Supporting Information:

Design of Efficient Thermally Activated Delayed Fluorescence Materials for Pure Blue Organic Light Emitting Diodes

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Table and Figures

Table S1. Photophysical and molecular orbital data for compounds **1**, **2** and **3** at room temperature.

	Emission in toluene (1×10^{-4} M)			Emission in DPEPO film (10 wt%)			HOMO[a]	LUMO[b]
	$\lambda_{max,}$ (nm)	ϕ	τ (ns/μs)	$\lambda_{max,}$ (nm)	ϕ	τ (ns/ms/ms)	(eV)	(eV)
1	402	0.57	2.2/90	421	0.60	3.5/0.85	5.89	2.62
2	419	0.65	3.1/140	430	0.66	3.2/0.84/8.2	5.65	2.46
3	404	0.69	5.3/270	423	0.80	7.6/0.54/2.6	5.81	2.52

(a) Recorded in a neat film by AC-3 (Figure S1); (b) Obtained from the HOMO value minus the optical band gap.

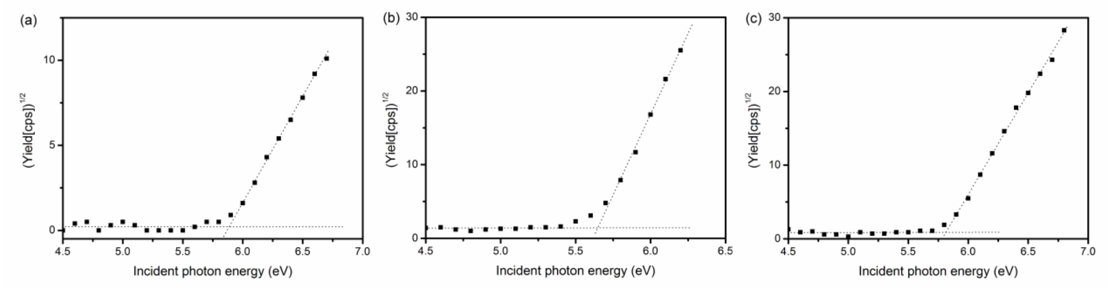


Figure S1. The photoelectron yield spectra of the neat films of compounds **1** (a), **2** (b) and **3** (c).

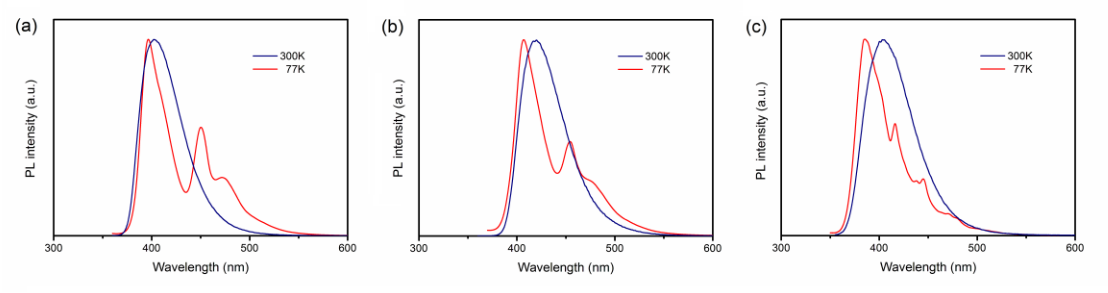


Figure S2. Emission spectra of compounds **1** (a), **2** (b) and **3** (c) in toluene at 77 K (without delay).

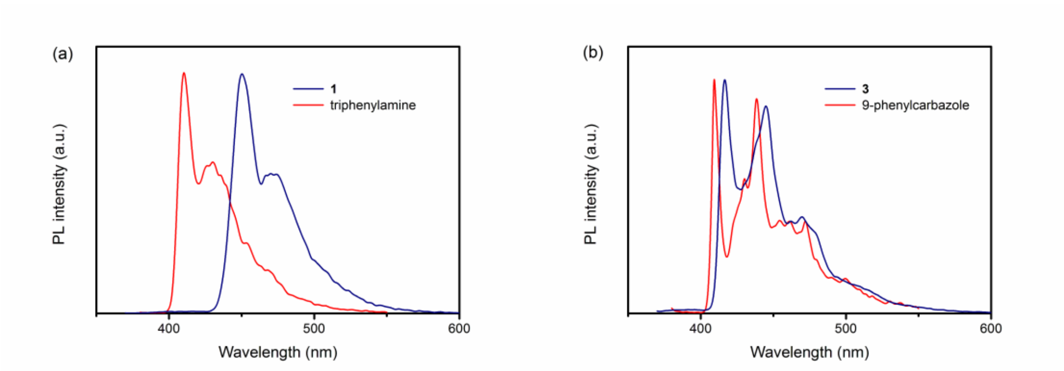


Figure S3. (a) Emission spectra of compound **1** and triphenylamine in toluene at 77 K with a 10 ms delay; (b) Emission spectra of compound **3** and 9-phenylcarbazole in toluene at 77 K with a 10 ms delay.

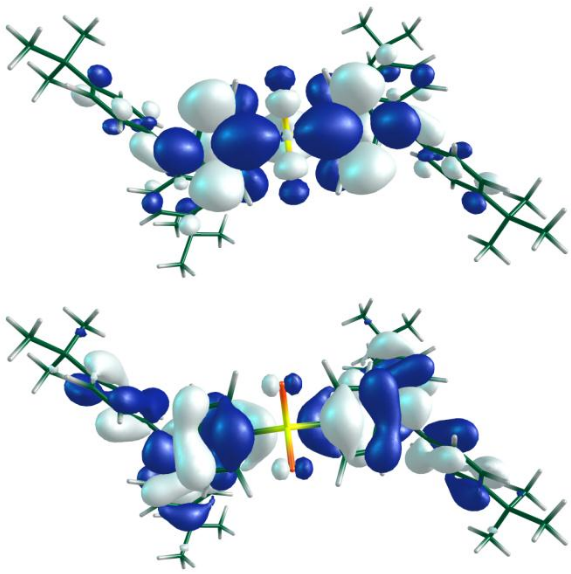


Figure S4. The HOMO (lower image) and LUMO (upper image) of compound **2** calculated at the B3LYP/6-31G* level. The calculated S_1 and T_1 energies of **2** are 3.46 and 2.86 eV, respectively, corresponding to the experimental values of 3.19 and 2.74 eV, respectively.

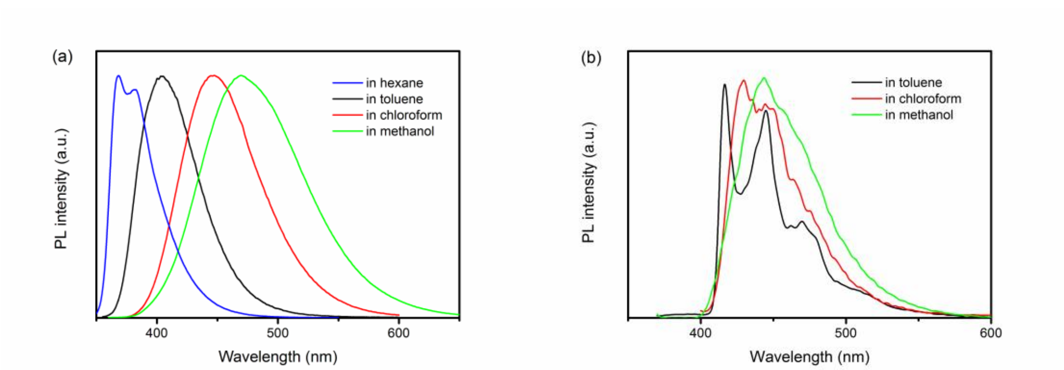


Figure S5. (a) Emission spectra of compound **3** in various solvents at 300 K; (b) Phosphorescent spectra of compound **3** in various solvents at 77 K (10 ms delay).

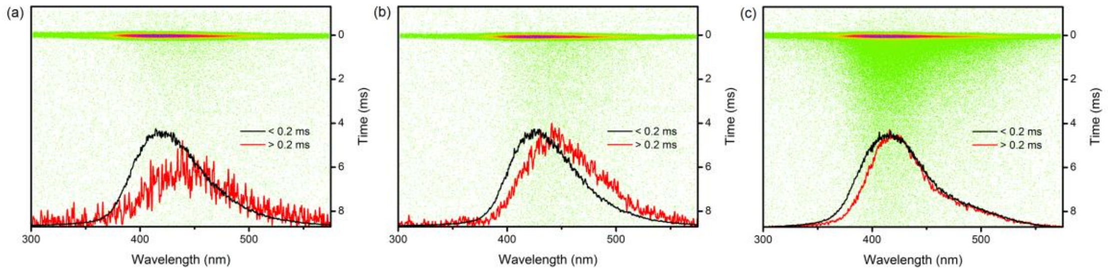


Figure S6. Streak image of a DPEPO film doped with 10 wt% of compounds **1** (a), **2** (b) or **3** (c) at 300 K.

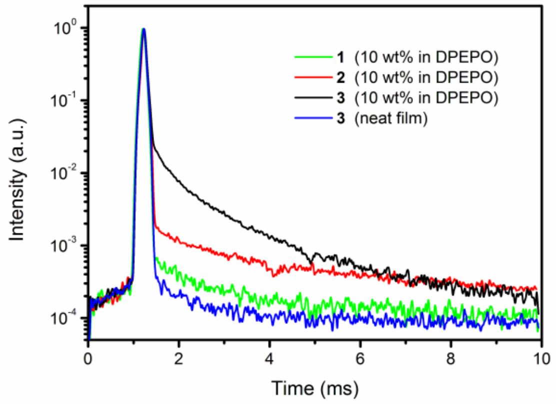


Figure S7. Emission decay of compounds **1**, **2** and **3** doped in DPEPO films at 300 K.

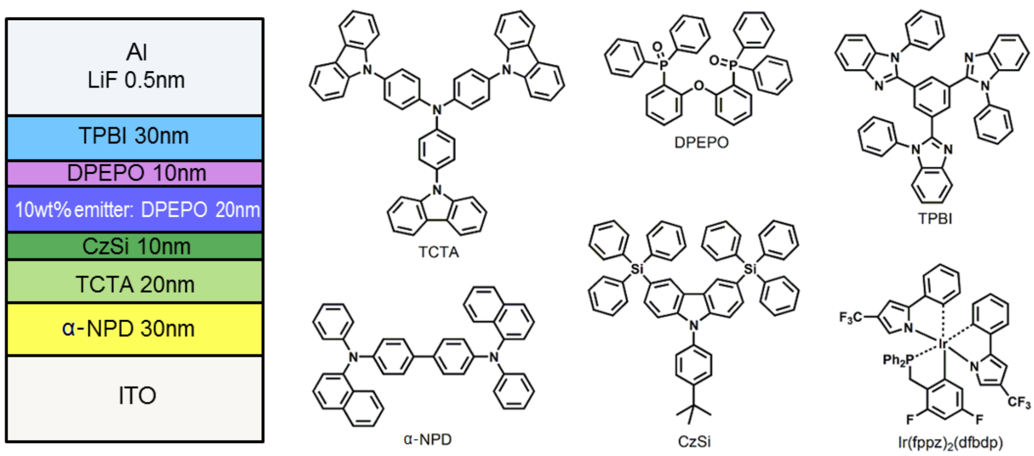


Figure S8. OLED device structure and the molecular structures of the compounds used in this device.

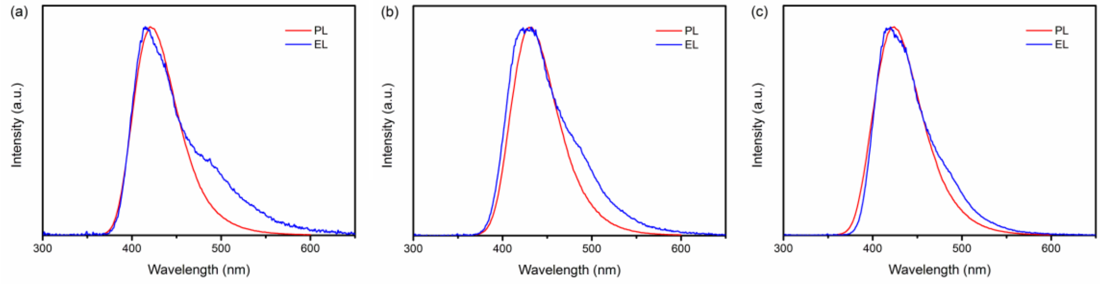


Figure S9. The EL and PL spectra of 10 wt% of compounds **1** (a), **2** (b) and **3** (c) doped in DPEPO layers.

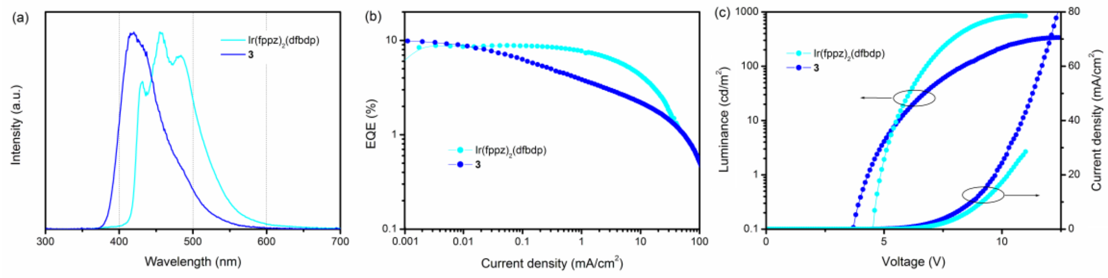


Figure S10. Comparison between the EL spectra, EQE-current density characteristics and luminance-current density-voltage characteristics of the OLEDs based on Ir(fppz)$_2$(dfbdp) and on compound **3**. It should be noted that the human eyes are insensitive to a pure blue emission. Therefore, the luminance of a pure blue OLED should be much lower than that of a green or sky-blue OLED with the same EQE at a same current density. For example, with an EQE of 9.0%, the current efficiency and luminance of a green OLED based on *fac*-tris(2-phenylpyridine) iridium (Ir(ppy)$_3$) are about 36 cd/A and 3.6 cd/m^2, respectively, at the current density of 0.01 mA/cm^2. However, the corresponding values are only 13 cd/A and 1.3 cd/m^2 for a deep blue OLED based on Ir(fppz)$_2$(dfbdp), and 5.0 cd/A and 0.5 cd/m^2 for a pure blue OLED based on compound **3**.

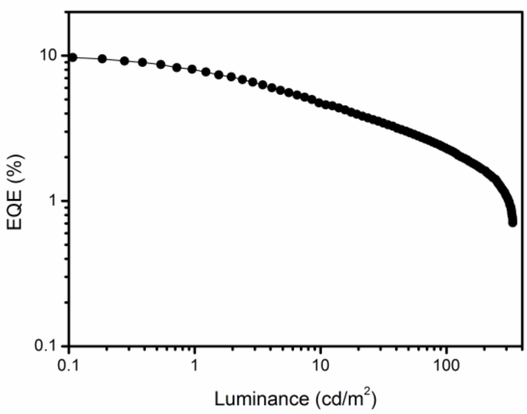


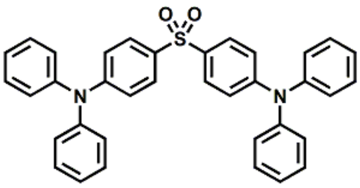
Figure S11. The EQE-luminance characteristics of the OLED based on compound **3**.

Experimental

1. Materials: Spectral grade solvents and all starting materials were purchased from commercial resources and were used as received. DPEPO was prepared by procedures given in the literature [1] and was further purified twice by sublimation. Other OLED materials including $Ir(fppz)_2(dfbdp)$ were purchased from Luminescence Technology Corporation and were used without further purification.

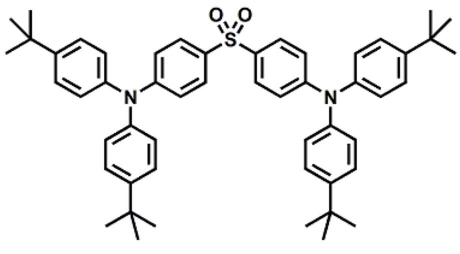
2. General: All reactions were carried out under N_2 atmospheres. ^1H nuclear magnetic resonance (NMR) and ^{13}C NMR spectra were recorded in $CDCl_3$ with a Bruker Avance 500 spectrometer operating at 500 MHz for ^1H NMR and 125 MHz for ^{13}C NMR. Chemical shifts (δ) are given in parts per million (ppm) relative to tetramethylsilane (TMS; δ=0) as the internal reference. ^1H NMR spectra data are reported as chemical shift, relative integral, multiplicity (s=singlet, d=doublet, m=multiplet), coupling constant (J in Hz) and assignment. Mass spectra were collected on a JEOL JMS-AX505HA by means of electronic impact at 70 eV ionization energy. Elemental analyses (C, H, N) were carried out with a Yanaco MT-5 CHN corder. The solution samples (0.1 mM) for the luminescence studies were degassed with nitrogen for several minutes prior to use unless otherwise indicated. Thin film samples (～100 nm) for the luminescence and photoelectron spectroscopy studies were deposited on quartz glass substrates by vacuum evaporation (pressure $<4\times10^{-4}$ Pa; rate≈0.2 nm/s). UV-VIS absorption spectra of the compounds in toluene were measured on a Perkin-Elmer Lambda 950-PKA UV/VIS spectrophotometer in the range of 280–600 nm. The photoluminescence spectra were recorded on a Jasco FP-6500 spectrofluorometer equipped with liquid nitrogen attachment at room temperature and 77 K. All samples were excited at 350 nm wavelength and measured at different time delays after the excitation. The absolute PL quantum yield (PLQY) was obtained by using an integrating sphere (C9920-02, Hamamatsu Photonics Co.) with a Xe lamp (λ_{max}=350 nm) as the excitation source and a multichannel spectrometer (Hamamatsu PMA-11) as the optical detector. The PLQY of the film samples was measured under nitrogen flow. The transient photoluminescence decay characteristics of the solution samples were recorded using a Quantaurus-Tau fluorescence lifetime measurement system (C11367-03, Hamamatsu Photonics Co.). The fast decay component was recorded in the TCC900 mode in conjunction with a 340 nm LED excitation source, while the slow decay component was recorded in the M9003-01 mode in conjunction with a flash lamp source. The transient photoluminescence decay characteristics of the film samples were investigated under vacuum conditions by using a streak camera (C4334, Hamamatsu Photonics Co.) equipped with a N_2 gas laser (MNL200, Laser Technik Berlin, λ=337 nm, pulse width≈500 ps, repetition rate=20 Hz) as the excitation source. The HOMO energy levels of the compounds in film state were determined by atmospheric ultraviolet photoelectron spectroscopy using a Riken Keiki AC-3.

3. Synthesis:



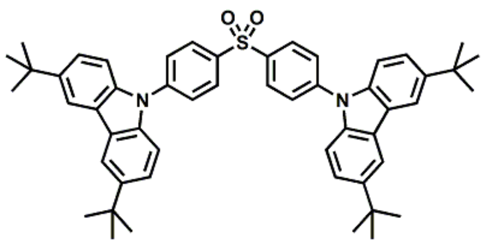
1

Synthesis of Bis[4-(diphenylamino)phenyl] sulfone (1): Diphenylamine (2.54 g, 15 mmol) was added to a solution of sodium hydride (0.72 g, 30 mmol) in dry dimethylformamide （DMF) (30 mL). After the solution was stirred at room temperature for 30 min, bis(p-fluorophenyl) sulfone (1.91 g, 7.5 mmol) in dry DMF (30 mL) was added, and then the mixture was stirred at 100 ℃ for an additional 1 h. After cooling, the mixture was poured into 400 ml of water, and the white precipitate was filtered and dried. The crude product was recrystallized from ethanol to produce white crystals (3.0 g) in 72% yield. ^{1}H NMR ($CDCl_3$, 500 MHz): δ [ppm] 7.68 (d, J = 9.0 Hz, 4H), 7.31 (t, J = 8.0 Hz, 8H), 7.16-7.12 (m, 12H), 6.98 (d, J = 9.0 Hz, 4H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ [ppm] 151.8, 146.2, 133.0, 129.7, 128.7, 126.1, 125.0, 119.7. FD-MS m/z: 552 $[M+1]^+$. Anal. Calcd for $C_{36}H_{28}N_2O_2S$: C, 78.23; H, 5.11; N, 5.07. Found: C, 78.25; H, 5.06; N, 5.13.



2

Synthesis of Bis{4-[bis(4-tert-butylphenyl)amine]phenyl} sulfone (2): A procedure similar to that used for **1** was followed but with bis(4-tert-butylphenyl)amine (4.22 g, 15 mmol) instead of diphenylamine. The crude product was recrystallized from chloroform and ethyl ether to produce white crystals (4.5 g) in 77% yield. ^{1}H NMR ($CDCl_3$, 500 MHz): δ [ppm] 7.64 (d, J = 9.0 Hz, 4H), 7.31 (d, J = 8.5 Hz, 8H), 7.05 (d, J = 8.5 Hz, 8H), 6.92 (d, J = 9.0 Hz, 4H), 1.32 (s, 36H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ [ppm] 152.0, 147.9, 143.4, 132.2, 128.6, 126.5, 125.7, 118.8, 34.5, 31.4. FD-MS m/z: 777 $[M+1]^+$. Anal. Calcd for $C_{52}H_{60}N_2O_2S$: C, 80.37; H, 7.78; N, 3.60. Found: C, 80.48; H, 7.76; N, 3.64.



3

Synthesis of Bis[4-(3,6-Di-tert-butylcarbazole)phenyl] sulfone (3): A procedure similar to that used for **1** was followed but with 3,6-Di-tert-butylcarbazole (4.19 g, 15 mmol) instead of diphenylamine. The crude product was recrystallized from chloroform and methanol to produce white crystals (4.2 g) in 73% yield. ^{1}H NMR ($CDCl_3$, 500 MHz): δ [ppm] 8.24 (d, J = 8.5 Hz, 4H), 8.13 (s, 4H), 7.81 (d, J = 9.0 Hz, 4H), 7.49-7.43 (m, 8H), 1.46 (s, 36H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ [ppm] 144.1, 143.2, 138.8, 138.3, 129.6, 126.6, 124.1, 124.0, 116.5, 109.2, 34.8, 31.9. FD-MS m/z: 773 $[M+1]^+$. Anal. Calcd for $C_{52}H_{56}N_2O_2S$: C, 80.79; H, 7.30; N, 3.62. Found: C, 80.74; H, 7.26; N, 3.63.

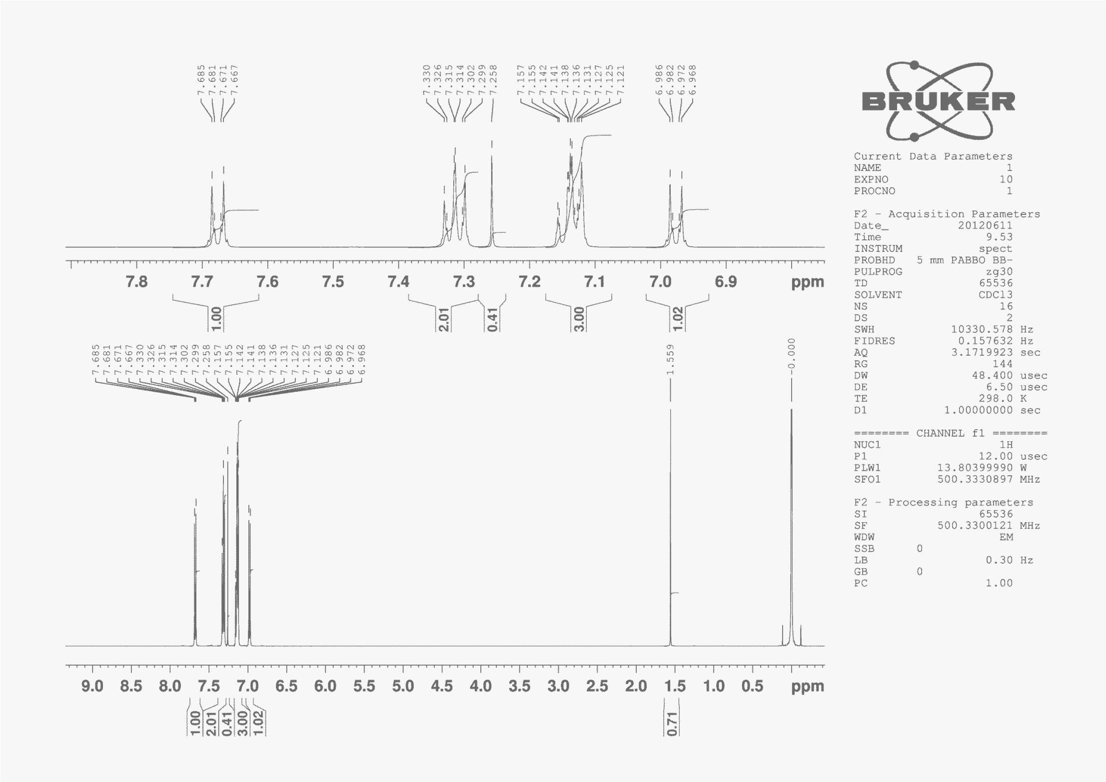


Figure S12. ^{1}H NMR spectra of compound **1**.

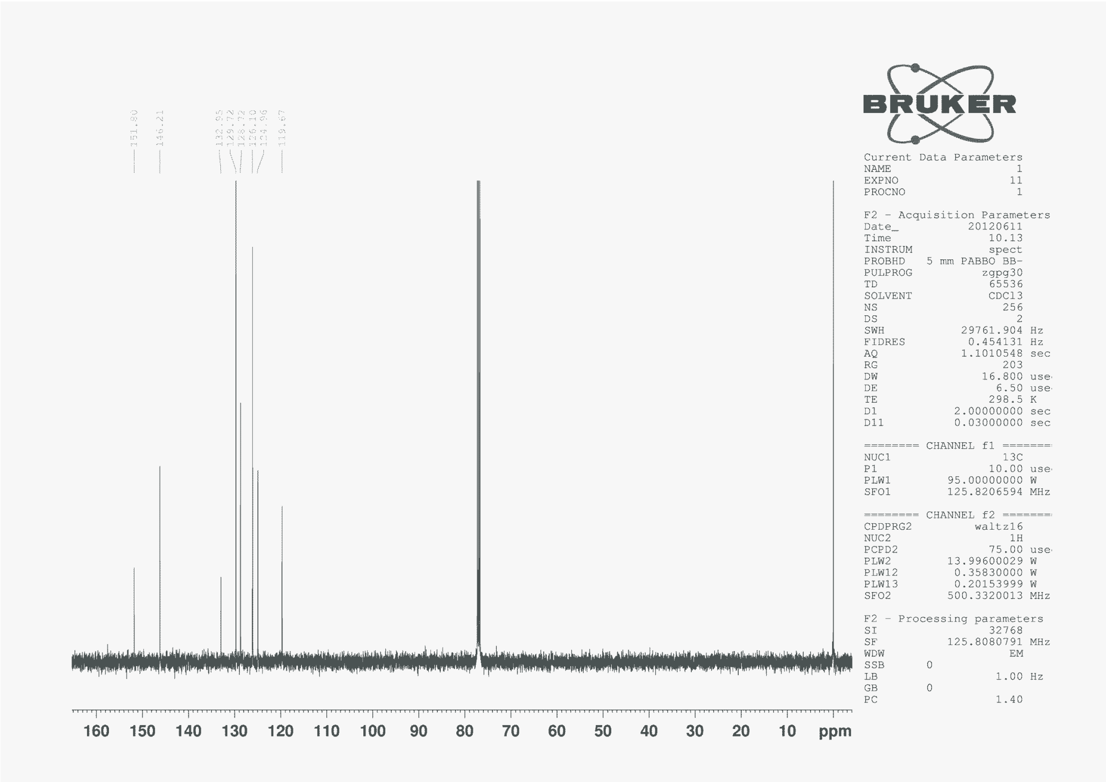


Figure S13. ^{13}C NMR spectra of compound **1**.

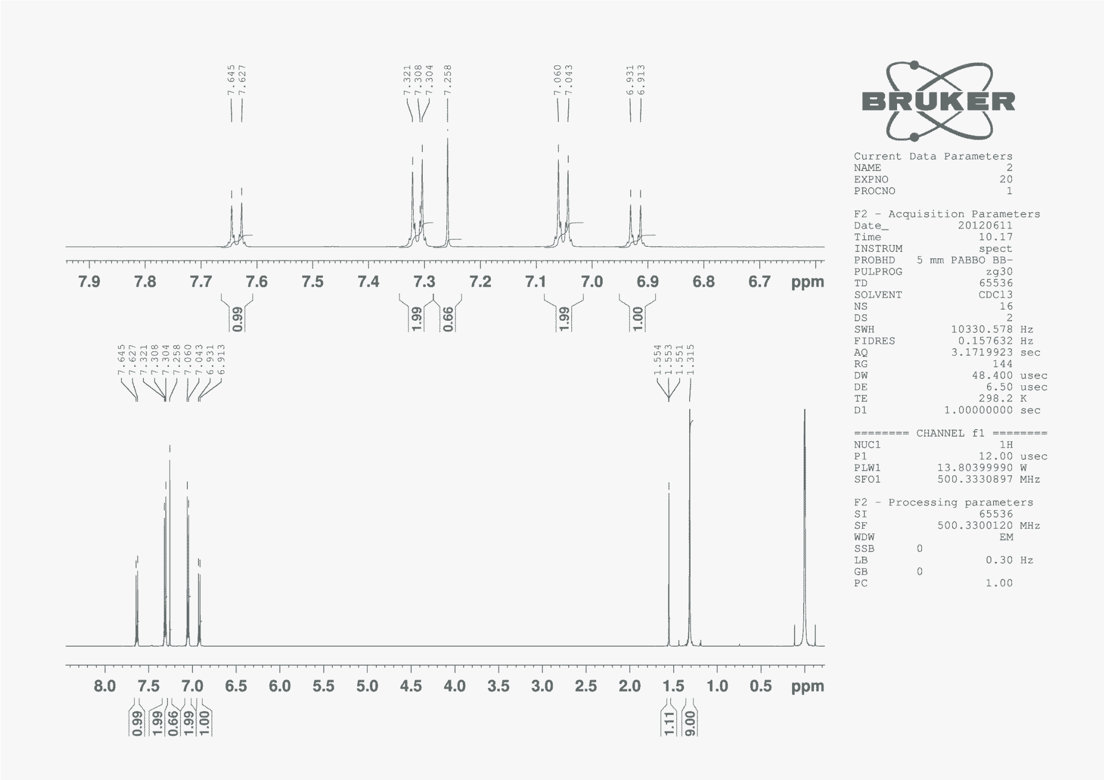


Figure S14. ^{1}H NMR spectra of compound **2**.

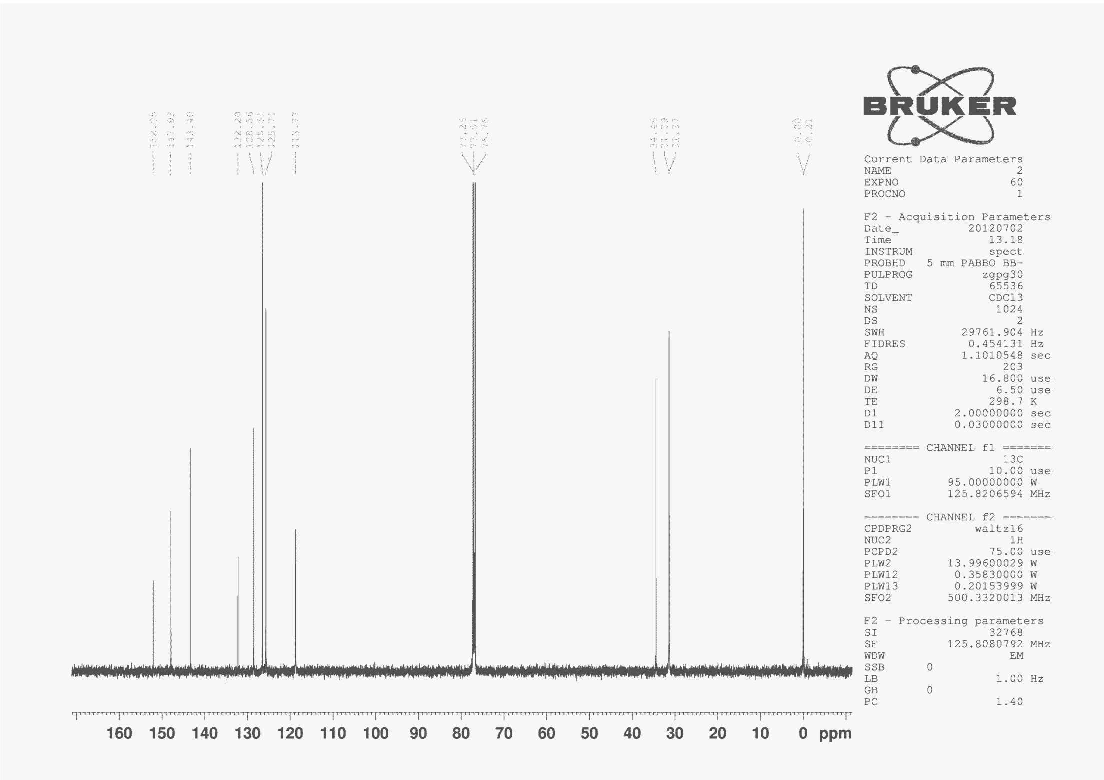


Figure S15. ^{13}C NMR spectra of compound **2**.

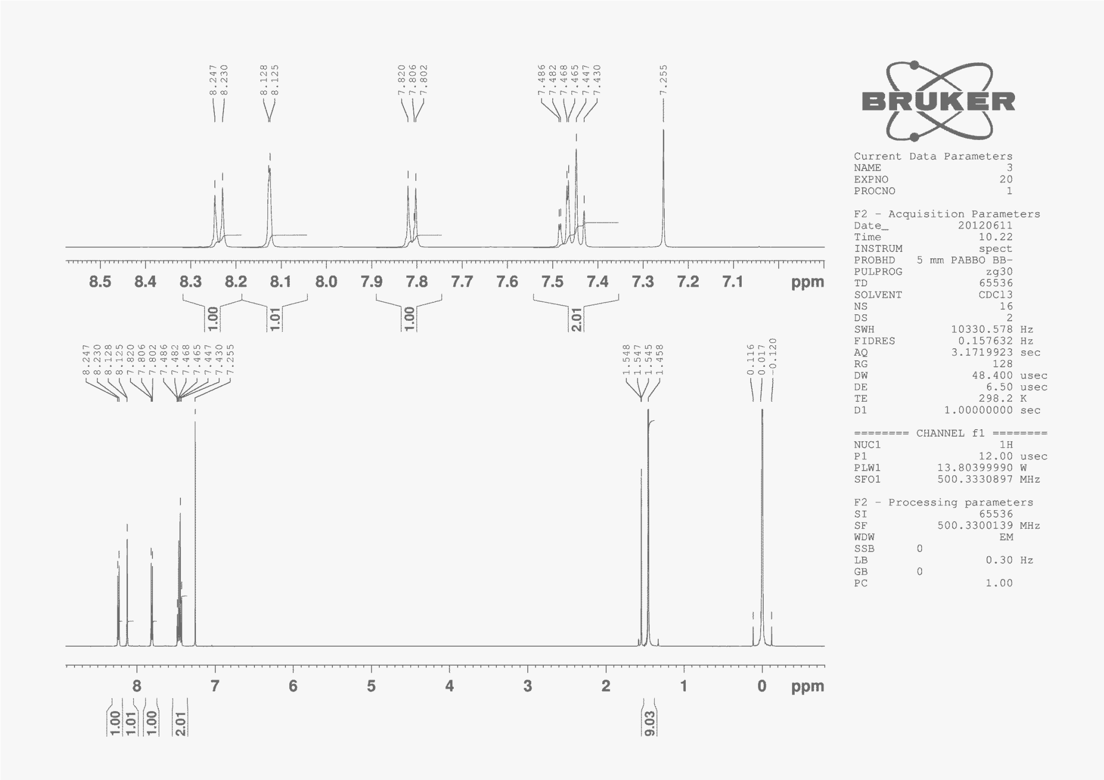


Figure S16. ^{1}H NMR spectra of compound **3**.

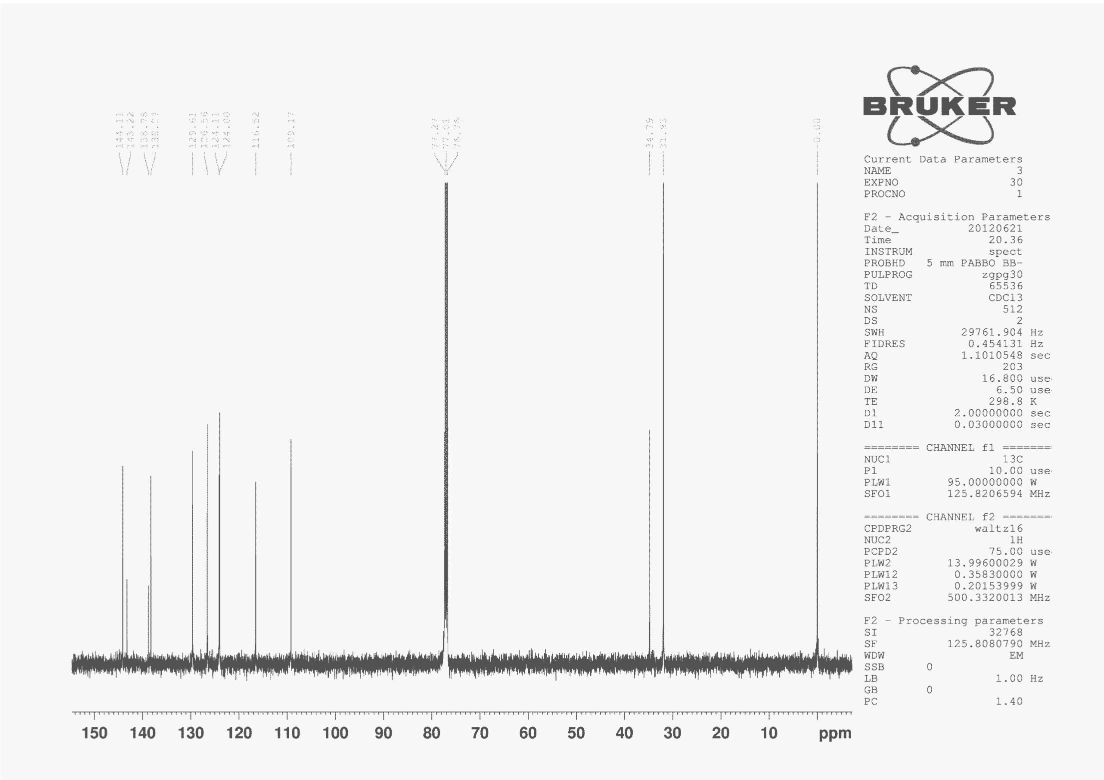


Figure S17. ^{13}C NMR spectra of compound **3**.

4. Quantum Chemical Calculations: All of the calculations were performed using the Gaussian 09 program package.[2] The geometries in the ground state were optimized via DFT calculations. The calculations for the excited state properties were based on TD-DFT level calculations. Both the ground and excited state calculations were performed with the B3LYP functional[3] using 6-31G* basis sets.[4]

Geometry Data for **1** (S_0 optimization: unit Å)

C	1.42860600	−1.71175100	−1.27270900
S	0.00000000	−2.58183700	−1.92166400
C	−1.42860600	−1.71175100	−1.27270900
C	−1.98385100	−2.09966000	−0.05069500
C	−3.08792800	−1.42390600	0.45437300
C	−3.66511100	−0.35607400	−0.26123200
C	−3.10128400	0.01128300	−1.49932200
C	−1.98991100	−0.65714400	−1.99754900
C	1.98385100	−2.09966000	−0.05069500
C	3.08792800	−1.42390600	0.45437300
C	3.66511100	−0.35607400	−0.26123200
C	3.10128500	0.01128300	−1.49932200
C	1.98991100	−0.65714400	−1.99755000
O	0.00000000	−3.92652800	−1.31887100
O	0.00000000	−2.38920400	−3.38265000
N	4.78975100	0.32499500	0.24620700
N	−4.78975100	0.32499500	0.24620700
C	5.76578000	−0.36445500	1.02636900
C	4.97989200	1.71345400	−0.01936000
C	−4.97989200	1.71345400	−0.01936000
C	−5.76578000	−0.36445500	1.02636900
C	6.27055000	−1.60401500	0.60511200
C	7.22564300	−2.26840800	1.37274400
C	7.70461200	−1.70070300	2.55539700
C	7.21170100	−0.46154300	2.96963800
C	6.24307400	0.20133900	2.21771000
C	6.23547300	2.18866400	−0.42607000
C	6.42673900	3.54858900	−0.66474900
C	5.37003300	4.44955400	−0.51817900
C	4.11768300	3.97742700	−0.11926300

C	3.92202100	2.62179000	0.13902000
C	−6.27055000	−1.60401500	0.60511200
C	−7.22564300	−2.26840800	1.37274400
C	−7.70461200	−1.70070400	2.55539600
C	−7.21170100	−0.46154400	2.96963800
C	−6.24307400	0.20133900	2.21771000
C	−6.23547300	2.18866400	−0.42607000
C	−6.42673900	3.54859000	−0.66474900
C	−5.37003300	4.44955400	−0.51817800
C	−4.11768300	3.97742800	−0.11926300
C	−3.92202100	2.62179000	0.13902000
H	−1.55539700	−2.93345300	0.49568100
H	−3.51247000	−1.72186400	1.40670800
H	−3.55010600	0.81374000	−2.07433500
H	−1.57788000	−0.39000500	−2.96513000
H	1.55539700	−2.93345300	0.49568100
H	3.51247000	−1.72186400	1.40670800
H	3.55010600	0.81373900	−2.07433600
H	1.57788000	−0.39000500	−2.96513000
H	5.91173100	−2.04087100	−0.32171000
H	7.60691000	−3.22827300	1.03476300
H	8.45455600	−2.21791800	3.14698100
H	7.57245500	−0.01100500	3.89047000
H	5.85230600	1.15938800	2.54606600
H	7.05505300	1.48812900	−0.55152100
H	7.40505200	3.90193800	−0.97948000
H	5.52084400	5.50774300	−0.71153900
H	3.28908000	4.66919500	0.00732400
H	2.95182500	2.25927600	0.46426300
H	−5.91173100	−2.04087000	−0.32171000
H	−7.60691100	−3.22827300	1.03476300
H	−8.45455600	−2.21791800	3.14698100
H	−7.57245500	−0.01100600	3.89047000
H	−5.85230600	1.15938800	2.54606600
H	−7.05505300	1.48812900	−0.55152000
H	−7.40505200	3.90193800	−0.97947900
H	−5.52084400	5.50774300	−0.71153900
H	−3.28908000	4.66919500	0.00732400
H	−2.95182500	2.25927600	0.46426300

Geometry Data for **2** (S_0 optimization: unit Å)

C	−1.41592800	0.13977400	−2.93032500
S	−0.00242800	−0.05443800	−4.01747500

C	1.41482800	-0.21999600	-2.93078700
O	0.15801500	1.21236000	-4.75354100
O	-0.16567800	-1.34012700	-4.71941200
C	1.82229500	-1.48737900	-2.50620100
C	2.91860400	-1.61645100	-1.66273300
C	3.62238000	-0.47863900	-1.21868000
C	3.20065600	0.79108200	-1.66253000
C	2.11136100	0.91781800	-2.51527800
C	-1.81202700	1.41720000	-2.52497700
C	-2.90437200	1.56831400	-1.68025100
C	-3.61600100	0.44333700	-1.21673600
C	-3.20656600	-0.83643400	-1.64186900
C	-2.12019900	-0.98564100	-2.49514200
N	-4.71757600	0.59711700	-0.35231400
N	4.72707200	-0.60890000	-0.35531600
C	-5.81301700	-0.31547200	-0.40261500
C	-4.74940800	1.65529300	0.60290200
C	4.78186900	-1.66336000	0.60320000
C	5.80985900	0.31873400	-0.41550800
C	-3.63322500	1.94780800	1.39474600
C	-3.67616200	2.98518100	2.32662000
C	-4.83033800	3.75561000	2.52401000
C	-5.94574600	3.43709700	1.72955500
C	-5.91236600	2.41826800	0.78329300
C	5.95446800	-2.40471700	0.78235400
C	6.01484600	-3.41767500	1.74024300
C	4.91307100	-3.74406400	2.54251300
C	3.74168000	-2.99196400	2.34354400
C	3.67195900	-1.96738200	1.40592900
C	6.38791000	0.67429900	-1.63891700
C	7.44146100	1.58796800	-1.68648100
C	7.97361900	2.16428400	-0.52484500
C	7.38945000	1.78213200	0.69572700
C	6.32680300	0.88711400	0.75747100
C	-6.39292700	-0.67870400	-1.62308300
C	-7.45879000	-1.57815200	-1.66201700
C	-8.00204900	-2.13236900	-0.49468900
C	-7.41620100	-1.74235900	0.72248800
C	-6.34137400	-0.86134200	0.77601900
C	-4.91102300	4.90233100	3.54696700
C	-3.59115800	5.09109800	4.31851900
C	-6.02991400	4.60218300	4.57300200
C	-9.17811200	-3.12476000	-0.50296400
C	-8.72869800	-4.46020800	0.13664100

C	-9.68245500	-3.42162600	-1.92794800
C	9.13711400	3.17129500	-0.54229700
C	9.63922300	3.45976000	-1.96974400
C	10.32070000	2.60786000	0.27997600
C	4.94307100	-4.86059300	3.60093000
C	3.87212200	-5.92409300	3.25923200
C	4.63992400	-4.25966100	4.99422700
C	6.31210100	-5.56327700	3.67053000
C	8.67086900	4.50755100	0.08327400
C	-10.35560500	-2.53882500	0.31219800
C	-5.23295700	6.22574400	2.81246300
H	1.30175900	-2.36821100	-2.86748600
H	3.24654300	-2.60249200	-1.35264600
H	3.73371400	1.67685500	-1.33550700
H	1.80216400	1.89691700	-2.86624700
H	-1.28600100	2.28815300	-2.90193900
H	-3.22310600	2.56150200	-1.38358700
H	-3.74634100	-1.71235600	-1.29953900
H	-1.81901500	-1.97247800	-2.83103900
H	-2.72600600	1.36245700	1.27978100
H	-2.78548300	3.17551000	2.91517300
H	-6.86564700	4.00527900	1.83769700
H	-6.78918300	2.20733400	0.17882600
H	6.82446500	-2.18484300	0.17123400
H	6.94596200	-3.96402300	1.84299100
H	2.86001400	-3.19602700	2.94491100
H	2.75516500	-1.39707000	1.29142700
H	6.00926800	0.23732200	-2.55801000
H	7.85497300	1.83532700	-2.65790700
H	7.76061000	2.20160800	1.62686600
H	5.89140500	0.62306900	1.71635000
H	-6.00588900	-0.25881900	-2.54662300
H	-7.87297000	-1.83217700	-2.63144300
H	-7.79562000	-2.14467500	1.65786400
H	-5.90493900	-0.59156200	1.73280900
H	-3.69503700	5.91639300	5.03183000
H	-2.75894800	5.33689800	3.64909000
H	-3.31951400	4.19515200	4.88837600
H	-6.10428800	5.41506300	5.30577300
H	-5.82476200	3.67258300	5.11618000
H	-7.00788000	4.49840500	4.09131900
H	-9.55828800	-5.17780100	0.14482500
H	-8.39537800	-4.32510900	1.17098200
H	-7.90023000	-4.90502900	-0.42628500

H	−10. 51433400	−4. 13351200	−1. 88409800
H	−8. 90025600	−3. 86674500	−2. 55336700
H	−10. 04781800	−2. 51768300	−2. 42847600
H	10. 46197500	4. 18254400	−1. 93248100
H	8. 85205300	3. 88841300	−2. 60040000
H	10. 01658600	2. 55544000	−2. 46056600
H	11. 15655600	3. 31819700	0. 28190500
H	10. 67868100	1. 66289900	−0. 14444300
H	10. 04102600	2. 42070200	1. 32214500
H	3. 87444300	−6. 72356800	4. 01027100
H	4. 06713200	−6. 37663200	2. 28029600
H	2. 86509200	−5. 49448600	3. 23356300
H	4. 65334900	−5. 04516400	5. 75980000
H	3. 65573300	−3. 78055500	5. 02717300
H	5. 38789200	−3. 50642700	5. 26699500
H	6. 28592500	−6. 34724500	4. 43563000
H	7. 11472700	−4. 86697500	3. 93915600
H	6. 57577800	−6. 03933800	2. 71924100
H	9. 49166000	5. 23520400	0. 08473900
H	8. 33828800	4. 37911500	1. 11869200
H	7. 83758700	4. 93643100	−0. 48489000
H	−11. 19980800	−3. 23914500	0. 32031600
H	−10. 70179500	−1. 59406900	−0. 12231300
H	−10. 07500300	−2. 34441700	1. 35278200
H	−5. 30372100	7. 05319600	3. 52910100
H	−6. 18372700	6. 17133100	2. 27182000
H	−4. 44957900	6. 47099700	2. 08628200

Geometry Data for **3** (S_0 optimization: unit Å)

C	−1. 42241700	−3. 24037900	0. 10091000
S	0. 00000500	−4. 33837200	0. 00001200
C	1. 42242300	−3. 24037500	−0. 10088900
O	−0. 09110300	−5. 05249200	−1. 28406000
O	0. 09111600	−5. 05248800	1. 28408700
C	2. 05428800	−2. 82100300	1. 07153900
C	3. 14463800	−1. 95995600	0. 99272700
C	3. 61817500	−1. 53118500	−0. 25750800
C	2. 98659500	−1. 97928000	−1. 42883800
C	1. 88553100	−2. 82653500	−1. 35158300
C	−2. 05427300	−2. 82100200	−1. 07152000
C	−3. 14462400	−1. 95995800	−0. 99271200
C	−3. 61817300	−1. 53119500	0. 25752100
C	−2. 98660300	−1. 97929600	1. 42885300

C	-1.88553500	-2.82654700	1.35160200
N	-4.72584200	-0.65989700	0.33739900
N	4.72584100	-0.65988500	-0.33739100
C	-5.95014400	-0.81331900	-0.33556000
C	-6.79794500	0.26992100	-0.00065300
C	-6.05658600	1.12120100	0.90958700
C	-4.79192500	0.52052300	1.09663500
C	5.95015200	-0.81331200	0.33555100
C	6.79795000	0.26993000	0.00064000
C	6.05657800	1.12121800	-0.90958100
C	4.79191400	0.52054100	-1.09661800
C	-6.39824200	-1.83515700	-1.17051600
C	-7.69105400	-1.74219800	-1.68748500
C	-8.55671300	-0.66872800	-1.39331100
C	-8.08687900	0.33273600	-0.53371700
C	-6.35941800	2.32990600	1.54861200
C	-5.41586900	2.95678300	2.36612500
C	-4.15366000	2.33532000	2.51286800
C	-3.82286200	1.13454600	1.89306500
C	6.39826100	-1.83515500	1.17049500
C	7.69108100	-1.74220200	1.68744500
C	8.55673900	-0.66873300	1.39326200
C	8.08689200	0.33273800	0.53368300
C	6.35940100	2.32992900	-1.54860000
C	5.41584000	2.95681300	-2.36609400
C	4.15363000	2.33535200	-2.51282400
C	3.82284100	1.13457200	-1.89302900
C	-9.98168000	-0.57017200	-1.97299400
C	-5.69347100	4.28600800	3.09311500
C	5.69343100	4.28604600	-3.09307300
C	9.98171400	-0.57018100	1.97292500
C	4.68700800	5.35887000	-2.61282600
C	5.53661000	4.08531200	-4.61944200
C	7.11605900	4.81275500	-2.82537900
C	11.01066400	-0.56398500	0.81749600
C	10.32097800	-1.74801900	2.90669400
C	10.11929600	0.73880900	2.78649900
C	-10.11920000	0.73873300	-2.78671500
C	-11.01063500	-0.56380200	-0.81757000
C	-5.53667500	4.08525600	4.61948500
C	-7.11609300	4.81272100	2.82540300
C	-10.32099300	-1.74809800	-2.90663400
C	-4.68703900	5.35883600	2.61289600
H	1.69526900	-3.17087500	2.03367800

H	3.62651900	−1.60496100	1.89732500
H	3.37897000	−1.68038000	−2.39498600
H	1.40974000	−3.19789400	−2.25306100
H	−1.69524500	−3.17086700	−2.03365900
H	−3.62649900	−1.60495800	−1.89731300
H	−3.37898600	−1.68040200	2.39500000
H	−1.40975100	−3.19791100	2.25308200
H	−5.77417000	−2.68902900	−1.41205400
H	−8.02782200	−2.54018500	−2.33890400
H	−8.72715000	1.16982400	−0.26914400
H	−7.33654000	2.77368900	1.39202200
H	−3.39736800	2.80881500	3.13215100
H	−2.83607400	0.70309800	2.02335400
H	5.77419100	−2.68902900	1.41203600
H	8.02785800	−2.54019500	2.33885200
H	8.72716000	1.16982800	0.26910800
H	7.33652400	2.77371100	−1.39201900
H	3.39732900	2.80885300	−3.13209300
H	2.83605000	0.70312500	−2.02330900
H	4.86627400	6.31013400	−3.12903800
H	4.78506400	5.53254200	−1.53513300
H	3.65088900	5.06413100	−2.80981800
H	5.72121600	5.02738300	−5.15030700
H	4.52992300	3.74623700	−4.88542500
H	6.24879300	3.33986300	−4.99139000
H	7.26868800	5.75519600	−3.36343700
H	7.88278400	4.10891100	−3.16892200
H	7.28422700	5.01069400	−1.76058200
H	12.03102600	−0.48737500	1.21313500
H	10.85339100	0.27932800	0.13669100
H	10.94256200	−1.48543100	0.22809500
H	11.33852300	−1.62827100	3.29549900
H	10.28023600	−2.71015800	2.38343400
H	9.64341900	−1.79676400	3.76692700
H	11.13060700	0.82682500	3.20250000
H	9.40618900	0.75993300	3.61857200
H	9.93596700	1.62417500	2.16855900
H	−11.13050100	0.82673900	−3.20274200
H	−9.40608000	0.75973900	−3.61877900
H	−9.93585100	1.62416200	−2.16887200
H	−12.03099100	−0.48717300	−1.21322000
H	−10.85331400	0.27957000	−0.13684800
H	−10.94258700	−1.48519300	−0.22807600
H	−5.72129000	5.02732100	5.15035700

H	−4.52999300	3.74617900	4.88548000
H	−6.24886500	3.33980300	4.99141200
H	−7.26873100	5.75515500	3.36347000
H	−7.88282500	4.10887200	3.16892400
H	−7.28424400	5.01067300	1.76060600
H	−11.33850100	−1.62830600	−3.29552000
H	−10.28037400	−2.71017400	−2.38325000
H	−9.64338100	−1.79701500	−3.76681700
H	−4.86631300	6.31009400	3.12911600
H	−4.78507600	5.53251900	1.53520300
H	−3.65092300	5.06409300	2.80990300

5. Device Fabrication and Measurements: After the pre-cleaned indium tin oxide (ITO) glass substrates were treated with ozone for 15 min, a 30 nm thick NPB layer, a 20 nm thick TCTA layer and a 10 nm thick CzSi layer were deposited consecutively on the substrates in an inert chamber under a pressure of $<4\times10^{-4}$ Pa. Next, the blue dopant materials and the DPEPO host were co-evaporated to form a 20 nm thick emitting layer, and then a 10 nm thick non-doped DPEPO layer and a 30 nm thick TPBI layer were deposited. Finally, the cathode was fabricated by thermal evaporation of a LiF layer (0.7 nm), followed by an Al layer (100 nm). The deposition rates of the organic layers and the Al layer were 0.1-0.2 nm/s, while that of the LiF layer was 0.01 nm/s. The intersection of the ITO and the metal electrodes gave an active device area of 4 mm^2. The current density (J), voltage (V) and brightness (B) characteristics of the OLEDs were measured in ambient air with a semiconductor parameter analyzer (E5273A, Agilent) and an optical power meter (1930C, Newport). The EL spectra were recorded using a multi-channel spectrometer (UBS2000, Ocean Optics).

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