_6 (396)	0.00	1.00	0.00	1.00	1.00	0.00
4_6 (51)	1.00	0.00	1.00	0.00	0.00	1.00