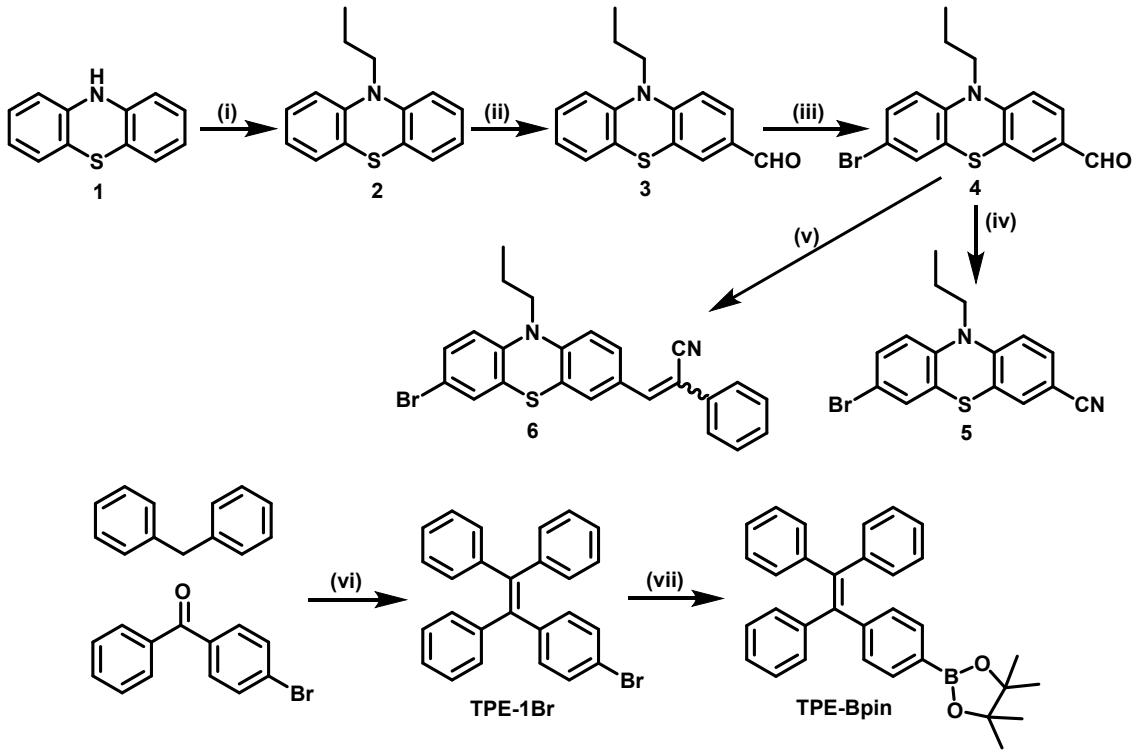
Supporting Information

Experimental details



Scheme S1. Synthetic route for intermediates (i). n-propyliodide, NaOH, DMSO, 12h, RT; (ii). DMF/$POCl_3$, DCE, 0 °C to reflux, overnight; (iii). NBS, THF, 0 °C to RT. 1.5h; (iv). $NH_2OH.HCl$, Pyridine, AcOH, DMF, reflux, 3.5h; (v). 2-phenylacetonitrile, NaOH(aq), THF, 70 °C, 12h; (vi). n-BuLi, THF, -5 °C to RT, overnight and then p-TSA, Toluene, 90 °C, 12 h; (vii). Bis(pinacolato)diboron, KOAc, Pd(dppf)Cl_2, 1,4-dioxane, 80 °C, 12 h.

Synthesis of 10-propyl-10H-phenothiazine (2)

Phenothiazine (5.0g, 25.1mmol) and propyl iodide (5.5g, 3.18mL, 32.6mmol) were dissolved in 50mL DMSO and stirred for 30min at room temperature. Sodium hydroxide (2.8g, 50mmol) was slowly added and stirred for overnight at room temperature. The reaction mixture was poured into water and extracted with dichloromethane. The organic layer was separated and dried over

anhydrous sodium sulfate. The product was purified using column chromatography with hexane. The product was obtained as white solid. Yield: 5.9g (97%).

Synthesis of 10-propyl-10H-phenothiazine-3-carbaldehyde (3)

Compound **2** (5 g, 1.0eq) and dry DMF (4.0eq) was dissolved in 1,2-dichloroethane then phosphorous oxychloride (4.0eq) was added slowly at 0 °C in an ice water bath. The mixture was heated to reflux for overnight and was quenched with water and extracted three times with dichloromethane. The combined organic fraction was washed with brine and dried over Na_2SO_4. The solvent was removed under reduced pressure and the residue was purified by column chromatography using silica gel and n-hexane/dichloromethane (1/1; v/v) as the eluent to give yellow solid (5.6 g, 79% yield).

Synthesis of 7-bromo-10-propyl-10H-phenothiazine-3-carbaldehyde (4)

NBS (1.1 eq) was added in one portion to the solution of **3** (1.5g, 1.0 eq) in THF (50 mL) at 0 °C. The mixture was allowed to room temperature and continued the stirring for 1.5 h Then the reaction was quenched by addition of water (50 mL) and extracted with DCM. The collected organic layer was evaporated under vacuum and the residue was purified by column chromatography to give the product as yellow solid (1.75g, 91% yield).

Synthesis of 7-bromo-10-propyl-10H-phenothiazine-3-carbonitrile (5)

A mixture of **4** (2.05 g, 1.0eq), hydroxylamine hydrochloride (1.2eq), acetic acid (3.3eq) and pyridine (1.5eq) in DMF (25 mL) was stirred and heated to 138 °C for 3.5 h under argon atmosphere. After cooling to room temperature, the reaction was quenched by water and the mixture was extracted with CH_2Cl_2. The organic layer was dried with anhydrous Na_2SO_4 and the solvent was removed by rotary evaporation. The crude product was further purified by column

chromatography (silica gel, hexane/dichloromethane 1/1 v/v) to give **5** as a light green solid (1.31 g, 66% yield).

Synthesis of 2-phenyl-3-(10-propyl-10H-phenothiazin-3-yl)acrylonitrile (6)

To a 50 mL schlenk flask capped with a rubber septum, 20 mL THF was injected via syringe. Compound **4 (**2.0g 1.0eq), phenyl acetonitrile (1.2eq), and aqueous solution of NaOH (2.0eq in 2 mL H_2O) were added to the flask. The resulting mixture was stirred for 12 h at 70 °C. The mixture was extracted with dichloromethane and aqueous solution of NH_4Cl and purified by silica gel column chromatograph with *n*-hexane/EtOAc (v/v = 10:2) to provide an isomeric E/Z form of **6** in 85% yield (1.61 g) as a red orange solid.

Synthesis of (2-(4-bromophenyl)ethene-1,1,2-triyl)tribenzene (TPE–1Br)

n-BuLi (5.8mL) was added dropwise to a solution of diphenylmethane (2.0 g, 11.8 mmol) in 30 mL THF and allowed to react for 30 minutes to produce an orange-red diphenyl lithium solution and cooled it to -5 °C and then 4-bromobenzophenone (2.48 g, 9.5 mmol) was added. The reaction mixture was stirred at room temperature for overnight, and then quenched with saturated NH_4Cl solution and extracted with dichloromethane; the organic phase was dried with anhydrous Na_2SO_4 and the desiccant was removed by suction filtration. The solvent was evaporated under reduced pressure to give the solid. Then the solid was dissolved in 25 mL toluene, and a catalytic amount of p-toluenesulfonic acid was added and allowed to reflux for 12 hours. The p-toluenesulfonic acid and the generated water were separated by an oil–water separator. The crude product was recrystallized from dichloromethane and methanol to give a white powder (3.0g). Yield: 61%.

Synthesis of 4,4,5,5-tetramethyl-2-(4-(1,2,2-triphenylvinyl)phenyl)-1,3,2-dioxaborolane (TPE–Bpin)

A mixture of **TPE-1Br** (1.5g, 1.0eq), Bis(pinacolato)diboron (1.2eq), KOAc (4.0eq) and Pd(dppf)Cl_2 (73mg, 0.1mmol) was dissolved in 40 mL 1,4-dioxane and purged with argon for 15 minutes and refluxed the reaction mixture for overnight. After completion of reaction solvents were dried and solid residue was worked up with dichloromethane/water. The organic layer was separated and dried over anhydrous sodium sulfate. The product was purified using column chromatography with hexane/dichloromethane (4/1 v/v). The product was obtained as white solid. Yield: 1.4g (84 %).

a). b)

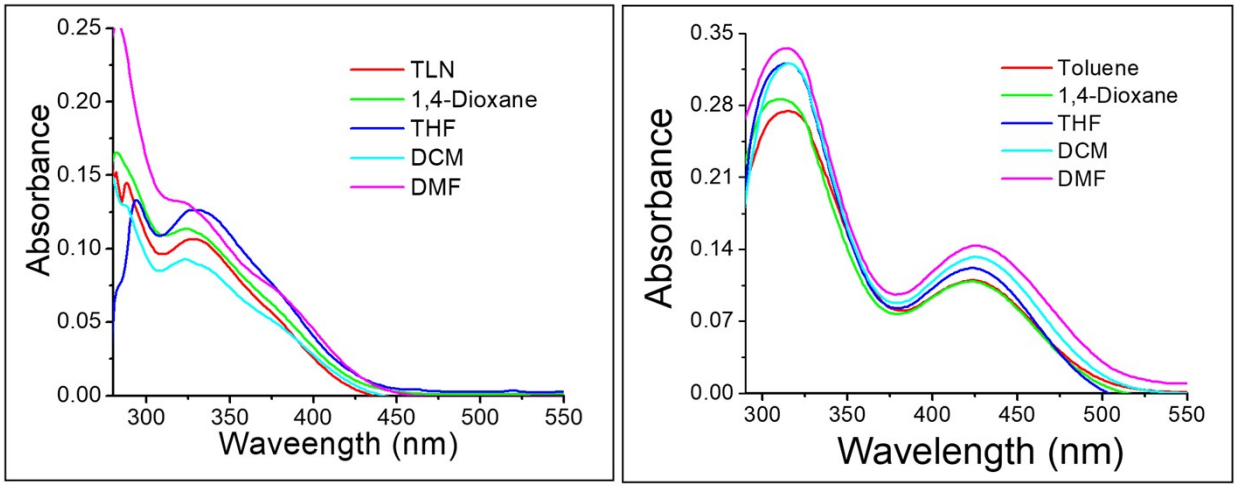


Figure S1 Absorption spectra of **PTZTPE-2** (a) and **PTZTPE-3** (b) in different polarity solvents.

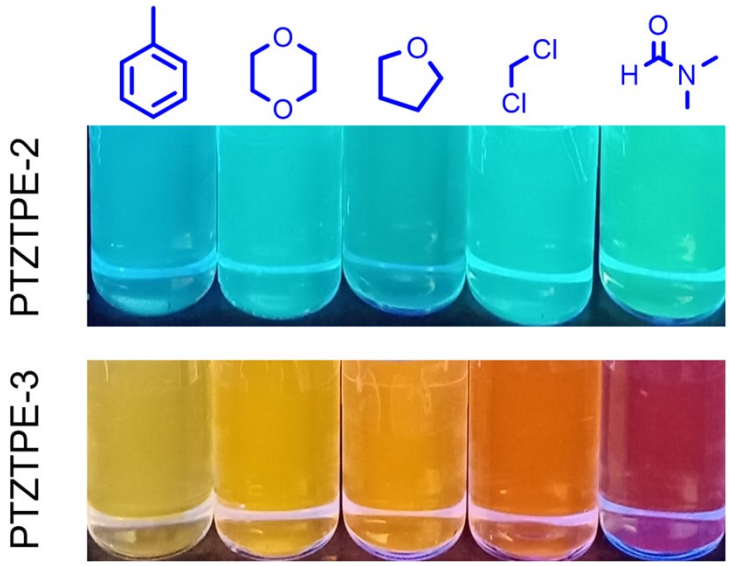


Figure S2 Photograph of compounds **PTZTPE-2** and **PTZTPE-3** in solvents of different polarity (from left to right, toluene to DMF) taken under 365 nm UV illumination.

Table S1 Photophysical properties of compounds **PTZTPE-2** and **PTZTPE-3**.

Compounds	**Solvent**	λ_{ab}**(nm)**[a]	λ_{em}**(nm)**[a]	**Stokes shift (cm^{-1})**
PTZTPE-2	Toluene	328	480	9655
	1,4-Dioxane	323	481	10170
	Tetrahydrofura	322	482	10309
	n	323	485	10341
	DCM	322	492	10731
	DMF			
PTZTPE-3	Toluene	424	563	5823
	1,4-Dioxane	423	573	6189
	Tetrahydrofura	423	585	6547
	n	425	598	6807
	DCM	425	613	7216

	DMF			

([a] absorption and emission maxima values recorded in different polarity solvents, [b] the fluorescence quantum yields were measured using quinine sulphate as a standard in 0.5 M H_2SO_4 solution for **PTZTPE-2** and rhodamine-6G as standard in ethanol for **PTZTPE-3**)

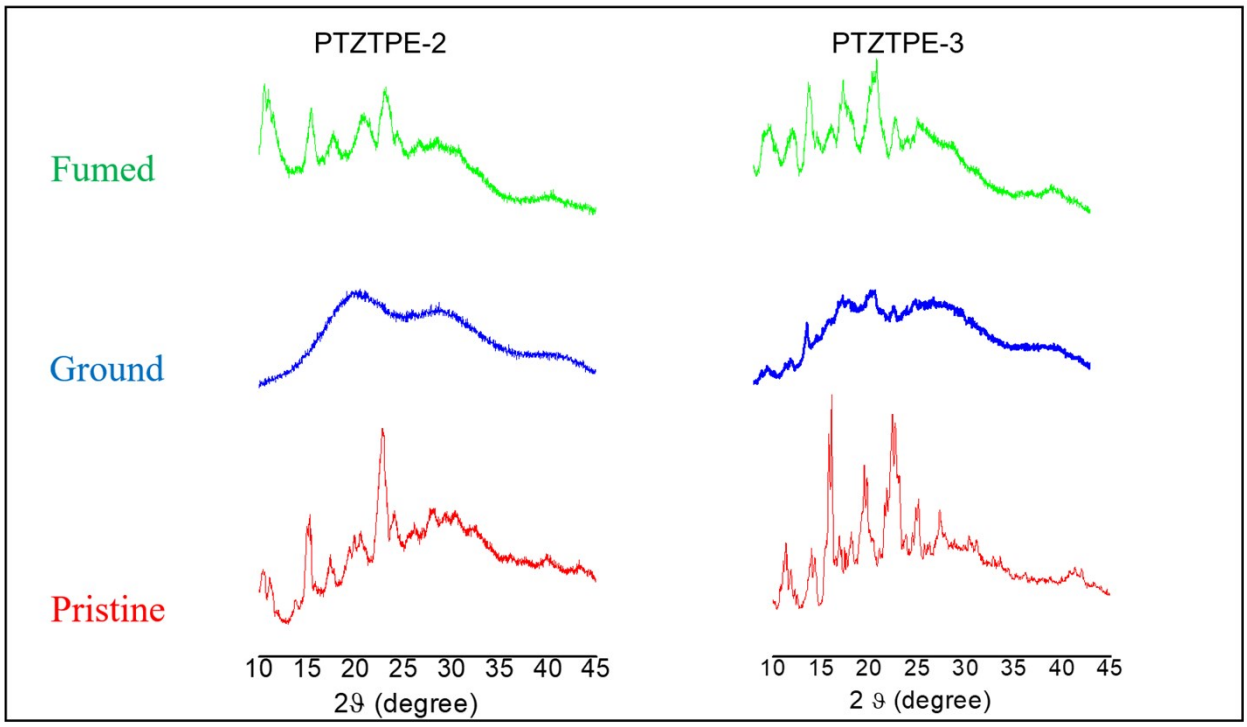


Figure S3 PXRD patterns of **PTZTPE-2** and **PTZTPE-3**.

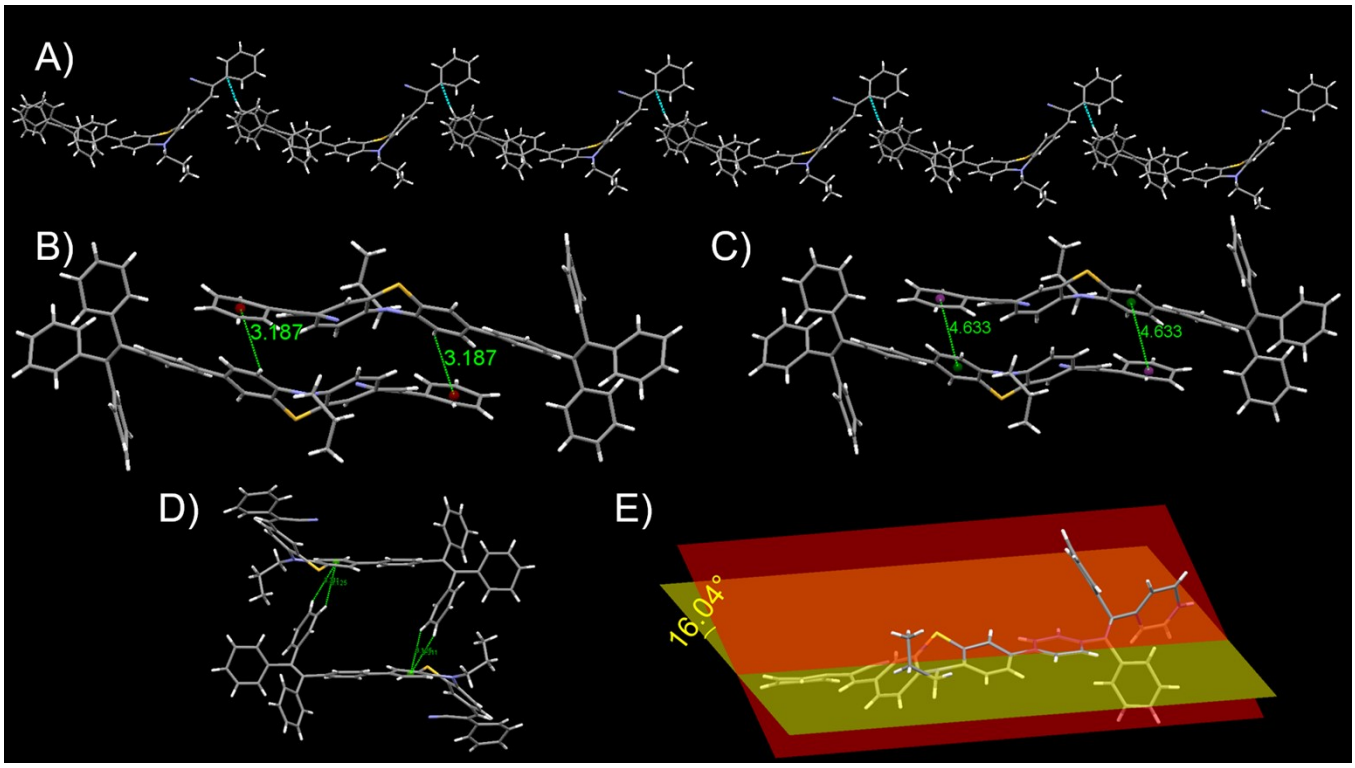


Figure S4 Packing diagram and dimeric interactions in the crystal structure of **PTZTPE-3**.

Crystallographic data

The crystal and refinement data are summarized in Table S2. The CCDC number 2011118 contains the supplementary crystallographic data for **PTZTPE-3**. These data can be obtained free of charge via www.ccdc.cam.ac.uk (or from the Cambridge Crystallographic Data Centre, 12 union Road, Cambridge CB21 EZ, UK; Fax: (+44) 1223- 336-033; or deposit@ccdc.cam.ac.uk).

Table S2 Crystal data and structure refinement for **PTZTPE-3**.

Identification code	**1**
Empirical formula	$C_{50}H_{38}N_2S.2O$
Formula weight	730.88
Temperature	293(2)K

Wavelength	154184 Å
Crystal system, space group	Triclinic, *P-1*
a/(Å)	9.744
b/(Å)	13.109
c/(Å)	16.277
Alpha/(°)	101.24
Beta/(°)	97.14
Gamma/(°)	92.17
Volume	2019.4(11) A^3
Z, calculated density	2, 1.202 mg/m^3
Absorption coefficient	1.034 mm^{-1}
F(000)	768
Crystal size	0.330 x 0.260 x 0.210
Θ range for data collection/(º)	3.975 to 70.709
Reflections collected / unique	14813 / 7421 [R(int) = 0.2796]
Completeness to theta	67.684 98.5%
Refinement method	Full-matrix least-squares on F^2
Data / restraints /parameters	7421/0/496
Goodness-of-fit on F2	0.836
Final R indices [I>2sigma(I)]	R1 = 0.1625, wR2 = 0.3730
R indices (all data)	R1 = 0.4214, wR2 = 0.5677
Extinction coefficient	n/a
Largest diff. peak and hole ($e.Å^{-3}$)	0.234 and -0.338

Table S3 Calculated major electronic transitions for **PTZTPE-2** and **PTZTPE-3** in the gas phase.

Compounds	Wavelength (nm)	Composition	Assignment	f^{a}
PTZTPE-2	372	HOMO-LUMO (0.65)	ICT	0.55
PTZTPE-3	477	HOMO-LUMO (0.69)	ICT	0.55

(Data obtained from TD-DFT calculations carried out using the Gaussian 09W program performed at the B3LYP/6-31G(d,p) level).

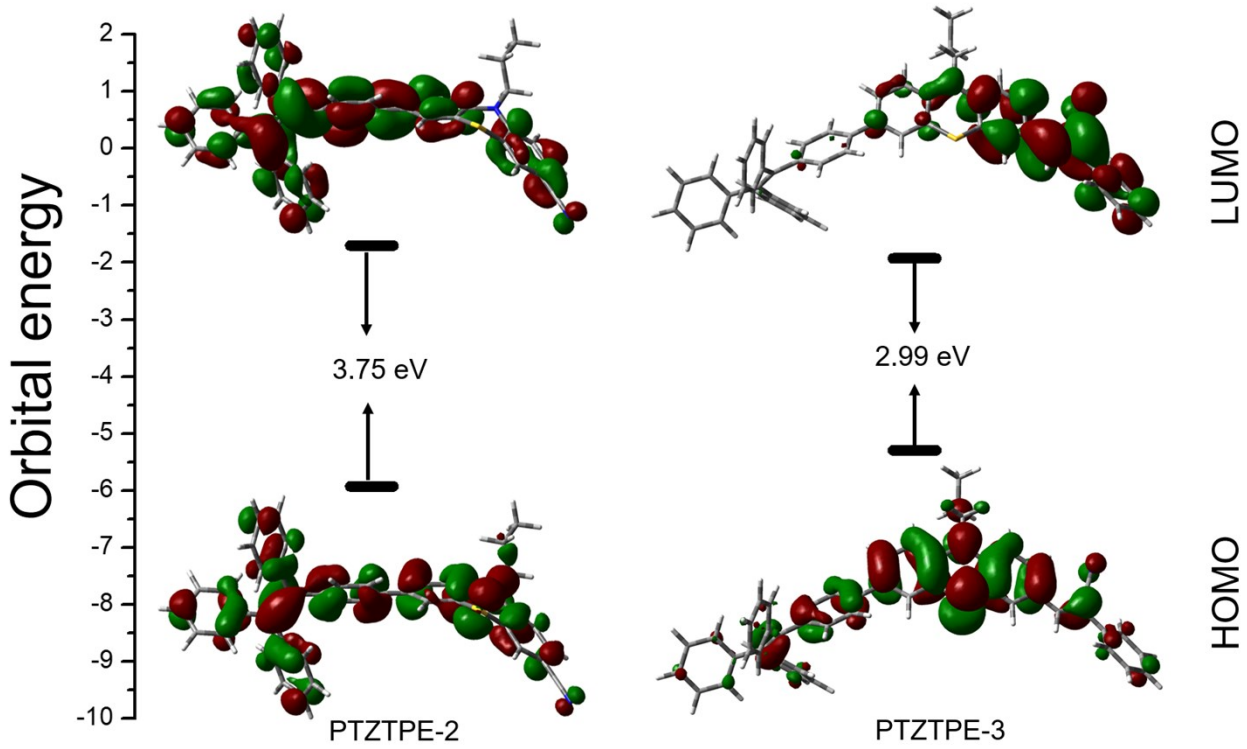


Figure S5 Energy level diagram of **PTZTPE-2** and **PTZTPE-3**.

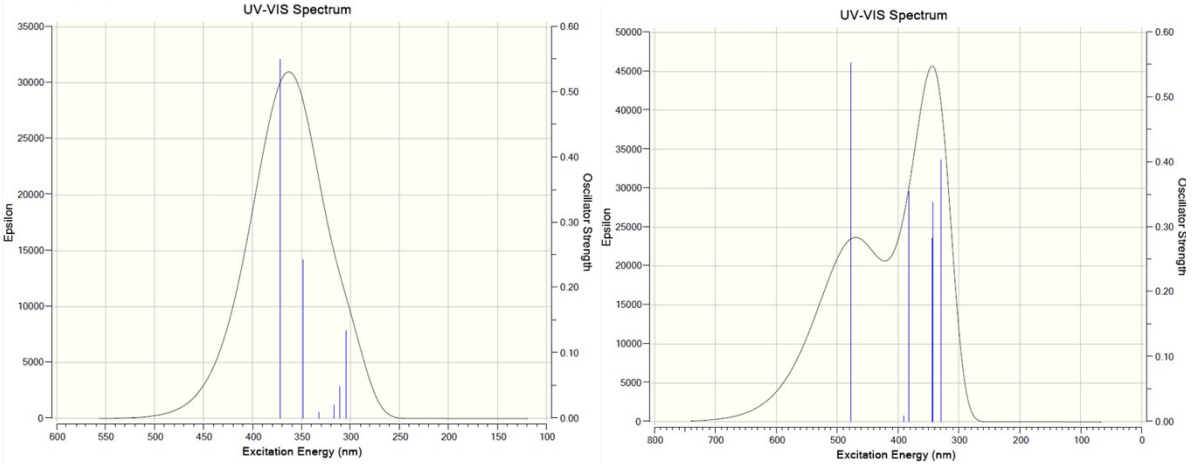


Figure S6 Simulated absorption spectra of **PTZTPE-2** (left) and **PTZTPE-3** (right).

Table S4. Theoretical data of **PTZTPE-2** and **PTZTPE-3.**

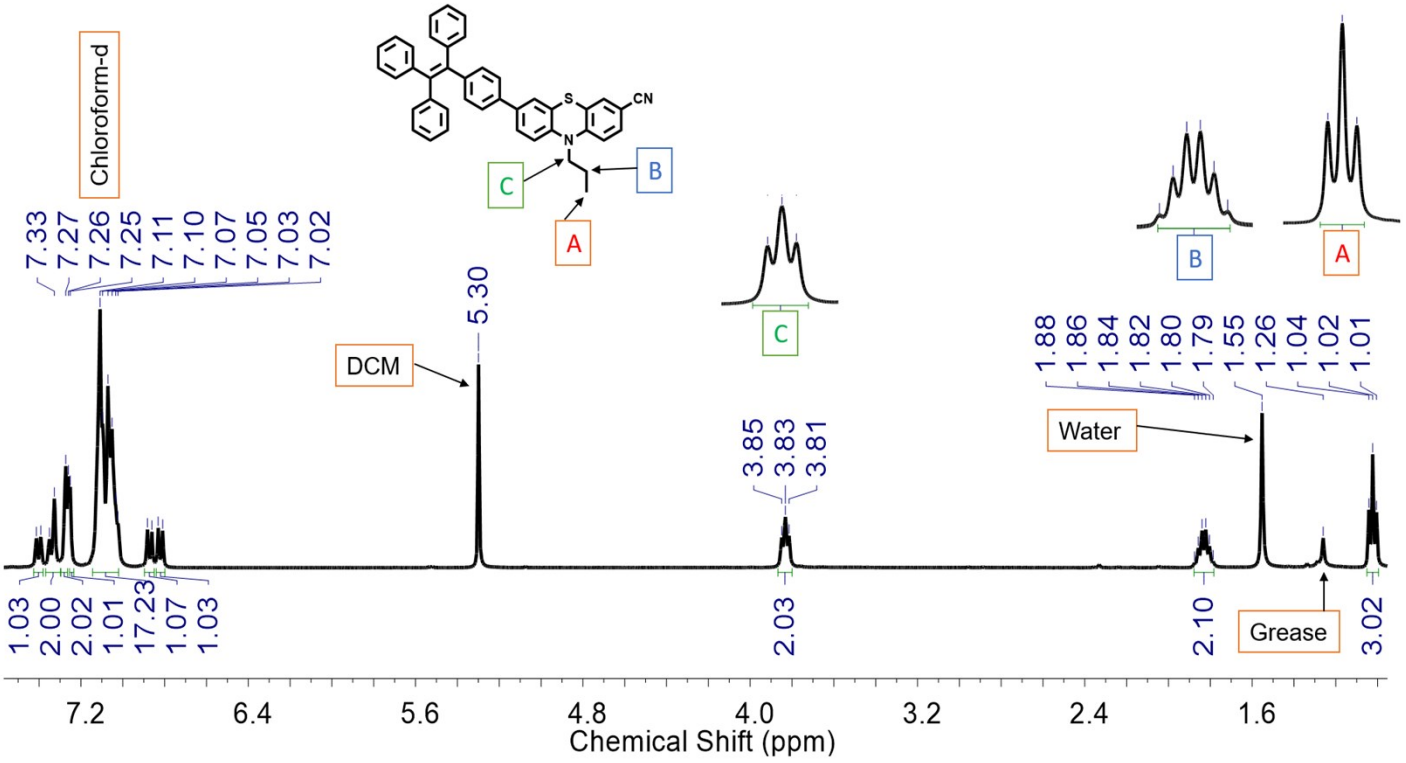
Compounds	$E_{HOMO}{}^{a}$ **(eV)**	$E_{LUMO}{}^{a}$ **(eV)**	$E_{g}{}^{a}$ **(eV)**
PTZTPE-2	-5.53	-1.78	3.75
PTZTPE-3	-4.97	-1.98	2.99

(**[a]** Theoretical data obtained from DFT calculations performed using the Gaussian 09W program at B3LYP/6-31G(d,p) level)

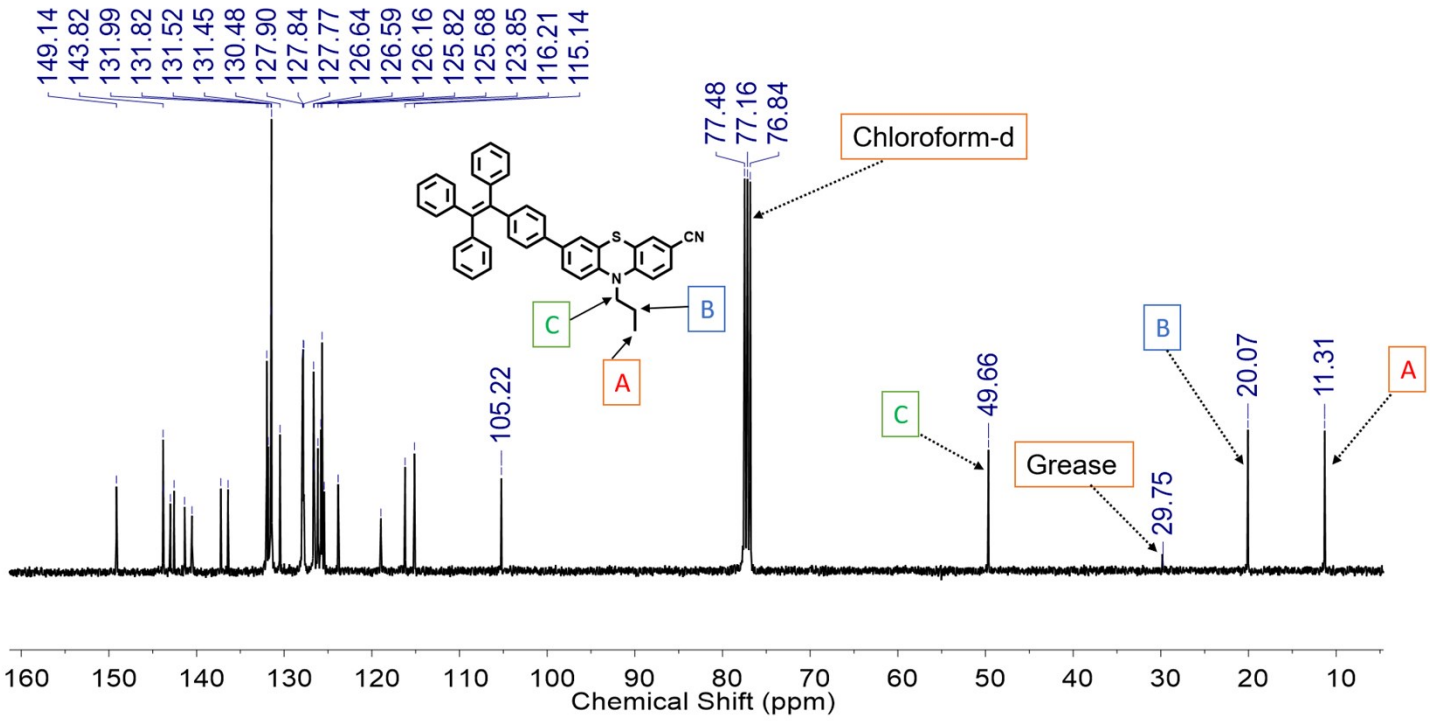
Table S5. Solid state emission maxima of compounds **PTZTPE-2** and **PTZTPE-3.**

Compounds	**Emission**			
	$\lambda_{pristine}$ **(nm)**	λ_{ground} **(nm)**	λ_{fumed} **(nm)**	**Λλ (nm)[a]**
PTZTPE-2	517	489	512	-28
PTZTPE-3	593[1], 590[2]	611	586	+21

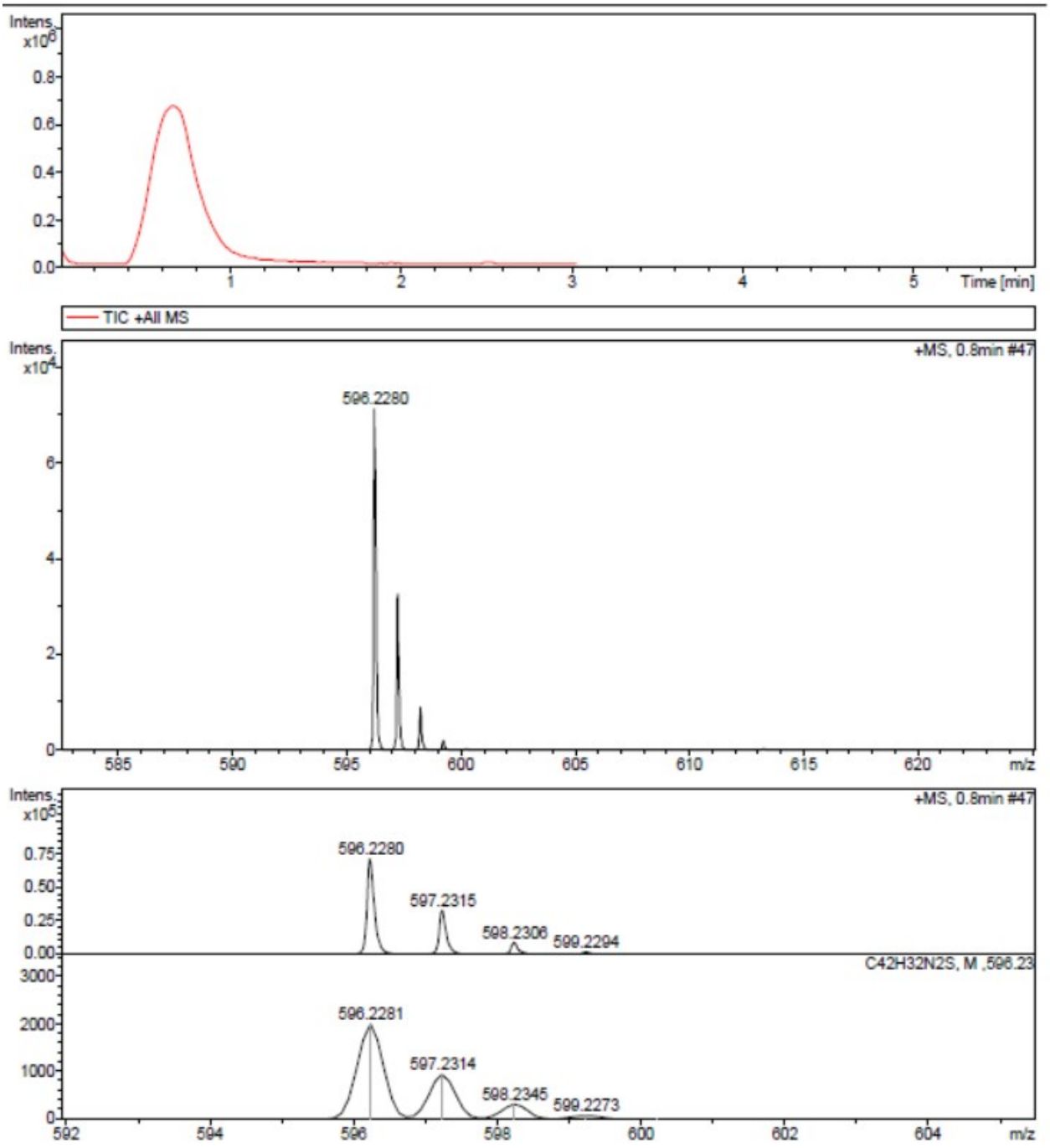
[1]For pristine-o form, [2]for pristine-y form, [a]grinding-induced spectral shift, [$\Lambda\lambda = \lambda_{ground} - \lambda_{pristine}$].



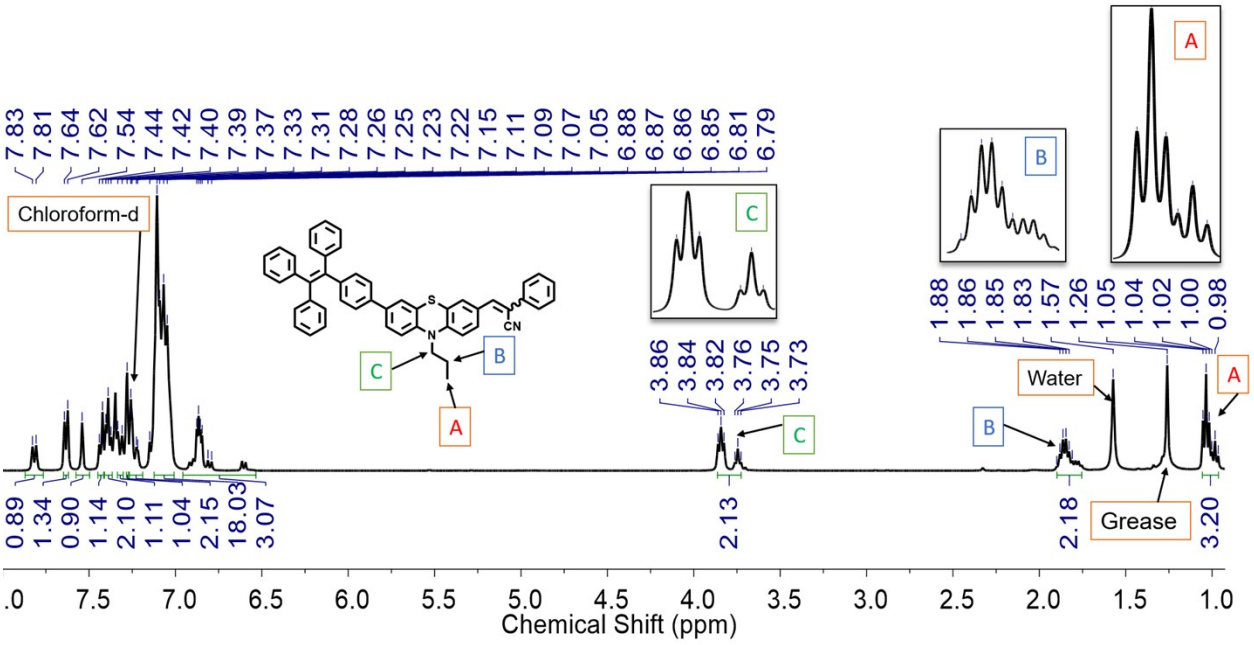
[1]H NMR spectrum of **PTZTPE-2**



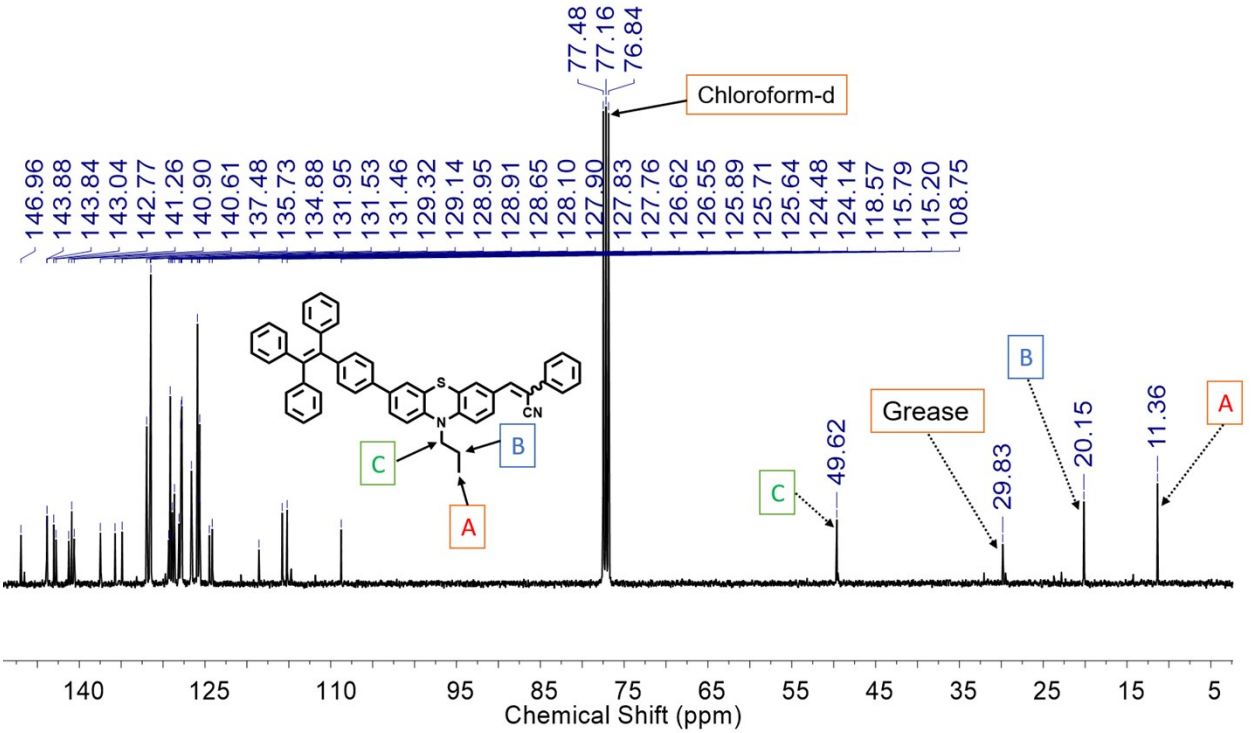
^{13}C NMR spectrum of **PTZTPE-2**



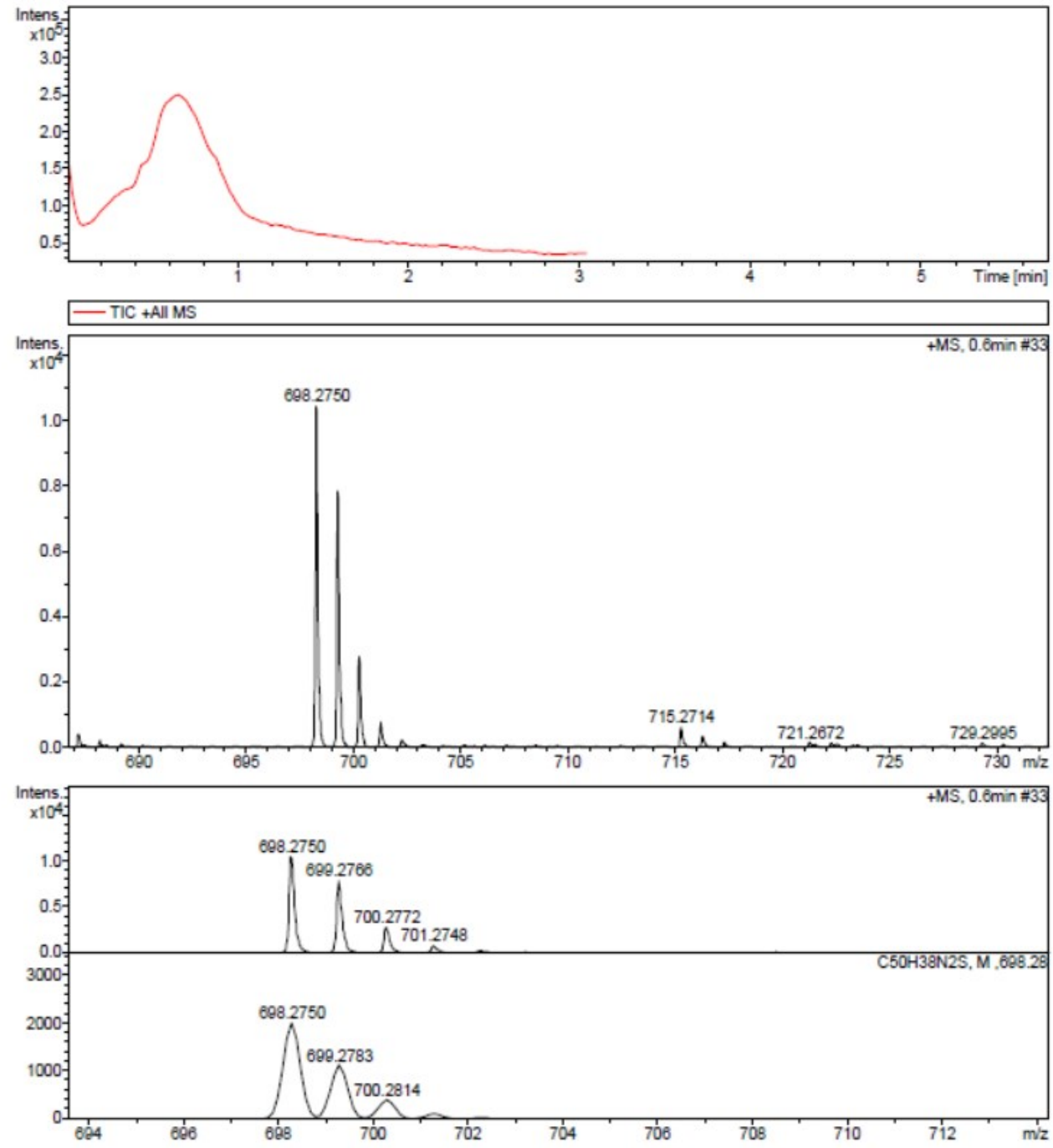
HRMS of **PTZTPE-2**



^{1}H NMR spectrum of **PTZTPE-3**



^{13}C NMR spectrum of **PTZTPE-3**



HRMS of **PTZTPE-3**

Processing and investigation methods of solid films and devices based on them.

Steady-state PL spectra of films were recorded using an Edinburgh Instruments FLS980 spectrometer. A PicoQuant LDH-D-C-375 laser (wavelength 374 nm) equipped to the FLS980 as the excitation source for the recording photoluminescence decay curves. Photoluminescence quantum yields (accuracy ± 2%) of the films were measured using the integrated sphere method.

The ionization potential of the solid-state sample was measured by photoelectron emission spectrometry in air. The experimental setup consisted a deep UV deuterium light source ASBN-D130-CM, a CM110 1/8m monochromator, and an electrometer 6517B Keithley. The charge carrier mobility (μ) measurements of vacuum deposited layer were carried out by the time of flight method (TOF). The thickness of the layer was measured utilizing a method of carrier extraction in linearly increasing voltage (CELIV). The TOF experimental setup consisted of a pulsed Nd:YAG laser (EKSPLA NL300, a wavelength of 355 nm, pulse duration 3-6 ns), a Keithley 6517B electrometer, a Tektronix TDS 3052C oscilloscope, and was as described in reference.The transit time (tt) with the applied bias (V) indicated the passage of charges through the entire thickness (d) of the samples. Hole mobility was calculated as $\mu=d_2 /U \cdot t_t$

OLEDs were prepared by vacuum deposition of organic and metal layers onto pre-cleaned ITO coated glass substrate under pressure lower than 2×10^{-6} mBar. ITO-coated glass substrates with a sheet resistance of 15 Ω/sq were patterned to get seven independent structures. The substrates were pre cleaned in acetone and isopropyl alcohol ultrasonic baths during ca. 10 min and by UV treatment during 15 min before deposition of the layers. Organic layers and aluminium layers were vacuum-deposited under the vacuum higher than 2×10^{-6} mBar using vacuum equipment from Kurt J. Lesker in-built in an MB EcoVap4G glove box. Devices based on hyperfluorescence emitting layer were fabricated with the following architecture ITO/MoO_3/TFB/EML/TSPO1/TPBi/LiF:Al.

The TFB and EML layers were fabricated by solution processing. The TBF layer was spin-coated using its 4 mg/ml solution. The EML layer containing three components co-hosts pCNBCzoCF$_3$ (15 wt %) and mCP (83 wt %) and emitter PTZTPE-1, PTZTPE-3, PTZTPE-4 (2 wt %) was spin-coated using their 5mg/ml solution. The fabricated layers were annealed for 30 minutes on the hot plate after each solution processing. Temperatures of 150 °C and 70 °C were used for TFB and EML layers, respectively. The density-voltage and luminance-voltage characteristics of the fabricated devices were simultaneously recorded using the Keithley 2400C sourcemeter and the certificated photodiode PH100-Si-HA-D0 together with the PCBased Power and Energy Monitor 11S-LINK in air without passivation immediately after taking out of the samples from inert atmosphere. Electroluminescence (EL) spectra were taken by an Aventes AvaSpec-2048XL spectrometer. External quantum efficiency was calculated from the luminance, current density, and EL spectrum. The chromaticity coordinates (x, y) of the devices were calculated using EL spectra.

Table S6. PL decay fitting results for the studied doped spin-coated films.

	t_1, ns	Influence %	t_2, ns	Influence %	χ^2
pCNBCzoCF$_3$:mCP (15:85 wt%)	12.44	92.21	253.21	7.79	1.12
PTZTPE-1:mCP (10:90wt%)	1.79	100	-	-	0.94
PTZTPE-1: pCNBCzoCF$_3$:mCP (2:15:83wt%)	1.8	55.47	9.54	44.53	1.04
PTZTPE-3:mCP (10:90wt%)	5.89	100	-	-	1.07
PTZTPE-3: pCNBCzoCF$_3$:mCP (2:15:83wt%)	6.7	100	-	-	0.93
PTZTPE-4:mCP (10:90wt%)	2.41	100	-	-	1.08
PTZTPE-4: pCNBCzoCF$_3$:mCP (2:15:83wt%)	2.95	80.25	12.23	19.75	1.14

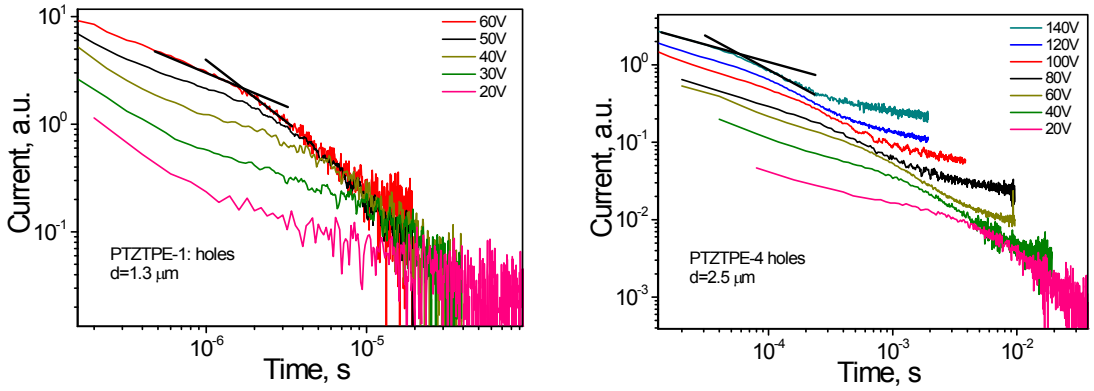
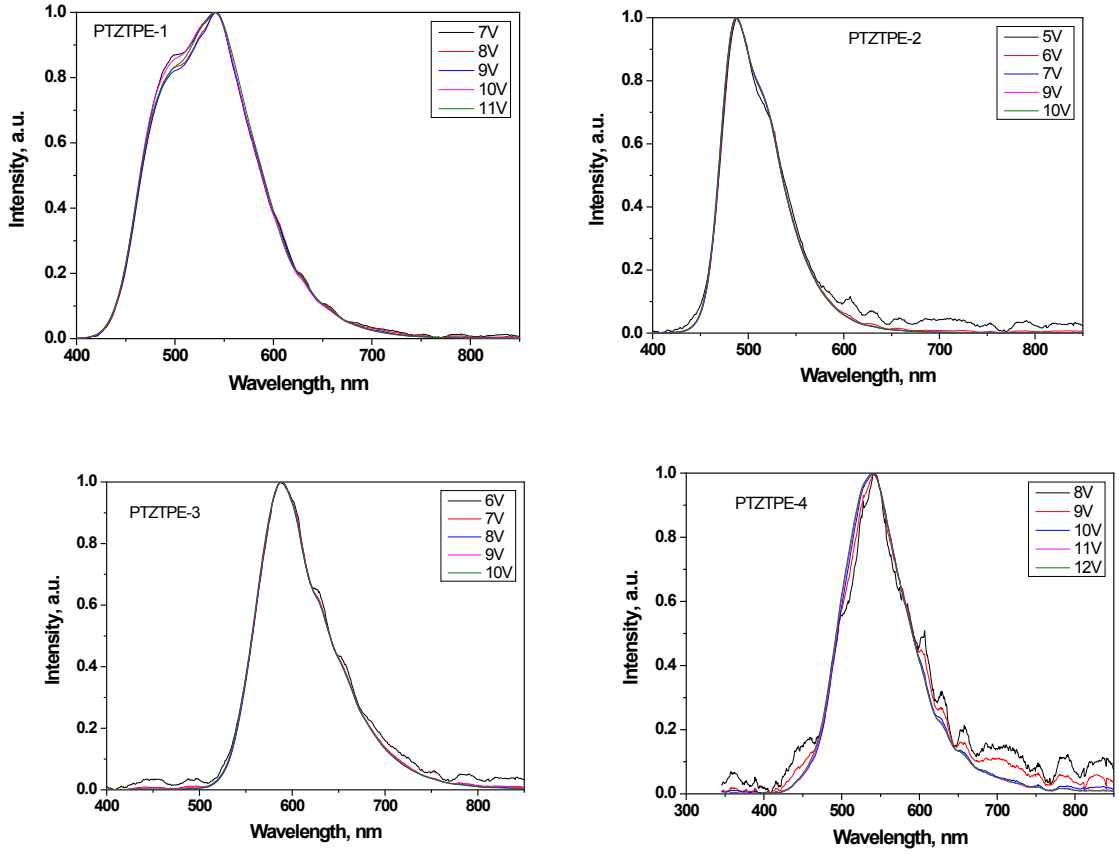
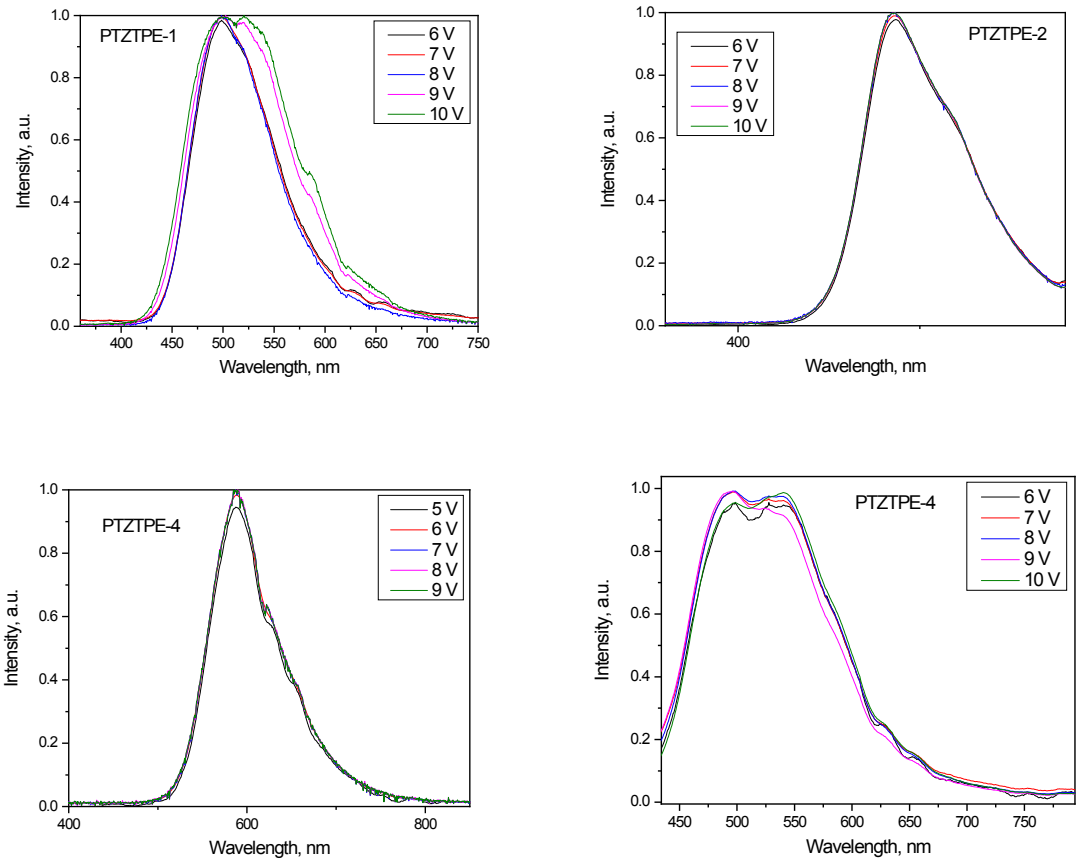


Figure S7. TOF signals for holes for the layers of **PTZTPE-1** and **PTZTPE-4**.



a)



b)

Figure S8. EL spectra of vacuum-processed (a) and solution-processed (b) non-doped OLEDs based on the corresponding **PTZTPE** emitters.

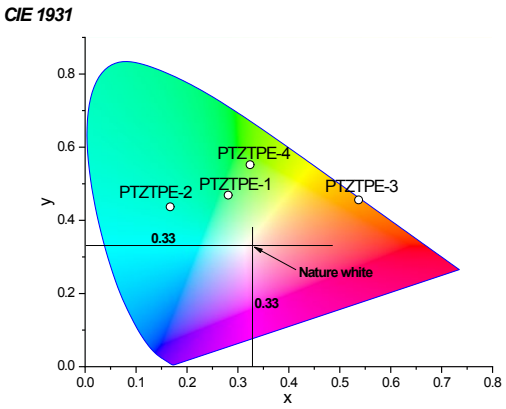


Figure S9. CIE colour coordinates at 6V of vacuum-processed non-doped OLEDs based on the corresponding **PTZTPE** emitters.

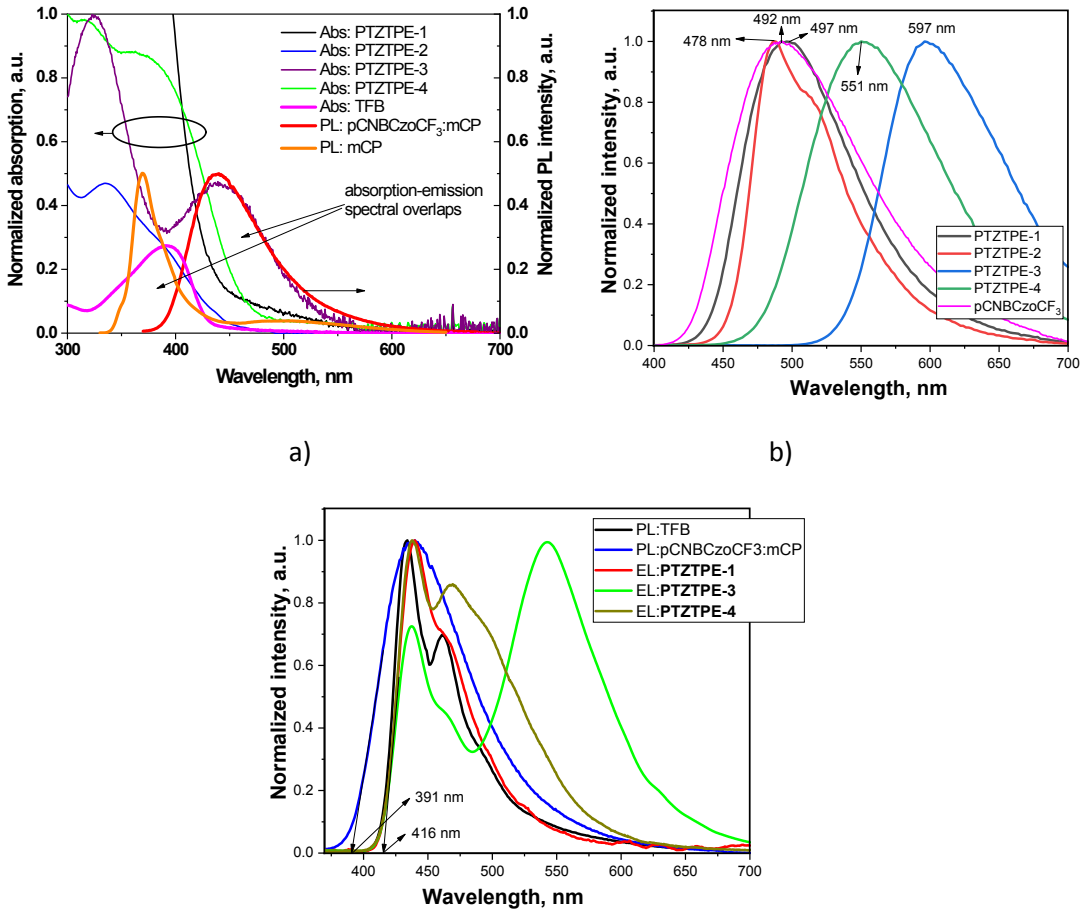


Figure S10. Absorption (a) and PL spectra of **PTZTPE** films and PL spectrum (b) of doped pCNBCzoCF$_3$:mCP or non-doped pCNBCzoCF$_3$ films as well as PL of TFB and pCNBCzoCF3:mCP films and EL spectra of **PTZTPE**-based devices (c).

DFT (PTZTPE-2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.238702	0.609160	1.068452
2	6	0	-6.972179	1.660212	1.608597
3	6	0	-8.115794	2.141445	0.946125
4	6	0	-8.482458	1.577703	-0.285849
5	6	0	-7.723942	0.552296	-0.842031
6	6	0	-6.601129	0.031651	-0.171088
7	1	0	-6.671263	2.097237	2.554869
8	1	0	-9.349553	1.957298	-0.815523

9	1	0	-8.005550	0.164071	-1.813348
10	6	0	-2.444040	-0.357885	0.713185
11	6	0	-3.827977	-0.478444	0.597970
12	6	0	-4.419581	-0.936943	-0.592651
13	6	0	-3.571338	-1.271230	-1.658661
14	6	0	-2.185942	-1.184460	-1.525931
15	1	0	-2.028700	0.042853	1.632506
16	1	0	-3.986976	-1.618238	-2.597694
17	1	0	-1.561159	-1.491340	-2.358773
18	7	0	-5.834489	-1.028283	-0.688556
19	16	0	-4.881510	-0.091964	1.984149
20	6	0	-6.427207	-1.943538	-1.671833
21	1	0	-6.165095	-1.655533	-2.702154
22	1	0	-7.510653	-1.845286	-1.586930
23	6	0	-6.068276	-3.414413	-1.414418
24	1	0	-4.982647	-3.551333	-1.430355
25	1	0	-6.400797	-3.676353	-0.403228
26	6	0	-6.721361	-4.342939	-2.444656
27	1	0	-6.385740	-4.112813	-3.462834
28	1	0	-7.814321	-4.258062	-2.427340
29	1	0	-6.468011	-5.388077	-2.242151
30	6	0	-1.589524	-0.728706	-0.339364
31	6	0	-0.115637	-0.630168	-0.198162
32	6	0	0.521851	-0.936588	1.017471
33	6	0	0.695906	-0.234527	-1.276245
34	6	0	1.905725	-0.848487	1.148111
35	1	0	-0.068411	-1.277240	1.863201
36	6	0	2.078659	-0.136073	-1.141403
37	1	0	0.238820	0.023928	-2.226988
38	6	0	2.715113	-0.429194	0.077166
39	1	0	2.368020	-1.112044	2.094873
40	1	0	2.675191	0.180776	-1.990689
41	6	0	4.200282	-0.356758	0.224150
42	6	0	4.932577	0.721246	-0.189697
43	6	0	4.824622	-1.555757	0.866123
44	6	0	6.425197	0.693856	-0.284455
45	6	0	4.303591	2.020179	-0.583638
46	6	0	4.503360	-2.852444	0.425736
47	6	0	5.700960	-1.423799	1.957317
48	6	0	7.195527	1.739700	0.255929
49	6	0	7.094087	-0.341149	-0.961119
50	6	0	4.677623	2.662560	-1.777971
51	6	0	3.366504	2.658719	0.247509
52	6	0	5.064561	-3.976762	1.032872
53	1	0	3.812298	-2.977054	-0.403075
54	6	0	6.253423	-2.547649	2.573825
55	1	0	5.947262	-0.432295	2.323746
56	6	0	8.587337	1.732748	0.154346
57	1	0	6.697447	2.560735	0.763428
58	6	0	8.485149	-0.342631	-1.075357

59	1	0	6.516741	-1.147374	-1.402101
60	6	0	4.107775	3.882090	-2.146452
61	1	0	5.417187	2.197123	-2.423195
62	6	0	2.805762	3.884977	-0.112929
63	1	0	3.079250	2.189132	1.182987
64	6	0	5.942631	-3.829240	2.110915
65	1	0	4.812138	-4.968202	0.667171
66	1	0	6.924797	-2.421060	3.418514
67	6	0	9.239057	0.690781	-0.512307
68	1	0	9.162463	2.544456	0.591079
69	1	0	8.979353	-1.151065	-1.606856
70	6	0	3.168110	4.499150	-1.315028
71	1	0	4.402008	4.353017	-3.080272
72	1	0	2.087114	4.361810	0.547699
73	1	0	6.374282	-4.703753	2.589148
74	1	0	10.321834	0.688507	-0.598405
75	1	0	2.729393	5.451935	-1.596969
76	6	0	-8.887666	3.203496	1.518576
77	7	0	-9.516708	4.067220	1.982056

Rotational constants (GHZ): 0.1328837 0.0251328 0.0231286

TD-DFT (PTZTPE-2)

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.3317 eV 372.14 nm f=0.5497
<S**2>=0.000
156 ->159 -0.17594
157 ->158 0.65435
157 ->159 0.15240
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -2127.36012459
Copying the excited state density for this state as the 1-particle RhoCI
density.

Excited State 2: Singlet-A 3.5582 eV 348.44 nm f=0.2436
<S**2>=0.000
156 ->158 -0.36320
156 ->159 -0.16288
157 ->158 -0.22678
157 ->159 0.51456

Excited State 3: Singlet-A 3.7333 eV 332.10 nm f=0.0089
<S**2>=0.000
156 ->158 0.57696
157 ->159 0.37778

Excited State 4: Singlet-A 3.9158 eV 316.62 nm f=0.0209
<S**2>=0.000

```
     155 ->159        -0.10590
     156 ->160        -0.28636
     156 ->161        -0.16291
     157 ->160         0.54051
     157 ->161         0.21161

 Excited State   5:      Singlet-A      3.9881 eV  310.88 nm  f=0.0488
<S**2>=0.000
     156 ->159         0.62924
     157 ->158         0.11696
     157 ->159         0.22744

 Excited State   6:      Singlet-A      4.0713 eV  304.53 nm  f=0.1345
<S**2>=0.000
     155 ->158        -0.18222
     156 ->159        -0.10062
     156 ->162         0.12730
     157 ->160        -0.30461
     157 ->161         0.44531
     157 ->162        -0.34317
 SavETr:  write IOETrn=   770 NScale= 10 NData=  16 NLR=1 NState=    6
LETran=     118.
```

DFT (PTZTPE-3)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.957636	-3.998109	-2.201012
2	1	0	-4.916043	-4.471256	-1.980451
3	1	0	-3.178173	-4.757390	-2.118554
4	1	0	-3.979498	-3.628798	-3.236637
5	7	0	-3.704687	-2.954079	-1.217132
6	6	0	-4.768556	-2.121396	-0.834958
7	6	0	-2.368324	-2.528782	-1.022086
8	6	0	-4.668031	-1.326188	0.326866
9	6	0	-5.963521	-2.051052	-1.573753
10	6	0	-2.014623	-1.797395	0.127466
11	6	0	-1.358033	-2.811991	-1.952446
12	6	0	-5.712822	-0.495548	0.703477
13	16	0	-3.241990	-1.489607	1.382344
14	6	0	-7.020969	-1.245265	-1.171625
15	1	0	-6.071701	-2.628606	-2.483687
16	6	0	-0.705972	-1.367960	0.325980
17	6	0	-0.042564	-2.412120	-1.727387
18	1	0	-1.590926	-3.354430	-2.861019
19	6	0	-6.923818	-0.438067	-0.021450

20	1	0	-5.597770	0.112735	1.596389
21	1	0	-7.919620	-1.239367	-1.773901
22	1	0	-0.481079	-0.770136	1.203365
23	6	0	0.315915	-1.681631	-0.586210
24	1	0	0.718289	-2.686267	-2.451070
25	6	0	-7.957243	0.448735	0.491268
26	6	0	1.713555	-1.249899	-0.347152
27	6	0	-9.190775	0.792262	0.020102
28	1	0	-7.678391	0.939036	1.420746
29	6	0	2.255867	-1.223106	0.949196
30	6	0	2.547665	-0.861869	-1.409531
31	6	0	-10.099929	1.711351	0.757943
32	6	0	-9.685513	0.310708	-1.235206
33	6	0	3.570840	-0.828234	1.170955
34	1	0	1.649696	-1.546054	1.790400
35	6	0	3.859175	-0.457022	-1.186295
36	1	0	2.156452	-0.855522	-2.422499
37	6	0	-11.034849	2.498157	0.063351
38	6	0	-10.050156	1.816372	2.159146
39	7	0	-10.120598	-0.052488	-2.253457
40	6	0	4.398766	-0.420466	0.110549
41	1	0	3.968486	-0.839257	2.181200
42	1	0	4.476400	-0.156113	-2.026162
43	6	0	-11.869546	3.381067	0.745070
44	1	0	-11.101518	2.420249	-1.017307
45	6	0	-10.882724	2.702987	2.837311
46	1	0	-9.377536	1.179980	2.725317
47	6	0	5.818011	-0.026787	0.357477
48	6	0	-11.794292	3.492804	2.133917
49	1	0	-12.579789	3.984072	0.187168
50	1	0	-10.830567	2.763966	3.920418
51	6	0	6.377043	1.097852	-0.182051
52	6	0	6.578537	-0.961228	1.243298
53	1	0	-12.447481	4.178807	2.664665
54	6	0	7.849037	1.357453	-0.159445
55	6	0	5.564374	2.166343	-0.840076
56	6	0	6.527296	-2.349612	1.027491
57	6	0	7.313397	-0.487723	2.343238
58	6	0	8.346141	2.614569	0.227389
59	6	0	8.768997	0.380217	-0.575557
60	6	0	5.950413	2.690244	-2.086512
61	6	0	4.434004	2.715166	-0.211265
62	6	0	7.213337	-3.230390	1.861780
63	1	0	5.947292	-2.735726	0.194604
64	6	0	7.989799	-1.369079	3.184808
65	1	0	7.349869	0.579389	2.535660
66	6	0	9.715453	2.873721	0.230074
67	1	0	7.649398	3.389544	0.532236
68	6	0	10.137597	0.643125	-0.584630
69	1	0	8.402865	-0.589861	-0.894805

```
     70          6           0        5.212777    3.702511   -2.697599
     71          1           0        6.834241    2.294141   -2.577396
     72          6           0        3.703151    3.735947   -0.816578
     73          1           0        4.132625    2.336408    0.759746
     74          6           0        7.947767   -2.743585    2.944776
     75          1           0        7.170250   -4.298533    1.668517
     76          1           0        8.547675   -0.980890    4.032209
     77          6           0       10.617704    1.888850   -0.176548
     78          1           0       10.077884    3.847986    0.545674
     79          1           0       10.829870   -0.125978   -0.915193
     80          6           0        4.085664    4.230363   -2.064798
     81          1           0        5.521787    4.083331   -3.666947
     82          1           0        2.835603    4.148684   -0.309642
     83          1           0        8.476507   -3.429803    3.599892
     84          1           0       11.684486    2.092776   -0.182091
     85          1           0        3.514929    5.024791   -2.536760
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.1113550      0.0152928      0.0145573
```

TD-DFT (PTZTPE-3)

```
Excitation energies and oscillator strengths:

 Excited State   1:      Singlet-A      2.7115 eV  457.26 nm  f=0.4812
<S**2>=0.000
     175 ->177         0.10013
     176 ->177         0.68590
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -2357.21925156
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:      Singlet-A      3.1830 eV  389.52 nm  f=0.0290
<S**2>=0.000
     175 ->177         0.68321
     176 ->177        -0.12174

 Excited State   3:      Singlet-A      3.3339 eV  371.89 nm  f=0.4743
<S**2>=0.000
     174 ->177        -0.13548
     175 ->178        -0.11590
     176 ->178         0.67205

 Excited State   4:      Singlet-A      3.6352 eV  341.06 nm  f=0.1894
<S**2>=0.000
     175 ->178         0.68201

 Excited State   5:      Singlet-A      3.6717 eV  337.67 nm  f=0.4776
<S**2>=0.000
```

```
     173 ->177         0.26266
     174 ->177         0.56519
     176 ->178         0.13169
     176 ->179         0.17372
     176 ->180        -0.12219
     176 ->181        -0.11370

 Excited State   6:      Singlet-A      3.8708 eV  320.30 nm  f=0.3414
<S**2>=0.000
     174 ->177        -0.28232
     175 ->180        -0.11647
     176 ->179         0.45123
     176 ->180        -0.35688
     176 ->181        -0.11521
 SavETr:  write IOETrn=   770 NScale= 10 NData=  16 NLR=1 NState=    6
LETran=     118.
```