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

Construction and Performance of OLED Devices Prepared from Liquid-crystalline TADF Materials

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Supporting Information

General methods

NMR spectra were recorded on a JEOL ECX spectrometer at 298 K. ^{1}H NMR (400 MHz) chemical shifts are referenced to residual, non-deuterated $CHCl_3$ (δ 7.26) in $CDCl_3$, DCM (δ 5.32) in methylene chloride-d_2 and DMSO in DMSO-d_6. ^{13}C NMR (100 MHz) chemical shifts are reported relative to $CDCl_3$ (δ 77.3), DCM-d_2 (δ 54.00) and DMSO-d_6 (δ 39.52). Elemental analysis was carried out on an Exeter Analytical Inc. CE-440 analyser. Accurate mass measurement analyses were conducted using matrix-assisted laser desorption/ionization (MALDI). Optical textures were recorded using an Olympus BX50 polarising microscope equipped with a Linkam scientific LTS350 heating stage, Linkam LNP2 cooling pump and Linkam TMS92 controller. DSC was performed on a Mettler DSC822e fitted with an autosampler operating with Mettler Star-E software and calibrated before use against an indium standard (onset = 156.55 ± 0.2°C, ΔH = 28.45 ± 0.40 J g^{-1}), with all runs performed under an atmosphere of dry nitrogen.

All reagents were purchased from commercial sources and used as received. Solvents were purified with drying cartridges through a solvent delivery system. Reactions were monitored by TLC using silica gel (F_{254} plates, 60 Å porosity). TLC analysis was visualized using UV light. The products were purified by chromatography on silica gel (60 Å porosity, 35-75 µm).

The UV-Vis absorption spectra were measured with a Varian Cary 300 double beam spectrometer. The emission and excitation spectra were measured with a Horiba Jobin Yvon Fluorolog-3 steady state fluorescence spectrometer. The emission decay times were measured with a PicoBright PB375 pulsed diode laser (λ_{exc} = 378 nm, pulse width 100 ps) used as the excitation source, and the PL signal was detected with a cooled photomultiplier attached to a FAST ComTec multichannel scalar PCI card with a time resolution of 250 ps. The PL quantum yield was determined with a Hamamatsu C9920-02 system equipped with a Spectralon® integrating sphere.

All calculations were carried out with the Gaussian 09 package utilising the DFT approach with the M06 functional and the def2-SVP basis set. Grimme's D3 empirical dispersion correction and C-

PCM polarisable continuum model to account for solvent effects. Geometry optimisations were conducted with 'tight' criteria.

Synthesis

***2,4,5,6-Tetra(3,6-bis-(3,4-didodecyloxybenzene)carbazolyl)-1,3-dicyanobenzene (3*)**

Sodium hydride (60% in oil) (23 mg, 0.57 mmol) was washed with anhydrous hexane (2x5 mL). To this white powder 3,6-bis-(3,4-didodecyloxybenzene)-9H-carbazole (500 mg, 0.47 mmol) in anhydrous THF (10 mL) was added. The yellow reaction mixture was stirred for 2 h at 70 °C. Then 2,4,5,6-tetrafluoro-1,4-dicyanobenzene (19 mg, 0.094 mmol) in anhydrous THF (2 mL) was added in dropwise. The reaction mixture was stirred 10 min at 70 °C. THF was evaporated and the product was purified by column chromatography (silica gel, hexane/ethyl acetate, 50/1) to obtain red powder with 32% of yield (110 mg). ^{1}H NMR (600 MHz, DCM-d_2): δ 8.51 (2H, s), 8.02 (6H, m), 7.85 (2H, d, *J* = 8.5 Hz), 7.61 (2H, s), 7.41-7.35 (12H, m), 7.10-6.82 (24H, m), 4.15 (4H, t, *J* = 6.6 Hz), 4.08 (4H, t, *J* = 6.6 Hz), 4.03 (4H, t, *J* = 6.6 Hz), 3.98 (16H, m), 3.89 (4H, t, *J* = 6.6 Hz), 1.88-1.79 (32H, m), 1.47-1.28 (288H, m), 0.88 (48H, m). ^{13}C NMR (150 MHz, DCM-d_2): δ 150.2, 150.1, 150.1, 149.9, 149.9, 149.7, 149.5, 149.4, 149.3, 149.1, 146.2, 140.0, 138.7, 137.8, 136.8, 136.2, 136.0, 135.3, 134.8, 134.7, 134.5, 127.0, 126.0, 125.9, 125.7, 125.5, 124.8, 121.5, 120.4, 120.1, 120.1, 120.0, 119.7, 119.1, 118.3, 116.9, 114.9, 114.8, 114.7, 114.7, 114.1, 113.7, 113.6, 113.4, 112.5, 111.1, 110.8, 110.6, 70.2, 70.1, 70.0, 70.0, 69.9, 69.8, 32.5, 30.4, 30.3, 30.3, 30.3, 30.2, 30.2, 30.1, 30.1, 30.1, 30.1, 30.1, 30.0, 30.0, 30.0, 30.0, 26.8, 26.8, 26.7, 26.7, 26.7, 23.3, 23.3, 14.5, 14.5.

Anal. Calcd for $C_{296}H_{448}N_6O_{16}$: C, 81.8; H, 10.4; N, 1.9; found: C, 81.8; H, 10.6; N, 1.9 %. MS (MALDI): $C_{296}H_{449}N_6NaO_{16}$, 4367.4435, found 4367.4397.

NMR spectra

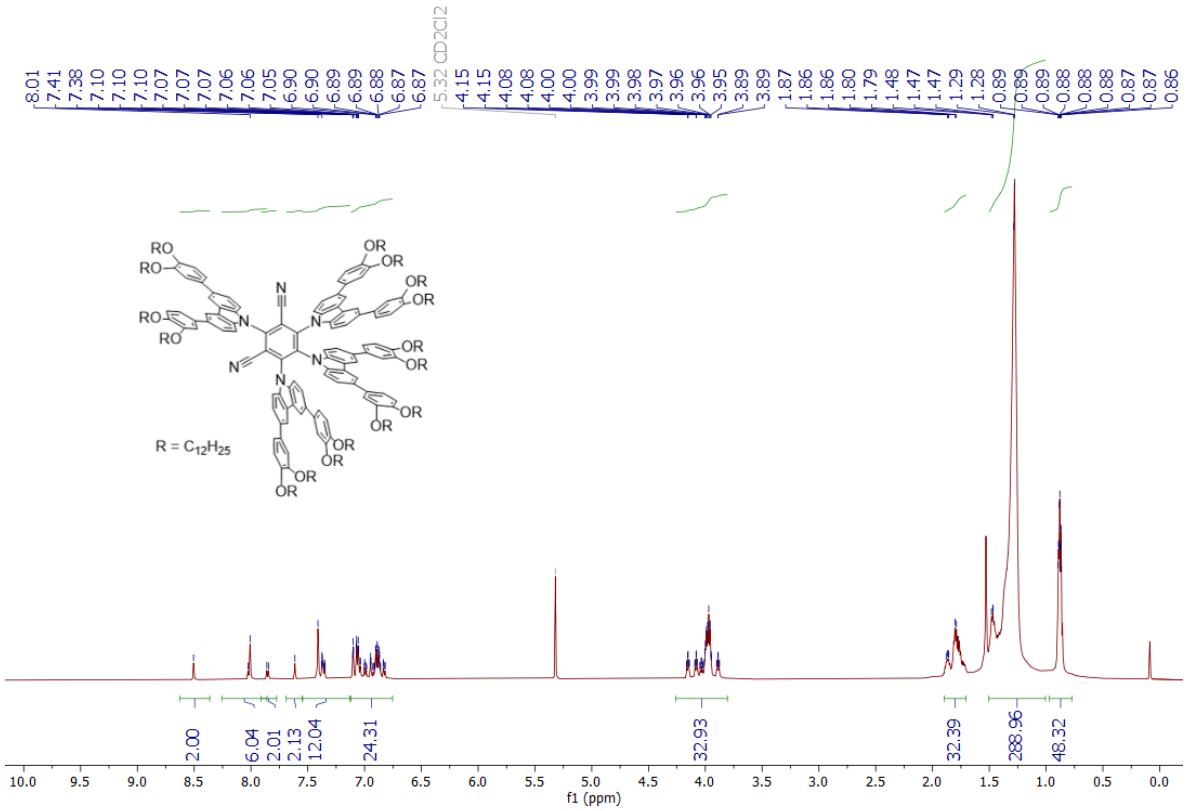

Figure S1. ^{1}H NMR spectrum of compound **3**

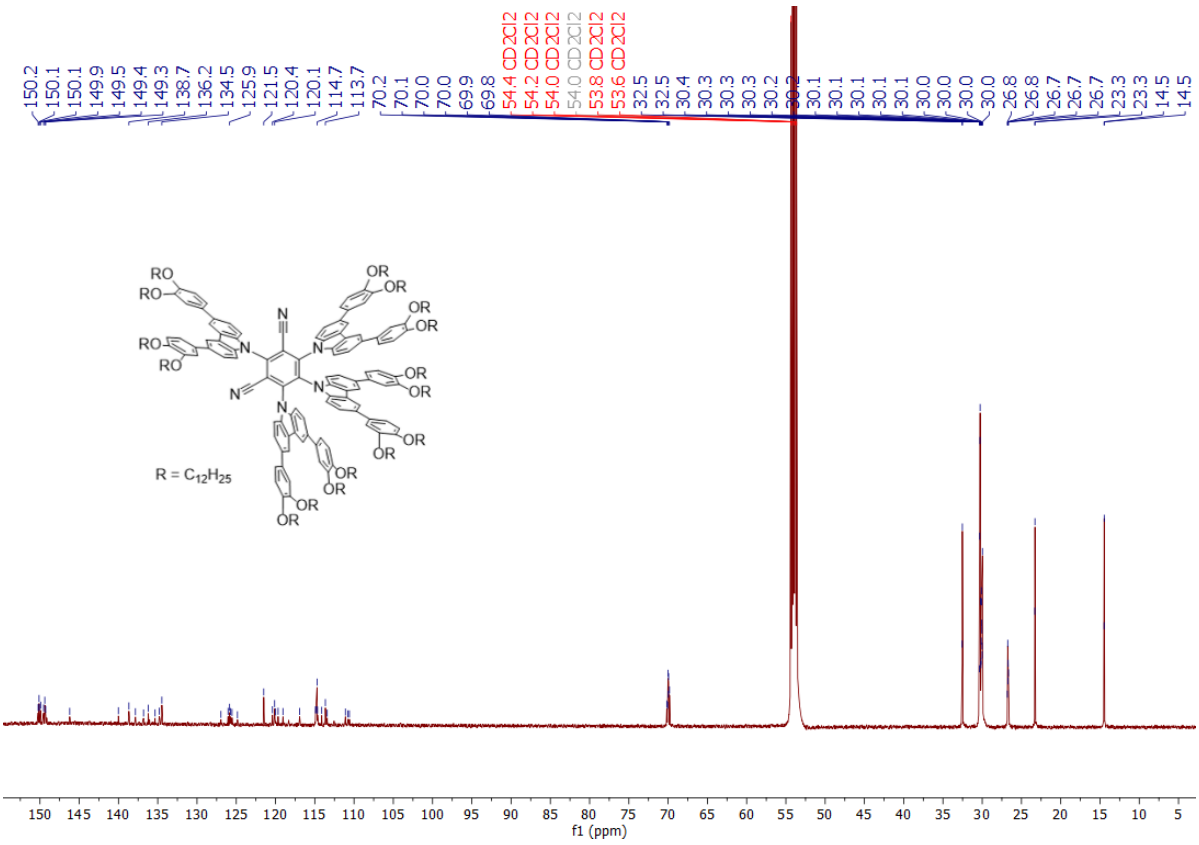

Figure S2. ^{13}C NMR spectrum of compound **3**

Liquid Crystal Data

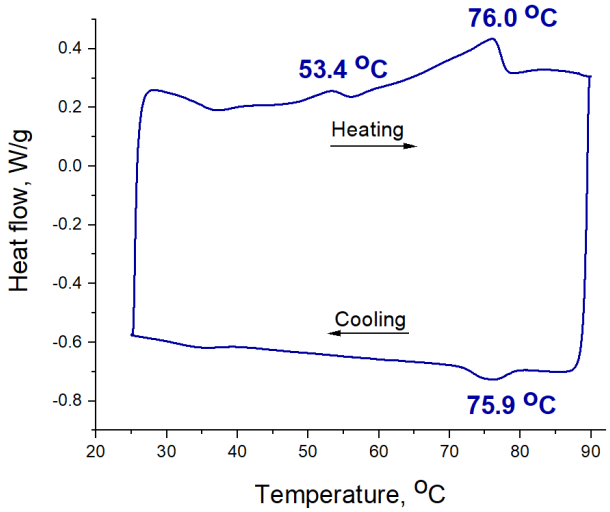

Figure S3. Differential scanning calorimetry trace - second heat-cool cycle (scan rate of 10 °C min^{-1}). The first and third traces are identical. ΔH(clearing) = 20.7 kJ mol^{-1}.

Cyclic voltammetry

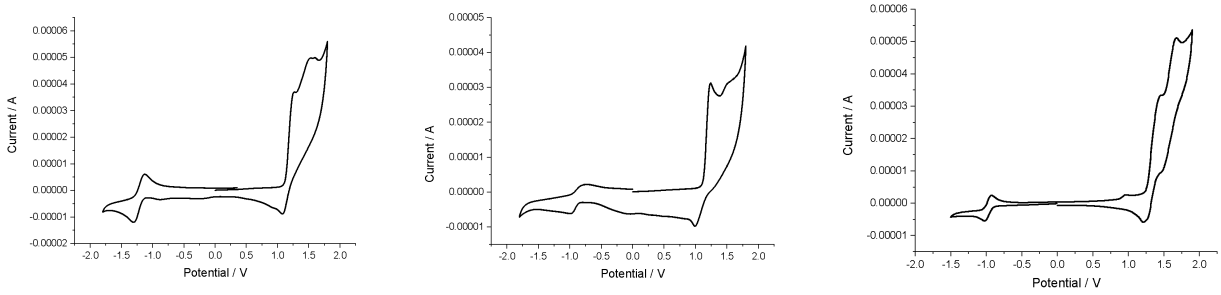

Figure S4. CV of compounds **1**, **2** and **3** in 0.1 M $TBAPF_6$ DCM solution(WE glassy carbon, CE platinum, RE Ag/AgCl).

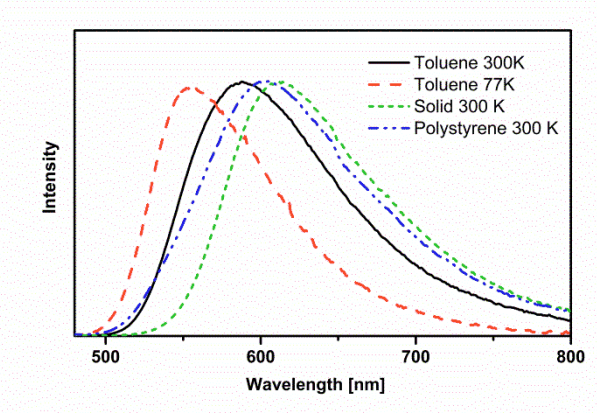

Figure S5 Room temperature photoluminescence spectra of compound **3** in toluene, polystyrene, and as powder and 77 K spectrum in frozen glassy toluene. The emission maxima shift from 585 nm in liquid toluene to 556 nm in frozen toluene at 77 K, 605 nm in polystyrene, and 610 nm in solid sample, respectively. The blue shift upon freezing to 77 K is a clear consequence of the charge-transfer character of the emitting state of compd. **3** and distinctly lower dynamic solvent polarity in frozen state at 77 K compared to a liquid solvent at room temperature. The red shifts observed for solid sample and in polystyrene polymer film combined with spectral broadening are most probably due to aggregation of compd. **3** and spectroscopic inhomogeneity of aggregated species.

Table S1 Photoluminescence data for **3**

	λ_{em}/nm	ϕ_{PL}	τ_{PF}/ns	τ_{DF}/µs
Toluene 300 K	585	11 %	7.5	0.92
Toluene 77 K	556	53 %	22	-[a]
Polystyrene 300 K	605	7 %	7.6-17[b]	1.04
Powder 300 K	610	5 %	4.9	-[a]

a) The long decay component is weak. A reliable fit of τ_{DF} was not obtained.

b) Non-monoexponential decay is observed due to sample inhomogeneity. The limiting values were obtained from fitting a biexponential decay function to the experimental decay trace.

Device fabrication and Measurements

In the device, poly(3,4-ethylenedioxythiophene):poly(styrenesulfonic acid) (PEDOT:PSS) serves as the hole injection layer, while bis[2-(diphenylphosphino)phenyl] ether oxide (DPEPO) and 1,3,5-tri(m-pyrid-3-yl-phenyl)benzene (TmPyPB) act as the hole-blocking and electron-transport S-3 layers, respectively. The emitter layer consists of a 9,9'-(1,3-phenylene)bis-9H-carbazole (mCP) host blended with the dopant at an optimized doping level of 20wt%. The patterned ITO substrates were washed with acetone and isopropyl alcohol under sonication for 15 min, followed

by 15 min of UV-ozone-treatment. After surface treatment, the PEDOT:PSS layer was spin-coated onto the ITO substrate as the hole-injecting layer, followed by annealing at 150 oC for 15 min. The emissive layers were prepared by spin-coating onto the PEDOT:PSS followed by annealing at 80 oC for 15 min. The hole blocking layer, the electron-transporting layer and the cathode materials were thermally evaporated and deposited onto the emitter layer in a vacuum chamber. The thermally evaporated deposition rates were 0.6-1 Å s-1 for the organic layers, 0.1 Å s -1 for Liq and 1.5-1.8 Å s-1 for the Al electrode, respectively. The current-voltage-luminance (J-V-L) characteristics and the electroluminescence spectra of the devices were obtained simultaneously by using a spectroradiometer (PR735) and a Keithley 2400 SourceMeter unit under ambient atmosphere at room temperature. In the devices, the emitter layer is a blend of the host matrix mCP and the dyes. Poly(3,4-ethylenedioxythiophene):poly(styrenesulfonic acid) (PEDOT:PSS) serves as the hole injection layer, while bis[2-(diphenylphosphino)phenyl] ether oxide (DPEPO) and 1,3,5-tri(*m*-pyrid-3-yl-phenyl)benzene (TmPyPB) act as the hole-blocking and electron-transport layers, respectively. LiF and Al serve as the cathode.

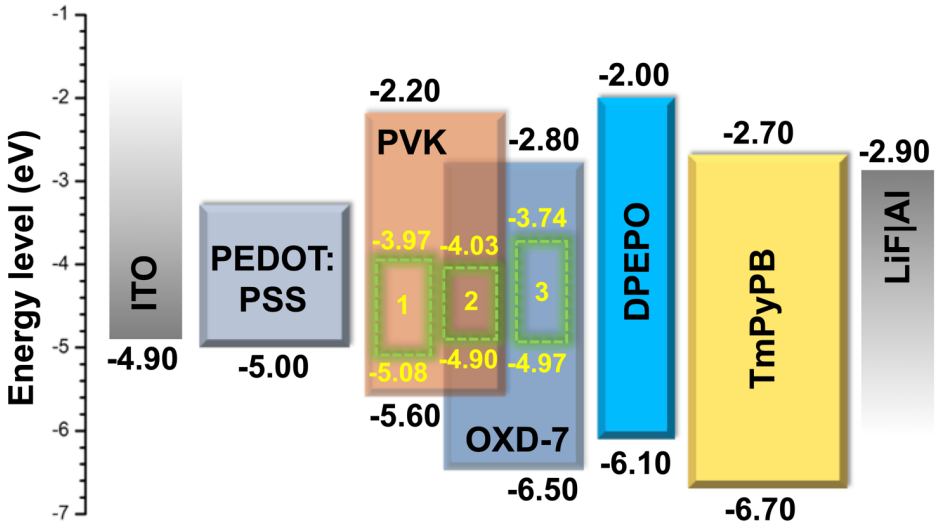

Figure S6 Energy levels of the materials used in the emissive device

Calculations

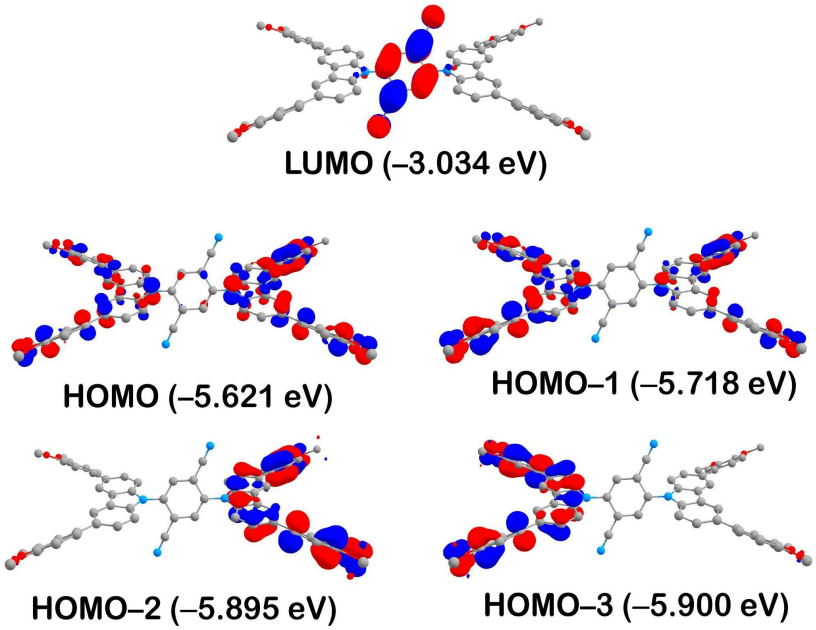

Figure S7. Iso-surface contour plots (iso-value = 0.03) of selected molecular orbitals of compound **1** in T_1 state geometry. Hydrogens are omitted for clarity. Calculated at M06/def2-SVP level with D3 correction and C-PCM (toluene) model.

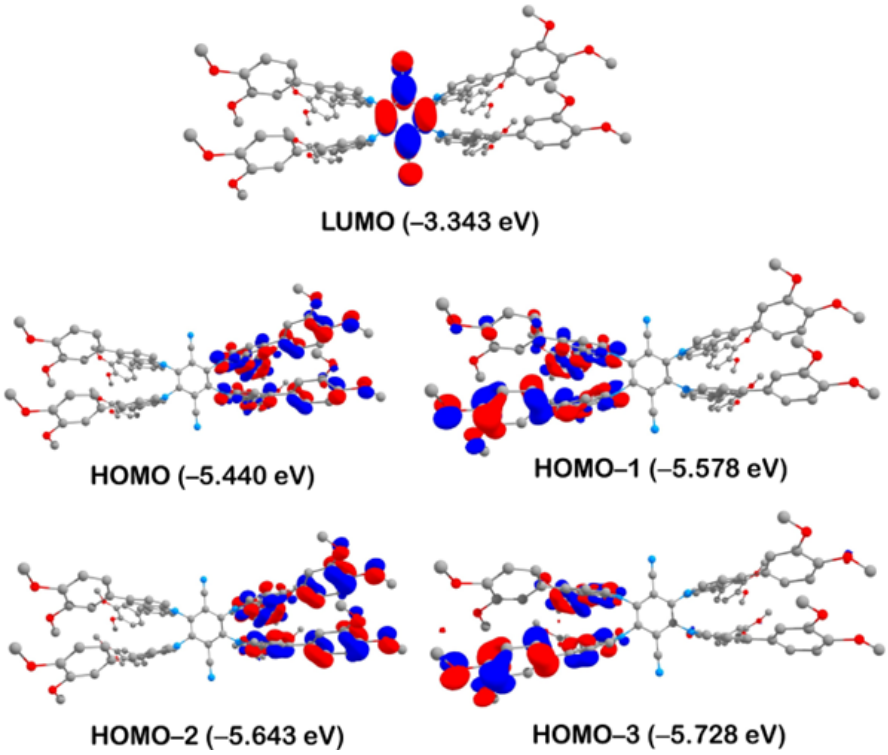

Figure S8. Iso-surface contour plots (iso-value = 0.03) of selected molecular orbitals of compound **2** in T_1 state geometry. Hydrogens are omitted for clarity. Calculated at M06/def2-SVP level with D3 correction and C-PCM (toluene) model.

Table S2 DFT calculated frontier orbital energies and atomic contributions in the T_1 state optimised geometry of **1** resulting from the Mulliken population analysis. Calculated at M06/def2-SVP level with D3 correction and C-PCM (toluene) model

Orbitals	Energy, eV	Contributions, %	
		Terephthalonitrile	Carbazole units
LUMO+4	−0.895	1	99
LUMO+3	−1.214	1	99
LUMO+2	−1.221	1	99
LUMO+1	−1.554	82	18
LUMO	−3.034	95	5
HOMO	−5.621	3	97
HOMO-1	−5.718	2	98
HOMO-2	−5.895	0	100
HOMO-3	−5.900	0	100
HOMO-4	−6.544	5	95

Table S3 DFT calculated frontier orbital energies and atomic contributions in the T_1 state optimized geometry of **2** resulting from the Mulliken population analysis. Calculated at M06/def2-SVP level with D3 correction and C-PCM (toluene) model.

Orbitals	Energy, eV	Contributions, %	
		Terephthalonitrile	Carbazole units
LUMO+4	−0.986	0	100
LUMO+3	−1.502	1	99
LUMO+2	−1.517	1	99
LUMO+1	−2.072	88	12
LUMO	−3.343	96	4
HOMO	−5.440	1	99
HOMO-1	−5.578	1	99
HOMO-2	−5.643	0	100
HOMO-3	−5.728	1	99
HOMO-4	−5.746	1	99

Table S4 DFT calculated frontier orbital energies and atomic contributions in the T_1 state optimized geometry of **3** resulting from the Mulliken population analysis. Calculated at M06/def2-SVP level with D3 correction and C-PCM (toluene) model.

Orbitals	Energy / eV	Contribution (Mulliken)				
		isophth	Cz1	Cz2	Cz3	Cz4
LUMO+4	−1.216	0	15	52	33	0
LUMO+3	−1.221	1	6	1	3	89
LUMO+2	−1.284	1	17	17	65	0
LUMO+1	−2.359	90	1	2	1	5
LUMO	−2.920	93	4	0	3	0
HOMO	−5.175	1	7	84	8	0
HOMO−1	−5.574	1	36	48	15	0
HOMO−2	−5.645	1	38	2	58	1
HOMO−3	−5.733	1	1	0	1	97
HOMO−4	−5.800	1	44	33	23	0

Table S5 TD-DFT calculated lowest triplet and singlet states of **1** in the T_1 state geometry. Calculated at M06/def2-SVP level with D3 correction and C-PCM (toluene) model.

State, energy (eV)	***f* / (oscillator strength)**	**Contributing transition coefficients***	**Character****
		triplets	
T_1, 1.793	(triplet)	HOMO→LUMO (0.65) HOMO–4→LUMO (0.21)	CT (Carbazoles→phth)
T_2, 2.022	(triplet)	HOMO–1→LUMO (0.68)	CT (Carbazoles→phth)
T_3, 2.331	(triplet)	HOMO–2→LUMO (0.67)	CT (Carbazoles→phth)
		singlets	
S_1, 1.951	0.1577	HOMO→LUMO (0.69)	CT (Carbazoles→phth)
S_2, 2.102	0.0006	HOMO–1→LUMO (0.69)	CT (Carbazoles→phth)
S_3, 1.742	0.0191	HOMO–2→LUMO (0.65) HOMO–3→LUMO (–0.23)	CT (Carbazoles→phth)

*Square of the coefficient multiplied by two gives percentage contribution of the transition to formation of the excited state. ** CT - Charge Transfer.

Table S6 TD-DFT calculated lowest triplet and singlet states of **2** in the T_1 state geometry. Calculated at M06/def2-SVP level with D3 correction and C-PCM (toluene) model.

State, energy (eV)	***f*** **(oscillator strength)**	**Contributing transition coefficients***	**Character****
		triplets	
T_1, 1.427	(triplet)	HOMO→LUMO (0.69)	CT (Carbazoles→phth)
T_2, 1.585	(triplet)	HOMO–1→LUMO (0.68)	CT (Carbazoles→phth)
T_3, 1.736	(triplet)	HOMO–2→LUMO (0.69)	CT (Carbazoles→phth)
		singlets	
S_1, 1.441	0.0097	HOMO→LUMO (0.69)	CT (Carbazoles→phth)
S_2, 1.600	0.0064	HOMO–1→LUMO (0.69)	CT (Carbazoles→phth)
S_3, 1.742	0.0008	HOMO–2→LUMO (0.69)	CT (Carbazoles→phth)

*Square of the coefficient multiplied by two gives a percentage contribution of the transition to formation of the excited state. ** CT - Charge Transfer.

Table S7 TD-DFT calculated lowest triplet and singlet states of **3** in the T_1 state geometry. Calculated at M06/def2-SVP level with D3 correction and C-PCM (toluene) model.

State, energy (eV)	***f* (oscillator strength)**	**Contributing transition coefficients***	**Character****
		triplets	
T_1, 1.618	(triplet)	HOMO→LUMO (0.69)	CT (Cz2→isophth)
T_2, 2.005	(triplet)	HOMO–1→LUMO (0.57) HOMO–2→LUMO (−0.32)	CT (Cz1/Cz2/Cz3→isophth)
T_3, 2.034	(triplet)	HOMO–2→LUMO (0.60) HOMO–1→LUMO (0.32)	CT (Cz1/Cz2/Cz3→isophth)
		singlets	
S_1, 1.632	0.0004	HOMO→LUMO (0.69)	CT (Cz2→isophth)
S_2, 2.042	0.0211	HOMO–1→LUMO (0.63) HOMO–2→LUMO (−0.25)	CT (Cz1/Cz2/Cz3→isophth)
S_3, 2.067	0.0171	HOMO–1→LUMO (0.25) HOMO–2→LUMO (0.64)	CT (Cz1/Cz2/Cz3→isophth)

*Square of the coefficient multiplied by two gives a percentage contribution of the transition to formation of the excited state. ** CT - Charge Transfer.

Table S8 The DFT calculated geometry of compound **1** in the S_0 and T_1 states given in *xyz* format. Calculated at M06/def2-SVP level with D3 correction and C-PCM (toluene) model.

S_0 geometry				T_1 geometry			
6	-1.370946000	1.058531000	-2.335205000	6	-1.418581000	1.209392000	-2.230481000
6	-0.732969000	0.510520000	-1.176105000	6	-0.774967000	0.649636000	-1.111250000
6	0.662652000	0.526330000	-1.097022000	6	0.641425000	0.622138000	-1.042168000
6	1.323582000	-0.063522000	-0.022879000	6	1.315580000	-0.053667000	-0.051850000
6	10.315824000	-3.489348000	2.052120000	6	10.361053000	-3.406290000	1.889231000
6	3.524440000	1.093498000	0.022010000	6	3.521923000	1.100010000	-0.042449000
6	3.157346000	2.437433000	0.046005000	6	3.157939000	2.447358000	-0.022692000
6	4.173394000	3.385332000	0.051118000	6	4.173773000	3.392849000	-0.008935000
6	5.540037000	3.030942000	0.043458000	6	5.540976000	3.037329000	-0.006961000
6	5.881504000	1.674371000	0.032287000	6	5.881041000	1.673716000	-0.010498000
6	4.880951000	0.703300000	0.021865000	6	4.881567000	0.710555000	-0.025537000
6	6.585464000	4.076284000	0.054179000	6	6.587826000	4.073586000	0.011087000
6	6.413813000	5.268518000	0.754153000	6	6.387388000	5.298892000	0.649227000
6	7.412927000	6.246283000	0.765426000	6	7.390102000	6.269626000	0.674029000
6	8.605523000	6.053205000	0.076273000	6	8.617061000	6.041503000	0.057219000
6	8.795764000	4.845332000	-0.641921000	6	8.837491000	4.801704000	-0.599129000
6	7.794100000	3.882776000	-0.643686000	6	7.832609000	3.844585000	-0.611247000
6	3.558866000	-1.174795000	0.026552000	6	3.546864000	-1.157494000	-0.011975000
6	3.233892000	-2.528556000	-0.025945000	6	3.210784000	-2.511516000	-0.070200000
6	4.278377000	-3.444000000	-0.048729000	6	4.245773000	-3.434094000	-0.074886000
6	5.633484000	-3.048154000	-0.030186000	6	5.605406000	-3.049690000	-0.038849000
6	5.933017000	-1.682535000	0.004390000	6	5.917391000	-1.679793000	-0.008259000
6	4.902554000	-0.743250000	0.028437000	6	4.897079000	-0.738644000	-0.000077000
6	6.710065000	-4.060953000	-0.058672000	6	6.672998000	-4.063714000	-0.052647000
6	7.909249000	-3.847070000	0.649224000	6	7.901290000	-3.819834000	0.596356000
6	8.939334000	-4.779216000	0.630659000	6	8.925115000	-4.756693000	0.588383000
6	8.788899000	-5.975009000	-0.116339000	6	8.741925000	-5.989897000	-0.091736000
6	7.605291000	-6.188371000	-0.814951000	6	7.531261000	-6.232738000	-0.734862000
6	6.576954000	-5.241748000	-0.785754000	6	6.509016000	-5.282974000	-0.713181000
6	9.487693000	8.149485000	0.707974000	6	9.479890000	8.159188000	0.645244000
6	10.221839000	3.561928000	-2.020031000	6	10.327121000	3.457412000	-1.845024000
6	9.735464000	-8.030381000	-0.788281000	6	9.657555000	-8.081127000	-0.694914000
7	-1.867227000	1.499522000	-3.286499000	7	-1.940929000	1.688713000	-3.161492000
7	2.723451000	-0.052117000	0.036909000	7	2.720606000	-0.038156000	-0.026364000
8	9.623395000	6.934221000	0.026253000	8	9.639558000	6.912605000	0.024615000
8	9.969115000	4.732474000	-1.294920000	8	10.041292000	4.658663000	-1.183723000
8	10.105350000	-4.646726000	1.293111000	8	10.114354000	-4.599676000	1.198220000
8	9.833242000	-6.825597000	-0.082140000	8	9.780865000	-6.840701000	-0.053834000
6	1.199025000	-1.218099000	2.154790000	6	1.236365000	-1.332799000	2.105247000
6	0.559293000	-0.668370000	0.997378000	6	0.591902000	-0.775527000	0.985106000
6	-0.836057000	-0.683644000	0.918861000	6	-0.823866000	-0.751253000	0.914430000
6	-1.497334000	-0.095181000	-0.156291000	6	-1.498197000	-0.077222000	-0.077271000
6	-6.542708000	7.510331000	1.915679000	6	-6.480622000	7.612137000	1.758376000
6	-3.691882000	-1.262217000	-0.184193000	6	-3.689228000	-1.255483000	-0.095257000
6	-3.317443000	-2.604307000	-0.191852000	6	-3.305810000	-2.597665000	-0.109792000
6	-4.328102000	-3.557789000	-0.181860000	6	-4.307743000	-3.557273000	-0.125400000
6	-5.696652000	-3.211042000	-0.175488000	6	-5.679934000	-3.221000000	-0.134339000
6	-6.045647000	-1.856307000	-0.181556000	6	-6.039454000	-1.861723000	-0.137817000
6	-5.050396000	-0.879675000	-0.186286000	6	-5.053975000	-0.884803000	-0.121294000
6	-6.735799000	-4.262659000	-0.170170000	6	-6.711501000	-4.271717000	-0.151217000
6	-6.557268000	-5.463642000	-0.853274000	6	-6.487623000	-5.500947000	-0.774492000
6	-7.549817000	-6.448047000	-0.848959000	6	-7.475379000	-6.486620000	-0.796806000
6	-8.742761000	-6.252952000	-0.160968000	6	-8.710539000	-6.270287000	-0.191892000
6	-8.940291000	-5.035897000	0.539575000	6	-8.954908000	-5.026665000	0.449114000
6	-7.944947000	-4.066877000	0.526138000	6	-7.964845000	-4.054482000	0.458320000
6	-3.738547000	1.005739000	-0.221786000	6	-3.743150000	1.000822000	-0.133673000
6	-3.421376000	2.361746000	-0.189256000	6	-3.424481000	2.358936000	-0.077862000
6	-4.471272000	3.271613000	-0.178046000	6	-4.471274000	3.268376000	-0.083953000

6	-5.824049000	2.868036000	-0.189356000	6	-5.825582000	2.866989000	-0.129336000
6	-6.115589000	1.500115000	-0.200340000	6	-6.119901000	1.492023000	-0.154887000
6	-5.079992000	0.566694000	-0.213919000	6	-5.088284000	0.564583000	-0.152835000
6	-6.910167000	3.871112000	-0.185289000	6	-6.908651000	3.863842000	-0.134063000
6	-6.766311000	5.080154000	0.523519000	6	-6.742415000	5.112085000	0.501334000
6	-7.774059000	6.036249000	0.540423000	6	-7.750621000	6.065364000	0.504009000
6	-8.978258000	5.797736000	-0.169300000	6	-8.980063000	5.788013000	-0.151376000
6	-9.121937000	4.605152000	-0.870382000	6	-9.146465000	4.557961000	-0.782119000
6	-8.098522000	3.652745000	-0.878867000	6	-8.125126000	3.607298000	-0.770918000
6	-9.611409000	-8.363964000	-0.761434000	6	-9.536239000	-8.407566000	-0.762077000
6	-10.374095000	-3.740871000	1.898657000	6	-10.474516000	-3.692269000	1.669008000
6	-11.116044000	6.590714000	-0.779539000	6	-11.139703000	6.548332000	-0.728335000
7	1.697957000	-1.660310000	3.104114000	7	1.759381000	-1.809461000	3.037160000
7	-2.896747000	-0.112467000	-0.217165000	7	-2.902982000	-0.107233000	-0.109659000
8	-9.754408000	-7.140215000	-0.096612000	8	-9.719572000	-7.156157000	-0.157393000
8	-10.113753000	-4.921044000	1.192060000	8	-10.165047000	-4.896015000	1.022799000
8	-7.709281000	7.207698000	1.203781000	8	-7.669328000	7.267933000	1.101402000
8	-9.904938000	6.773403000	-0.101497000	8	-9.902694000	6.762567000	-0.104322000

Table S9 The DFT calculated geometry of compound **2** in the S_0 and T_1 states given in *xyz* format. Calculated at M06/def2-SVP level with D3 correction and C-PCM (toluene) model.

S_0 geometry				T_1 geometry			
6	0.046427000	-0.753860000	-2.724461000	6	0.070908000	-0.662354000	-2.830620000
6	0.070863000	-0.452874000	-1.324056000	6	0.078520000	-0.458370000	-1.439004000
6	-1.144412000	-0.296199000	-0.636795000	6	-1.140296000	-0.337291000	-0.687176000
6	-1.122437000	0.042591000	0.730846000	6	-1.124210000	-0.126763000	0.680679000
6	-3.167151000	-1.508749000	-1.512211000	6	-3.202216000	-1.430653000	-1.628435000
6	-2.834769000	-2.857732000	-1.441264000	6	-2.905306000	-2.792013000	-1.611286000
6	-3.859775000	-3.786208000	-1.584466000	6	-3.949753000	-3.687175000	-1.802597000
6	-5.200877000	-3.400434000	-1.792516000	6	-5.280283000	-3.260032000	-2.005584000
6	-5.499527000	-2.038188000	-1.906802000	6	-5.542815000	-1.885353000	-2.075455000
6	-4.488819000	-1.088361000	-1.776026000	6	-4.511059000	-0.967603000	-1.899749000
6	-6.289771000	-4.398293000	-1.835172000	6	-6.393417000	-4.226271000	-2.084187000
6	-6.295518000	-5.503981000	-0.988239000	6	-6.410197000	-5.384937000	-1.308451000
6	-7.390113000	-6.373566000	-0.950812000	6	-7.524289000	-6.229375000	-1.301664000
6	-8.501024000	-6.156283000	-1.760164000	6	-8.647089000	-5.934232000	-2.069514000
6	-8.499790000	-5.046363000	-2.641006000	6	-8.636642000	-4.769948000	-2.878270000
6	-7.404194000	-4.194026000	-2.672041000	6	-7.521357000	-3.944252000	-2.880520000
6	-3.150914000	0.758156000	-1.567481000	6	-3.120895000	0.821463000	-1.581205000
6	-2.767320000	2.093904000	-1.592893000	6	-2.698978000	2.146608000	-1.525994000
6	-3.759104000	3.041596000	-1.802759000	6	-3.658295000	3.134530000	-1.691392000
6	-5.112345000	2.686533000	-1.985548000	6	-5.020722000	2.831946000	-1.902633000
6	-9.509132000	3.997649000	4.174509000	6	-9.451259000	3.786041000	4.367393000
6	-5.463817000	1.332012000	-2.001508000	6	-5.411610000	1.490932000	-2.007887000
6	-4.481240000	0.359755000	-1.806049000	6	-4.461315000	0.479600000	-1.863766000
6	-6.126264000	3.752357000	-2.132944000	6	-6.007610000	3.929152000	-1.971181000
6	-7.365925000	3.658057000	-1.473069000	6	-7.251872000	3.810260000	-1.322964000
6	-8.301669000	4.683776000	-1.544335000	6	-8.166933000	4.856397000	-1.317099000
6	-8.022263000	5.828577000	-2.330618000	6	-7.861620000	6.053097000	-2.010909000
6	-6.799923000	5.921741000	-2.986321000	6	-6.633521000	6.173355000	-2.651795000
6	-5.858634000	4.894421000	-2.884329000	6	-5.713550000	5.122275000	-2.628681000
6	-9.754613000	-7.905955000	-0.796078000	6	-9.912022000	-7.728744000	-1.207136000
6	-9.712988000	-3.757958000	-4.203727000	6	-9.855595000	-3.349457000	-4.316699000
6	-9.790647000	3.629950000	-0.038582000	6	-9.682420000	3.717445000	0.097327000
6	-8.704547000	7.987411000	-3.005845000	6	-8.502384000	8.268957000	-2.523766000
6	-3.182121000	-0.916881000	1.666994000	6	-3.207580000	-1.110974000	1.587310000
6	-2.883586000	-2.273919000	1.695074000	6	-2.928524000	-2.472945000	1.527049000
6	-3.936169000	-3.159230000	1.881769000	6	-3.985638000	-3.354848000	1.695797000
6	-5.267989000	-2.721432000	2.039673000	6	-5.307482000	-2.911452000	1.915785000
6	-5.534016000	-1.347404000	2.055469000	6	-5.554521000	-1.537140000	2.025020000
6	-4.489425000	-0.438131000	1.883311000	6	-4.503692000	-0.631283000	1.878426000
6	-6.351684000	-3.719643000	2.160531000	6	-6.402034000	-3.900598000	1.993857000
6	-6.176881000	-4.880792000	2.910342000	6	-6.226814000	-5.114408000	2.656230000
6	-7.188039000	-5.841762000	2.988750000	6	-7.247863000	-6.067039000	2.689503000
6	-8.389030000	-5.661685000	2.312029000	6	-8.460714000	-5.826475000	2.053452000
6	-8.574916000	-4.496381000	1.528197000	6	-8.647408000	-4.607903000	1.355915000
6	-7.569195000	-3.538305000	1.477575000	6	-7.631682000	-3.659135000	1.351554000
6	-3.059659000	1.347266000	1.622346000	6	-3.053302000	1.137140000	1.648246000
6	-2.645528000	2.673361000	1.551873000	6	-2.614309000	2.459525000	1.627504000
6	-3.615636000	3.662707000	1.669832000	6	-3.558277000	3.459350000	1.820177000
6	-4.981038000	3.358793000	1.852717000	6	-4.925384000	3.173953000	2.028705000
6	-5.362819000	2.017265000	1.966508000	6	-5.331357000	1.834714000	2.101524000
6	-4.408660000	1.008087000	1.858869000	6	-4.402268000	0.813238000	1.921808000
6	-6.011222000	4.418213000	1.866481000	6	-5.928864000	4.253513000	2.106394000
6	-7.151243000	4.284997000	2.683306000	6	-7.076777000	4.102519000	2.909882000
6	-8.193669000	5.200145000	2.626382000	6	-8.091491000	5.049391000	2.909175000
6	-8.114624000	6.301490000	1.738422000	6	-7.975803000	6.204246000	2.095417000
6	-6.979478000	6.446607000	0.946720000	6	-6.833961000	6.365898000	1.316038000
6	-5.938216000	5.514969000	1.010784000	6	-5.821773000	5.401718000	1.322381000
6	-9.234978000	-7.768176000	2.967933000	6	-9.313114000	-7.970935000	2.561063000

6	-9.966694000	-3.329113000	0.013648000	6	-10.052992000	-3.324534000	-0.048561000
6	-9.239394000	8.131303000	0.761374000	6	-9.037749000	8.129869000	1.241019000
7	0.027024000	-1.014095000	-3.854287000	7	0.078494000	-0.845044000	-3.985878000
7	-2.356883000	-0.374581000	-1.347541000	7	-2.372470000	-0.336909000	-1.390070000
7	-2.313629000	0.165279000	1.470374000	7	-2.341861000	-0.036417000	1.401854000
8	-9.612486000	-6.914702000	-1.777813000	8	-9.777517000	-6.662320000	-2.108249000
8	-9.615845000	-4.886727000	-3.382800000	8	-9.764338000	-4.536744000	-3.582061000
8	-9.476711000	4.702125000	-0.884880000	8	-9.344187000	4.846770000	-0.660612000
8	-8.986931000	6.774030000	-2.366417000	8	-8.808439000	7.017365000	-1.976471000
8	-9.417315000	-6.537896000	2.324402000	8	-9.499511000	-6.690927000	2.025619000
8	-9.737786000	-4.429734000	0.850491000	8	-9.820459000	-4.484284000	0.703275000
8	-9.329894000	5.113194000	3.349435000	8	-9.233386000	4.949433000	3.621291000
8	-9.179193000	7.124188000	1.735380000	8	-9.015425000	7.056384000	2.143153000
6	0.136173000	0.530005000	2.772027000	6	0.139584000	0.180243000	2.796656000
6	0.114424000	0.220249000	1.373694000	6	0.110821000	-0.004285000	1.402436000
6	1.329724000	0.073466000	0.684009000	6	1.320058000	-0.077194000	0.641297000
6	1.307119000	-0.257352000	-0.686648000	6	1.305705000	-0.291679000	-0.722506000
6	3.266096000	1.407735000	1.548216000	6	3.268537000	1.241177000	1.486479000
6	2.817702000	2.724572000	1.541200000	6	2.801583000	2.556455000	1.447708000
6	3.766278000	3.733900000	1.666002000	6	3.732028000	3.576211000	1.573891000
6	5.143756000	3.458922000	1.794602000	6	5.113951000	3.320199000	1.724888000
6	5.562481000	2.124444000	1.841209000	6	5.550413000	1.983759000	1.813114000
6	4.631020000	1.095585000	1.724127000	6	4.636894000	0.946514000	1.708554000
6	6.148026000	4.542320000	1.824289000	6	6.096846000	4.411744000	1.738615000
6	6.028091000	5.669531000	1.014814000	6	5.899006000	5.581668000	0.998704000
6	7.048212000	6.624741000	0.958835000	6	6.886776000	6.564826000	0.931030000
6	8.207364000	6.473784000	1.713839000	6	8.095192000	6.406395000	1.607148000
6	8.332415000	5.342755000	2.558047000	6	8.302631000	5.232534000	2.381628000
6	7.311088000	4.403924000	2.606813000	6	7.313920000	4.263667000	2.437370000
6	3.448607000	-0.852834000	1.504877000	6	3.452051000	-1.001985000	1.495451000
6	3.183943000	-2.217216000	1.500659000	6	3.179207000	-2.367741000	1.500708000
6	4.264145000	-3.080845000	1.618781000	6	4.249512000	-3.234088000	1.664537000
6	5.590150000	-2.613657000	1.736115000	6	5.576878000	-2.773112000	1.798625000
6	6.585972000	-7.793954000	-0.015164000	6	6.630053000	-7.790500000	-0.153324000
6	5.823444000	-1.235002000	1.789750000	6	5.818300000	-1.387958000	1.836479000
6	4.750478000	-0.347724000	1.689554000	6	4.756547000	-0.500269000	1.707989000
6	6.703697000	-3.585393000	1.763163000	6	6.686131000	-3.739107000	1.865466000
6	6.591899000	-4.766208000	2.522177000	6	6.521739000	-4.963627000	2.544378000
6	7.593520000	-5.727926000	2.512049000	6	7.527049000	-5.919071000	2.562092000
6	8.748831000	-5.531634000	1.714791000	6	8.744079000	-5.672891000	1.872942000
6	8.861989000	-4.362515000	0.968818000	6	8.910353000	-4.460912000	1.207320000
6	7.850897000	-3.396148000	0.996705000	6	7.895084000	-3.501693000	1.209721000
6	9.269588000	8.356454000	0.769840000	6	9.035947000	8.388739000	0.739451000
6	9.711616000	4.113285000	4.027548000	6	9.794499000	3.991100000	3.725937000
6	6.405989000	-7.174466000	3.952208000	6	6.252470000	-7.440004000	3.842705000
6	10.762659000	-6.447625000	0.893300000	6	10.817936000	-6.540414000	1.157622000
6	3.252651000	0.872175000	-1.647985000	6	3.236174000	0.922297000	-1.665234000
6	2.833305000	2.196957000	-1.619121000	6	2.760007000	2.231631000	-1.651737000
6	3.793104000	3.177525000	-1.825104000	6	3.677811000	3.249530000	-1.859174000
6	5.149223000	2.865201000	-2.057343000	6	5.051429000	2.995225000	-2.063142000
6	5.535494000	1.521713000	-2.128471000	6	5.498143000	1.663230000	-2.115176000
6	4.584769000	0.517124000	-1.937361000	6	4.591249000	0.623976000	-1.936679000
6	6.129619000	3.963421000	-2.194745000	6	5.991707000	4.121104000	-2.202767000
6	5.810619000	5.121638000	-2.900094000	6	5.611008000	5.296324000	-2.852604000
6	6.718356000	6.179851000	-2.988063000	6	6.492782000	6.371285000	-2.965096000
6	7.958133000	6.101910000	-2.363802000	6	7.771365000	6.297993000	-2.420825000
6	8.290831000	4.939308000	-1.625788000	6	8.166909000	5.121366000	-1.735450000
6	7.387655000	3.883857000	-1.568297000	6	7.287532000	4.049399000	-1.653031000
6	3.324590000	-1.393912000	-1.675218000	6	3.397928000	-1.322615000	-1.654317000
6	3.027292000	-2.752116000	-1.646575000	6	3.140671000	-2.692537000	-1.610828000
6	4.069505000	-3.648290000	-1.856620000	6	4.210112000	-3.557892000	-1.793694000
6	5.394599000	-3.222577000	-2.088549000	6	5.528959000	-3.095827000	-2.000652000
6	5.656615000	-1.849491000	-2.154695000	6	5.750503000	-1.709108000	-2.088574000

6	4.627922000	-0.931150000	-1.960235000	6	4.693628000	-0.823683000	-1.934901000
6	6.502064000	-4.192340000	-2.223494000	6	6.664906000	-4.029148000	-2.087743000
6	6.502924000	-5.388889000	-1.481554000	6	6.630641000	-5.274320000	-1.427296000
6	7.573291000	-6.273300000	-1.534498000	6	7.716752000	-6.138481000	-1.450910000
6	8.676604000	-5.985726000	-2.375294000	6	8.880226000	-5.780356000	-2.179477000
6	8.675062000	-4.809273000	-3.116253000	6	8.917704000	-4.554267000	-2.837468000
6	7.597857000	-3.922786000	-3.041329000	6	7.824320000	-3.690604000	-2.791375000
6	8.562618000	8.299833000	-2.985803000	6	8.308069000	8.516432000	-3.033316000
6	9.851293000	3.876205000	-0.200738000	6	9.848629000	4.033872000	-0.476933000
6	10.834132000	-6.609581000	-3.105250000	6	11.092827000	-6.336868000	-2.792914000
7	0.153880000	0.793735000	3.901069000	7	0.179561000	0.349243000	3.953236000
7	2.545450000	0.211849000	1.378573000	7	2.574670000	0.056008000	1.301578000
7	2.492296000	-0.287060000	-1.445031000	7	2.538179000	-0.255280000	-1.435253000
8	9.256180000	7.316519000	1.710535000	8	9.113738000	7.274405000	1.591843000
8	9.489132000	5.253227000	3.247528000	8	9.497325000	5.148698000	2.995060000
8	7.550318000	-6.888871000	3.199636000	8	7.440844000	-7.114667000	3.176471000
8	9.653694000	-6.526584000	1.747012000	8	9.647519000	-6.662710000	1.922094000
8	8.892729000	7.077516000	-2.387834000	8	8.687027000	7.286082000	-2.478134000
8	9.480951000	4.970298000	-0.994599000	8	9.391997000	5.159398000	-1.176594000
8	7.672120000	-7.406257000	-0.810975000	8	7.778759000	-7.316915000	-0.803305000
8	9.673477000	-6.898002000	-2.377234000	8	9.884383000	-6.677853000	-2.168877000

Table S10 The DFT calculated geometry of compound **3** in the S_0 and T_1 states given in *xyz* format. Calculated at M06/def2-SVP level with D3 correction and C-PCM (toluene) model.

S_0 geometry				T_1 geometry			
6	-0.952620000	-3.249325000	-1.908231000	6	-0.904698000	-3.281104000	-2.130393000
6	-0.208186000	-4.423299000	-1.937857000	6	-0.156052000	-4.449502000	-2.167467000
6	1.151994000	-4.446738000	-2.314625000	6	1.209593000	-4.465440000	-2.534173000
6	1.727735000	-3.268040000	-2.803925000	6	1.784588000	-3.279942000	-3.007047000
6	0.995750000	-2.082993000	-2.800976000	6	1.044291000	-2.098178000	-3.005503000
6	-0.318517000	-2.074299000	-2.293371000	6	-0.274597000	-2.097097000	-2.503134000
6	1.356741000	-0.702563000	-3.058615000	6	1.392652000	-0.711121000	-3.242357000
6	0.246157000	0.082298000	-2.692996000	6	0.254869000	0.050369000	-2.895235000
6	0.256471000	1.460908000	-2.858845000	6	0.255771000	1.434302000	-3.031805000
6	1.444960000	2.058410000	-3.262404000	6	1.454657000	2.056669000	-3.356202000
6	2.616884000	1.315123000	-3.514056000	6	2.653063000	1.335863000	-3.552142000
6	2.535268000	-0.084393000	-3.469307000	6	2.584421000	-0.065294000	-3.565157000
6	1.989885000	-5.632949000	-2.033473000	6	2.042672000	-5.658417000	-2.265711000
6	1.656295000	-6.462440000	-0.944441000	6	1.677086000	-6.529425000	-1.219214000
6	2.475802000	-7.505124000	-0.539865000	6	2.476270000	-7.597029000	-0.839230000
6	3.689601000	-7.751714000	-1.225195000	6	3.705395000	-7.826426000	-1.502771000
6	4.017836000	-6.945234000	-2.311888000	6	4.070089000	-6.974313000	-2.541974000
6	3.177771000	-5.901541000	-2.711768000	6	3.247577000	-5.908756000	-2.921525000
6	3.918485000	1.997238000	-3.704720000	6	3.957322000	2.038719000	-3.581213000
6	5.110661000	1.348291000	-3.382269000	6	5.127262000	1.374152000	-3.203195000
6	3.996201000	3.345777000	-4.108105000	6	4.056860000	3.416508000	-3.864067000
6	5.207170000	4.025783000	-4.159630000	6	5.258710000	4.104962000	-3.741567000
6	6.405230000	3.344237000	-3.836386000	6	6.433368000	3.406120000	-3.369241000
6	6.339435000	2.009061000	-3.456357000	6	6.348947000	2.043070000	-3.108574000
7	-0.777582000	-0.741415000	-2.182196000	7	-0.745601000	-0.781566000	-2.380916000
8	4.445612000	-8.752433000	-0.739847000	8	4.434859000	-8.861429000	-1.048067000
8	2.220669000	-8.303083000	0.522141000	8	2.185722000	-8.440352000	0.177244000
6	1.193821000	-7.930672000	1.397149000	6	1.099299000	-8.131950000	1.003947000
8	7.540492000	4.073346000	-3.901039000	8	7.561653000	4.142286000	-3.273044000
6	5.717833000	-8.966071000	-1.293544000	6	5.724549000	-9.052965000	-1.566357000
6	8.731257000	3.494587000	-3.448497000	6	8.722682000	3.520048000	-2.796744000
8	5.346465000	5.327233000	-4.482831000	8	5.408913000	5.431699000	-3.930365000
6	4.195163000	6.107595000	-4.656894000	6	4.282842000	6.201271000	-4.256662000
6	-5.509933000	-2.625908000	-0.585280000	6	-5.550026000	-2.594687000	-0.472347000
6	-6.489608000	-3.582952000	-0.819743000	6	-6.536805000	-3.569891000	-0.528611000
6	-7.861945000	-3.259574000	-0.885508000	6	-7.913041000	-3.253044000	-0.554435000
6	-8.248568000	-1.928191000	-0.696304000	6	-8.295799000	-1.908185000	-0.515977000
6	-7.284516000	-0.947982000	-0.466066000	6	-7.324922000	-0.908222000	-0.458069000
6	-5.921127000	-1.305945000	-0.423825000	6	-5.957356000	-1.262607000	-0.442767000
6	-7.355982000	0.477015000	-0.218217000	6	-7.380633000	0.535848000	-0.380169000
6	-6.033324000	0.930354000	-0.034140000	6	-6.044429000	0.991230000	-0.317048000
6	-5.748519000	2.273653000	0.194685000	6	-5.740952000	2.349042000	-0.237621000
6	-6.818885000	3.156828000	0.262645000	6	-6.800353000	3.245937000	-0.209200000
6	-8.156605000	2.737025000	0.099606000	6	-8.148381000	2.826800000	-0.262393000
6	-8.412360000	1.384104000	-0.147739000	6	-8.425956000	1.458968000	-0.352540000
6	-8.871957000	-4.305569000	-1.153263000	6	-8.929876000	-4.324490000	-0.620630000
6	-8.701618000	-5.613977000	-0.659591000	6	-8.729577000	-5.544726000	0.054432000
6	-9.638414000	-6.610354000	-0.905390000	6	-9.671227000	-6.565188000	0.006303000
6	-10.795361000	-6.311671000	-1.668772000	6	-10.864311000	-6.383713000	-0.736685000
6	-10.964832000	-5.020584000	-2.157533000	6	-11.064836000	-5.180015000	-1.403981000
6	-10.012941000	-4.029093000	-1.903144000	6	-10.107879000	-4.162355000	-1.346958000
6	-9.265287000	3.711753000	0.178349000	6	-9.244437000	3.818350000	-0.222981000
6	-10.387537000	3.597717000	-0.639038000	6	-10.413477000	3.639351000	-0.959691000
6	-9.209461000	4.786193000	1.087736000	6	-9.130883000	4.977279000	0.569925000
6	-10.240043000	5.713496000	1.178723000	6	-10.147390000	5.922728000	0.625279000
6	-11.375510000	5.583711000	0.339474000	6	-11.329912000	5.725591000	-0.130382000
6	-11.431750000	4.523878000	-0.559559000	6	-11.445282000	4.581861000	-0.913311000
7	-5.161431000	-0.158623000	-0.161943000	7	-5.189058000	-0.104741000	-0.365432000

8	-11.654561000	-7.331697000	-1.860452000	8	-11.725965000	-7.421789000	-0.732037000
8	-9.544968000	-7.878090000	-0.457279000	8	-9.549441000	-7.751742000	0.636704000
6	-8.421375000	-8.241248000	0.294157000	6	-8.392914000	-7.994148000	1.385892000
8	-12.329121000	6.523592000	0.490305000	8	-12.267758000	6.689402000	-0.021150000
6	-12.817888000	-7.093056000	-2.601835000	6	-12.925952000	-7.292389000	-1.439641000
6	-13.480454000	6.438181000	-0.301439000	6	-13.462024000	6.538046000	-0.733981000
8	-10.260547000	6.756173000	2.032236000	8	-10.109745000	7.046290000	1.371129000
6	-9.171320000	6.937773000	2.892719000	6	-8.972044000	7.293694000	2.147290000
6	-0.953781000	0.019767000	0.162037000	6	-0.992087000	0.002289000	-0.059324000
6	-1.554176000	-0.374246000	-1.055399000	6	-1.563361000	-0.391922000	-1.279367000
6	-1.767295000	0.337620000	1.272973000	6	-1.757523000	0.378115000	1.054081000
6	-3.165095000	0.267231000	1.160604000	6	-3.202927000	0.323615000	0.955405000
6	-3.770219000	-0.105443000	-0.052935000	6	-3.782850000	-0.060960000	-0.264646000
6	-2.956282000	-0.423474000	-1.154450000	6	-3.011631000	-0.410847000	-1.383583000
6	-3.967875000	0.524716000	2.317515000	6	-4.000972000	0.615170000	2.084915000
7	-4.623957000	0.731787000	3.251191000	7	-4.640803000	0.874414000	3.026187000
6	-3.550669000	-0.741773000	-2.417309000	6	-3.627585000	-0.747105000	-2.611381000
7	-4.036403000	-0.996672000	-3.439144000	7	-4.117465000	-1.040832000	-3.628982000
6	-0.288584000	-1.554153000	3.189451000	6	-0.295239000	-1.524559000	2.960263000
6	0.854403000	-2.213340000	3.623137000	6	0.823188000	-2.212728000	3.407353000
6	2.040665000	-1.522369000	3.942625000	6	2.020181000	-1.553017000	3.764555000
6	2.025416000	-0.120754000	3.954329000	6	2.032044000	-0.153452000	3.803411000
6	0.884959000	0.561450000	3.532936000	6	0.912086000	0.560627000	3.372404000
6	-0.230592000	-0.171727000	3.085532000	6	-0.207507000	-0.140652000	2.877314000
6	0.582040000	1.961553000	3.292513000	6	0.641877000	1.967029000	3.141668000
6	-0.699092000	2.006183000	2.707030000	6	-0.617418000	2.031745000	2.497927000
6	-1.284979000	3.208999000	2.337401000	6	-1.178654000	3.254319000	2.133706000
6	-0.517212000	4.362894000	2.450087000	6	-0.415154000	4.396841000	2.315211000
6	0.811530000	4.343088000	2.926161000	6	0.897319000	4.358051000	2.846017000
6	1.328573000	3.132407000	3.406828000	6	1.391392000	3.130044000	3.308219000
6	3.301797000	-2.281240000	4.079335000	6	3.259922000	-2.344774000	3.907393000
6	3.317613000	-3.584813000	4.610035000	6	3.229820000	-3.664163000	4.397344000
6	4.460376000	-4.372667000	4.558464000	6	4.352450000	-4.480111000	4.352743000
6	5.626952000	-3.879259000	3.923125000	6	5.551379000	-3.996647000	3.772461000
6	5.630429000	-2.572118000	3.448099000	6	5.600941000	-2.676327000	3.337842000
6	4.481327000	-1.782261000	3.528750000	6	4.468330000	-1.860923000	3.405943000
6	1.671390000	5.539951000	2.782216000	6	1.755088000	5.561997000	2.796029000
6	3.048066000	5.413875000	2.594879000	6	3.147846000	5.459446000	2.747698000
6	1.113152000	6.830840000	2.689453000	6	1.192629000	6.849840000	2.678490000
6	1.891184000	7.940152000	2.384280000	6	1.980428000	7.975026000	2.479245000
6	3.283409000	7.786843000	2.166633000	6	3.389680000	7.843071000	2.390699000
6	3.844694000	6.521619000	2.294366000	6	3.954527000	6.583397000	2.555325000
7	-1.191989000	0.692248000	2.523391000	7	-1.113289000	0.743635000	2.275826000
8	6.648518000	-4.749790000	3.802922000	8	6.555609000	-4.888759000	3.662240000
8	4.545774000	-5.627408000	5.053019000	8	4.388099000	-5.752796000	4.803849000
6	3.367483000	-6.264402000	5.459716000	6	3.178705000	-6.376468000	5.135997000
8	3.950380000	8.903843000	1.816965000	8	4.068547000	8.973788000	2.121134000
6	7.778794000	-4.356615000	3.071413000	6	7.711412000	-4.512043000	2.963995000
6	5.325707000	8.813530000	1.553536000	6	5.461640000	8.904944000	1.984119000
8	1.414141000	9.195405000	2.244934000	8	1.502787000	9.226774000	2.325135000
6	0.041960000	9.412480000	2.413931000	6	0.115106000	9.419469000	2.331527000
6	1.168678000	-2.292314000	0.482210000	6	1.111938000	-2.341191000	0.289881000
6	2.275442000	-3.130149000	0.445224000	6	2.211903000	-3.192883000	0.291304000
6	3.581510000	-2.641756000	0.232913000	6	3.527772000	-2.717843000	0.133405000
6	3.771212000	-1.259300000	0.129289000	6	3.739811000	-1.327408000	0.063557000
6	2.675367000	-0.398164000	0.177974000	6	2.656325000	-0.462320000	0.078565000
6	1.374110000	-0.927646000	0.311080000	6	1.343574000	-0.978920000	0.137280000
6	2.538183000	1.037647000	0.067939000	6	2.529514000	0.980145000	-0.005013000
6	1.159078000	1.319742000	0.106490000	6	1.134863000	1.252866000	-0.047331000
6	0.690707000	2.614063000	-0.072862000	6	0.657761000	2.557680000	-0.219100000
6	1.618819000	3.625298000	-0.260698000	6	1.576568000	3.580387000	-0.280086000
6	3.010475000	3.388257000	-0.308053000	6	2.978640000	3.354612000	-0.227499000
6	3.451722000	2.070565000	-0.130727000	6	3.433961000	2.016504000	-0.088137000

6	4.718911000	-3.569736000	0.059048000	6	4.662844000	-3.643776000	-0.027147000
6	4.789831000	-4.794242000	0.753176000	6	4.699542000	-4.899666000	0.612332000
6	5.850462000	-5.672534000	0.558123000	6	5.757304000	-5.778179000	0.408506000
6	6.886793000	-5.330974000	-0.347659000	6	6.824483000	-5.405389000	-0.451498000
6	6.818168000	-4.126882000	-1.036739000	6	6.788977000	-4.169786000	-1.086486000
6	5.742923000	-3.256739000	-0.834907000	6	5.719559000	-3.298399000	-0.872875000
6	3.962567000	4.479664000	-0.622504000	6	3.920671000	4.451949000	-0.392391000
6	5.334398000	4.247378000	-0.727321000	6	5.313961000	4.229811000	-0.371323000
6	3.509989000	5.787906000	-0.887193000	6	3.478937000	5.775494000	-0.630800000
6	4.373317000	6.796063000	-1.293012000	6	4.364829000	6.799969000	-0.902994000
6	5.747991000	6.515541000	-1.469079000	6	5.761824000	6.522250000	-0.980682000
6	6.212799000	5.246325000	-1.147040000	6	6.214708000	5.243573000	-0.654701000
7	0.446938000	0.124667000	0.262742000	7	0.434138000	0.082084000	0.042810000
8	7.885560000	-6.235581000	-0.466742000	8	7.816316000	-6.310043000	-0.580647000
8	6.006458000	-6.854624000	1.178978000	8	5.884270000	-6.988473000	0.973208000
6	5.048292000	-7.268753000	2.120615000	6	4.923473000	-7.414248000	1.908503000
8	6.510421000	7.523248000	-1.939318000	8	6.539492000	7.534274000	-1.357816000
6	8.940418000	-5.945623000	-1.339789000	6	8.885505000	-6.010019000	-1.435130000
6	7.791661000	7.203708000	-2.419995000	6	7.886788000	7.266367000	-1.684325000
8	3.998293000	8.065409000	-1.565595000	8	4.026034000	8.074040000	-1.143667000
6	2.654732000	8.422943000	-1.393626000	6	2.671436000	8.444870000	-1.081722000