Electronic Supplementary Material (ESI) for Materials Advances.

Towards deep-blue organic light-emitting diodes: A computational and experimental investigation of tetraaryl-benzobis[1,2-*d*:4,5-*d*']oxazoles

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Supplemental Information

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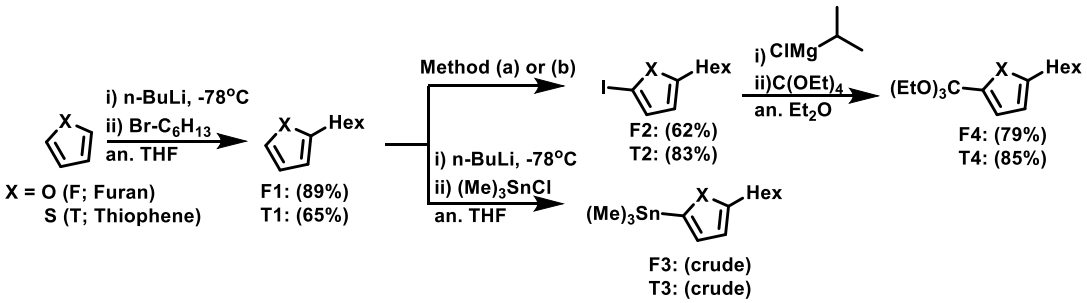
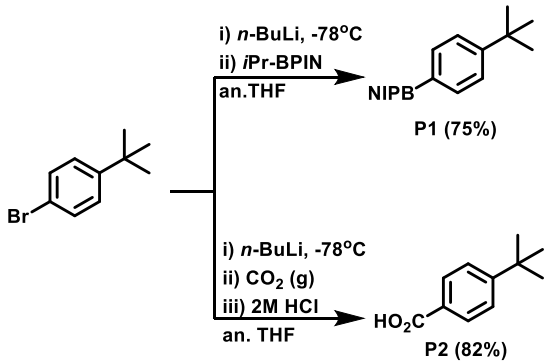
Synthesis of Precursor Compounds



Scheme S1. Synthesis of precursor furanyl- and thiophenyl-based stannanes and orthoesters.



Scheme S2. Synthesis of precursor phenyl-based boronic ester and benzoic acid.

NMR Spectra

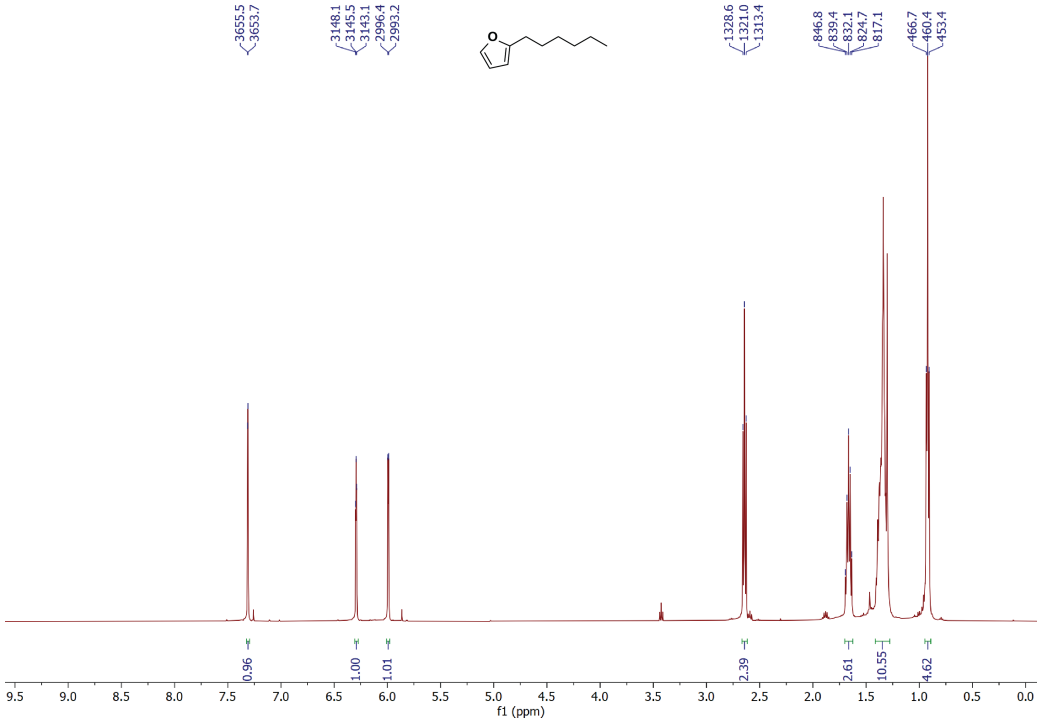


Figure S1. ^{1}H NMR of **F1**

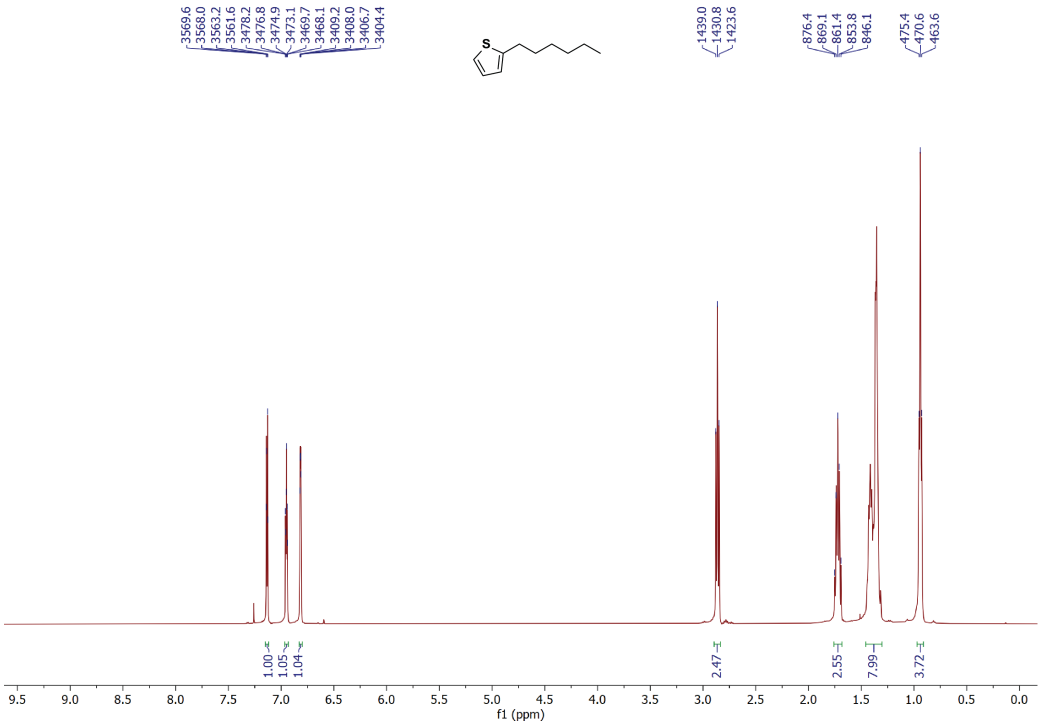


Figure S2. ^{1}H NMR of **T1**

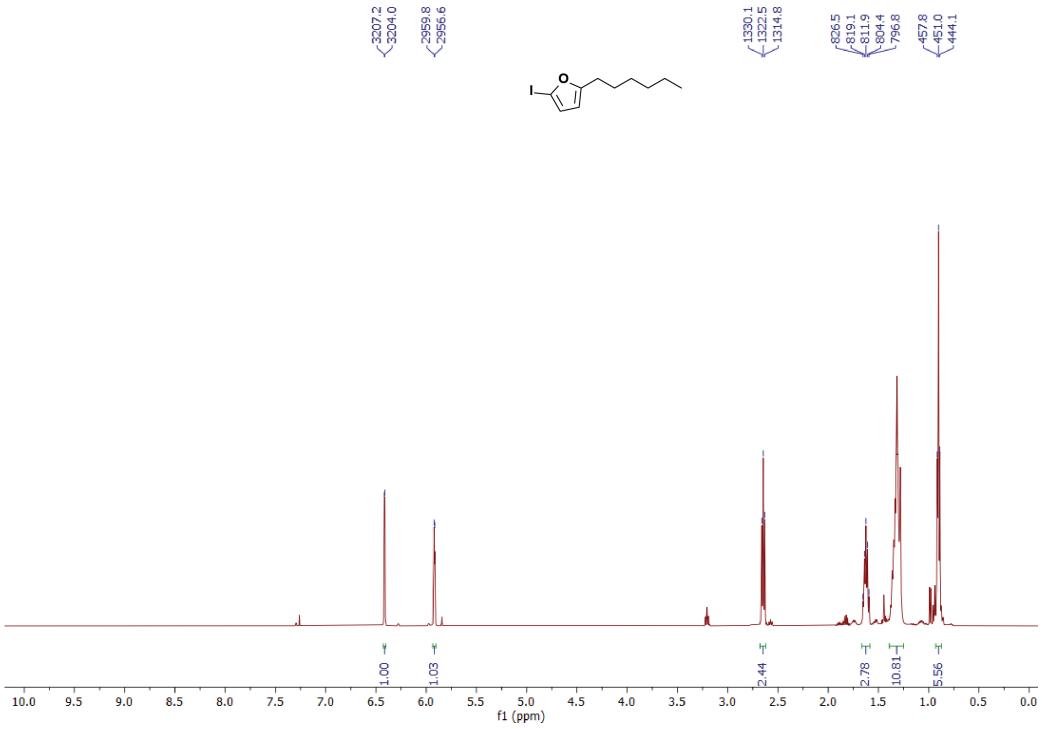


Figure S3. ^{1}H NMR of **F2**

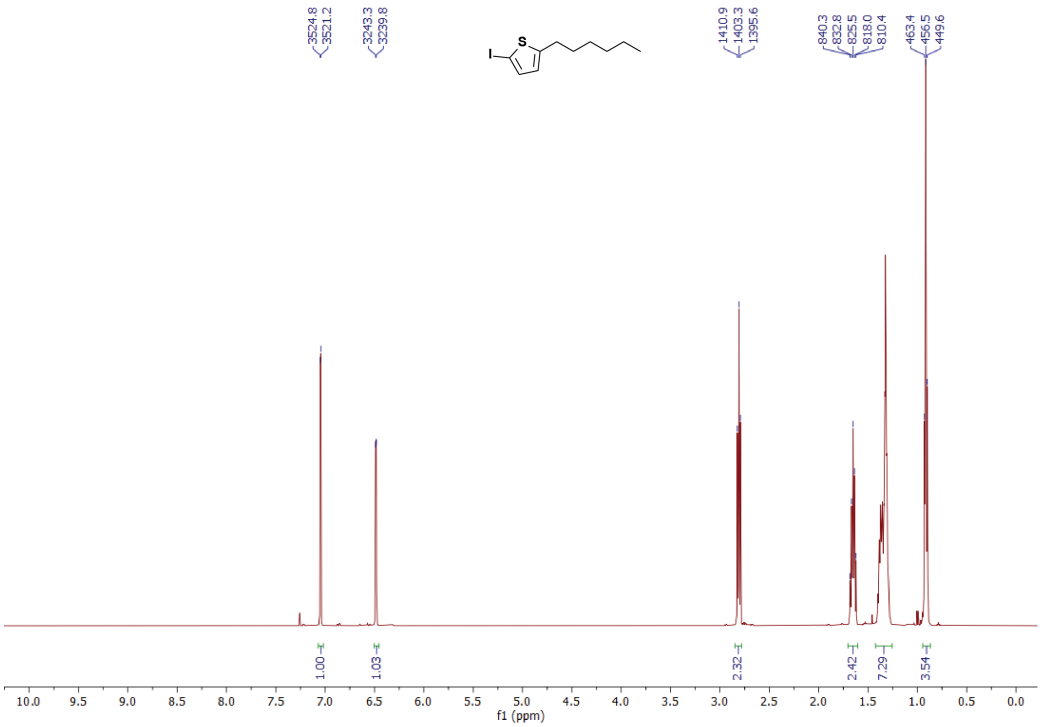


Figure S4. ^{1}H NMR of **T2**

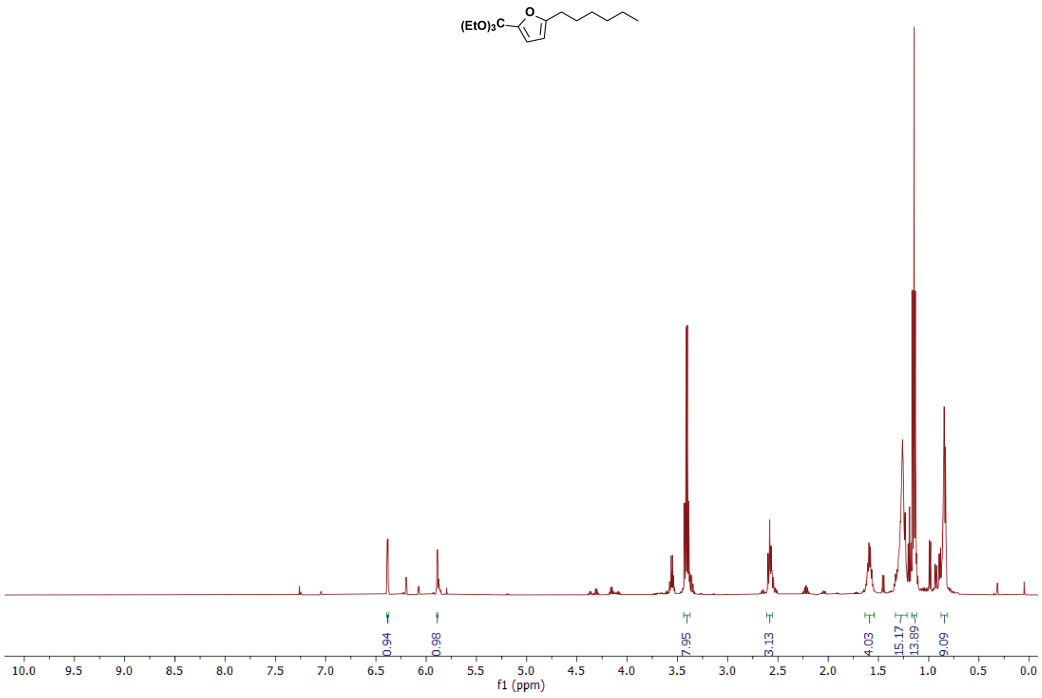


Figure S5. ^{1}H NMR of **F4**

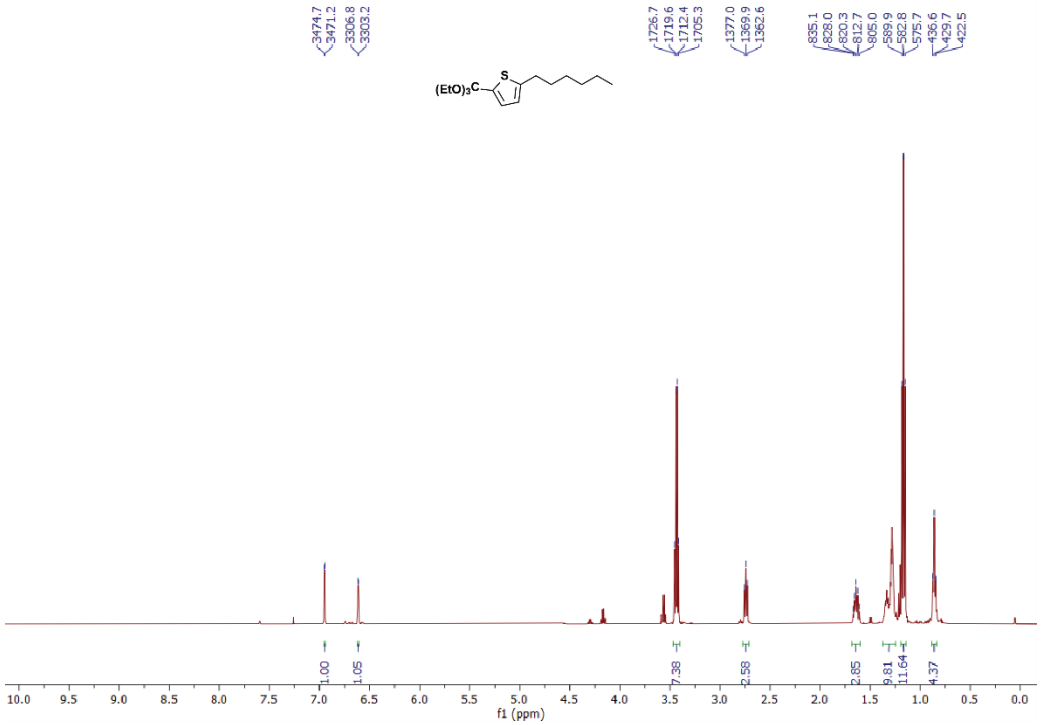


Figure S6. ^{1}H NMR of **T4**

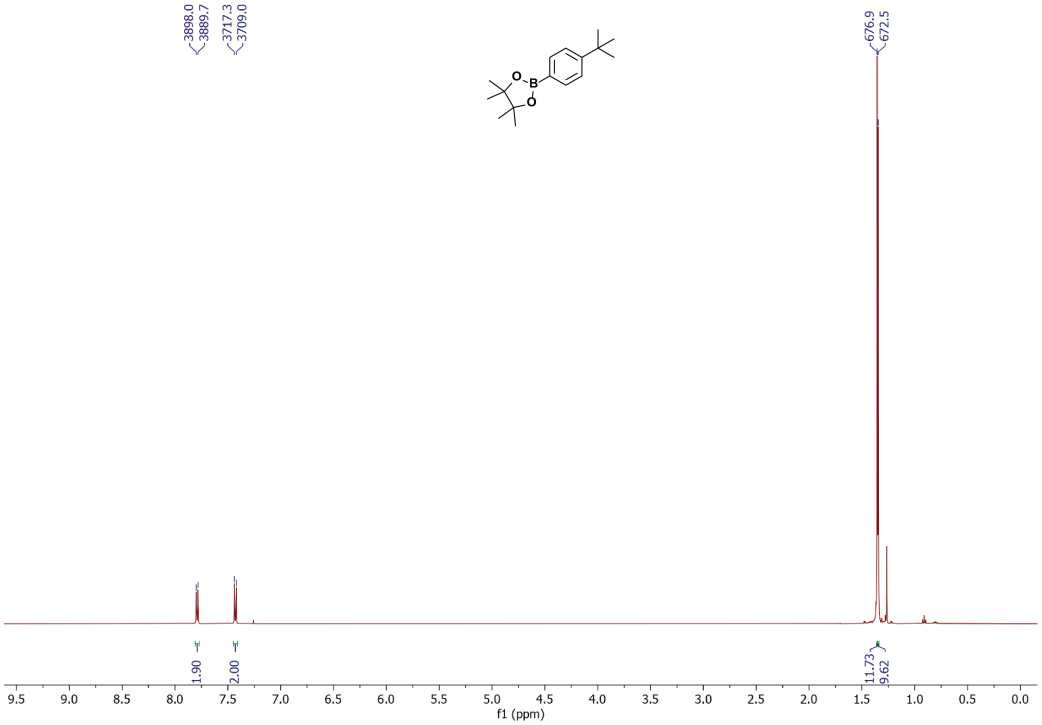


Figure S7. ^{1}H NMR of **P1**

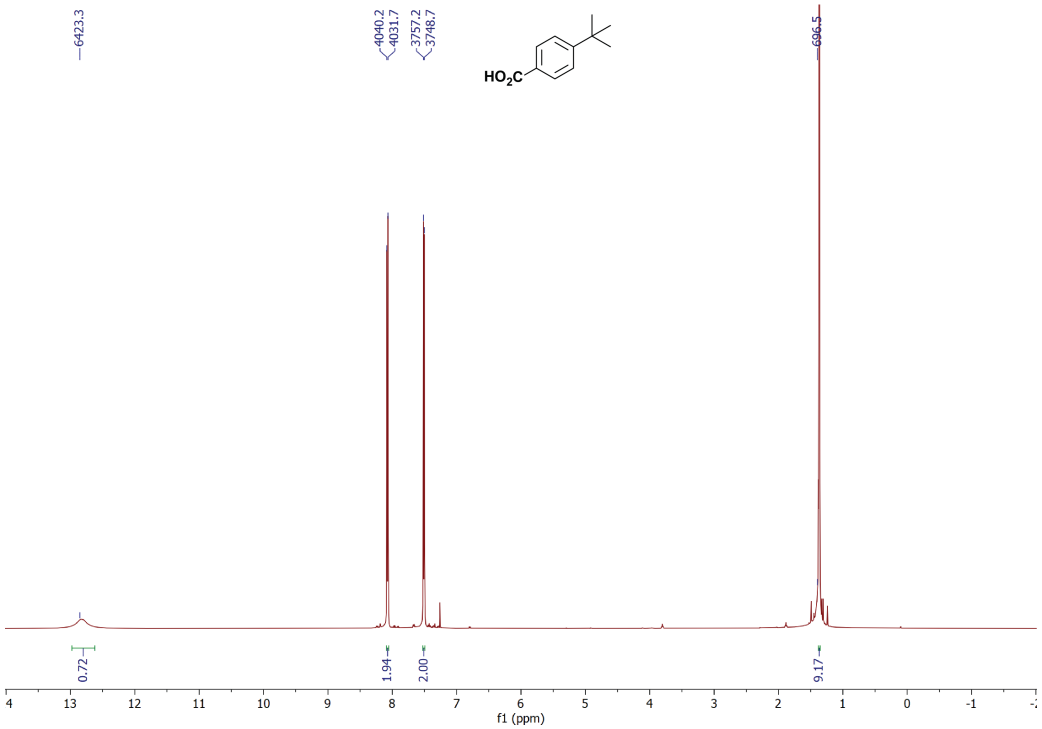


Figure S8. ^{1}H NMR of **P2**

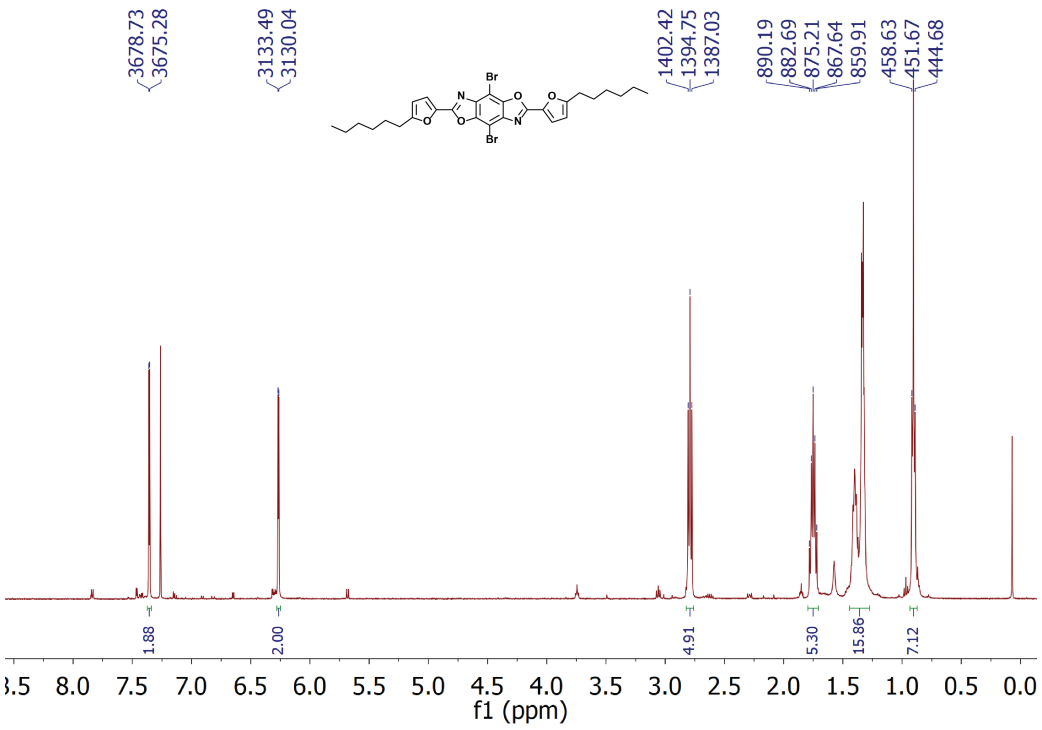


Figure S9. ^{1}H NMR of **26F48Br**

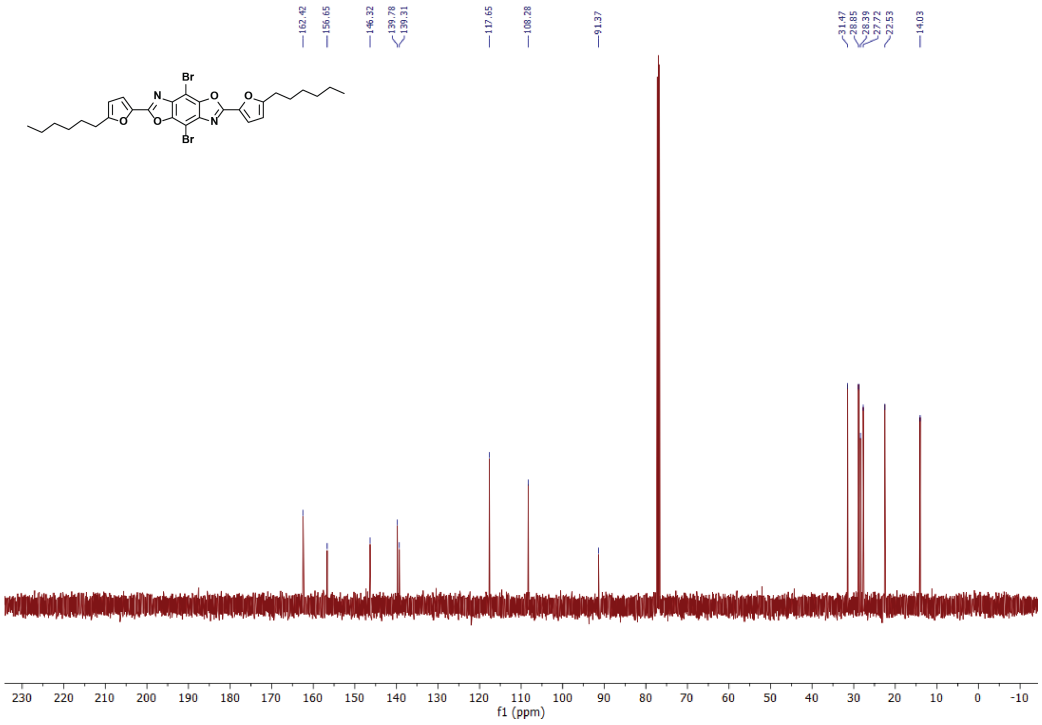


Figure S10. ^{13}C NMR of **26F48Br**

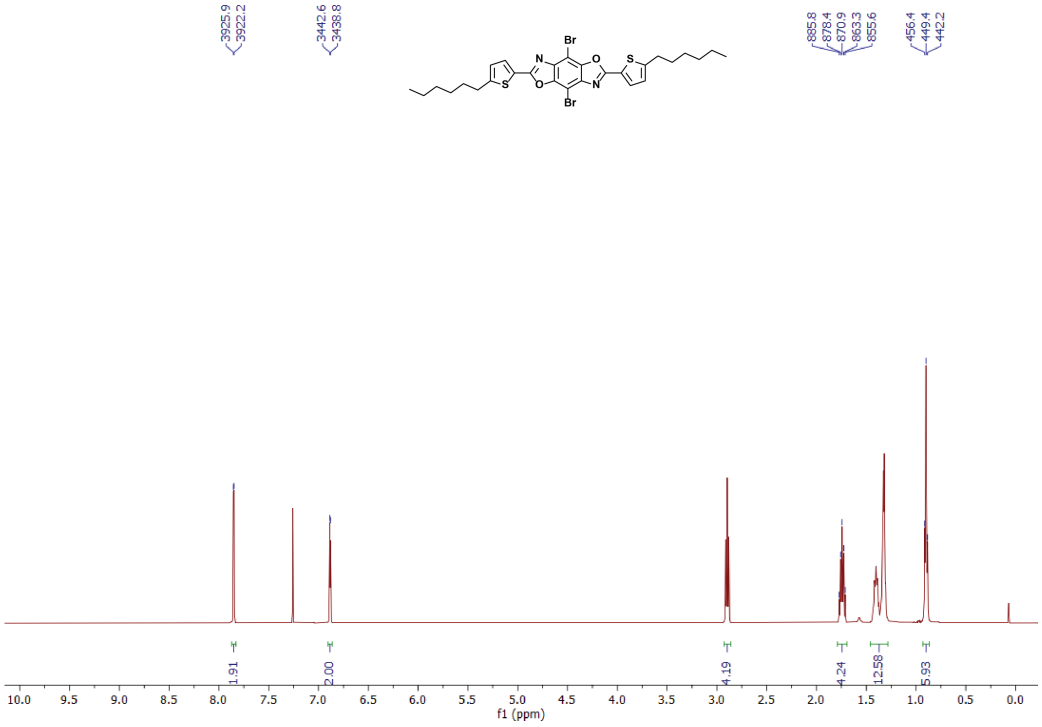


Figure S11. ^{1}H NMR of **26T48Br**

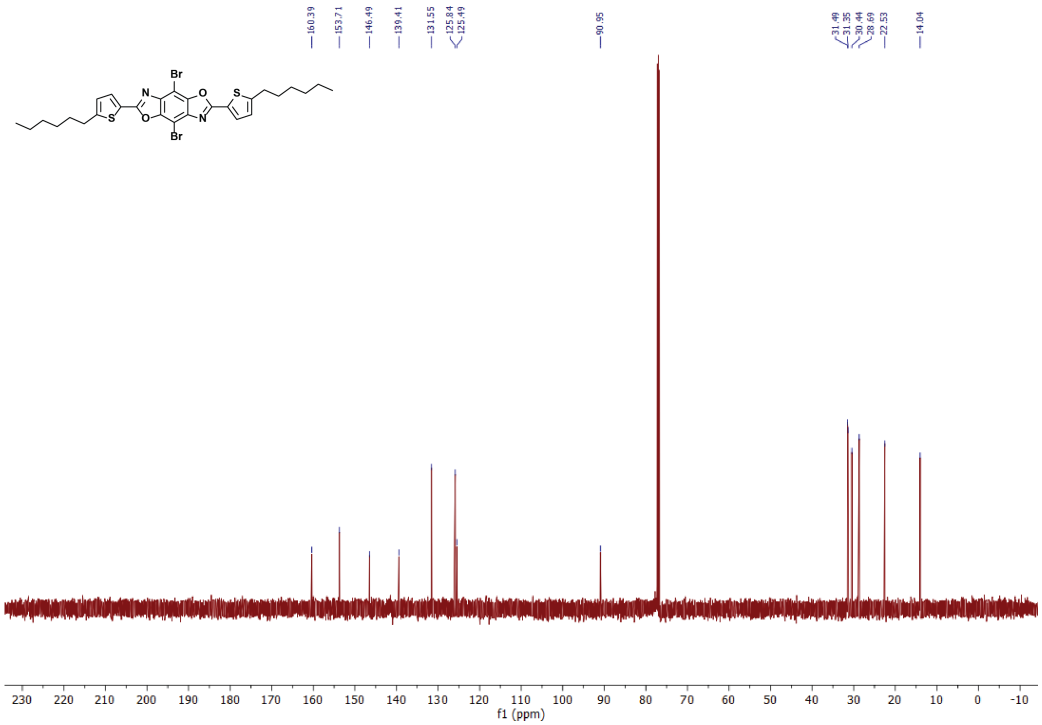


Figure S12. ^{13}C NMR of **26T48Br**

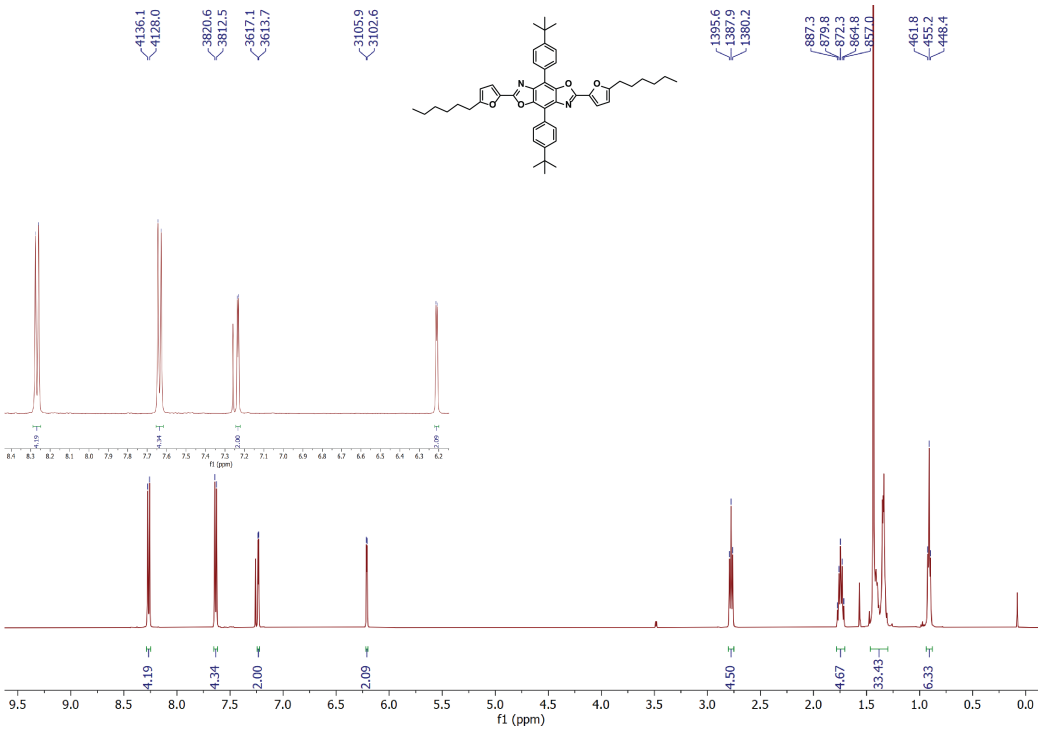


Figure S13. ^{1}H NMR of **FP**

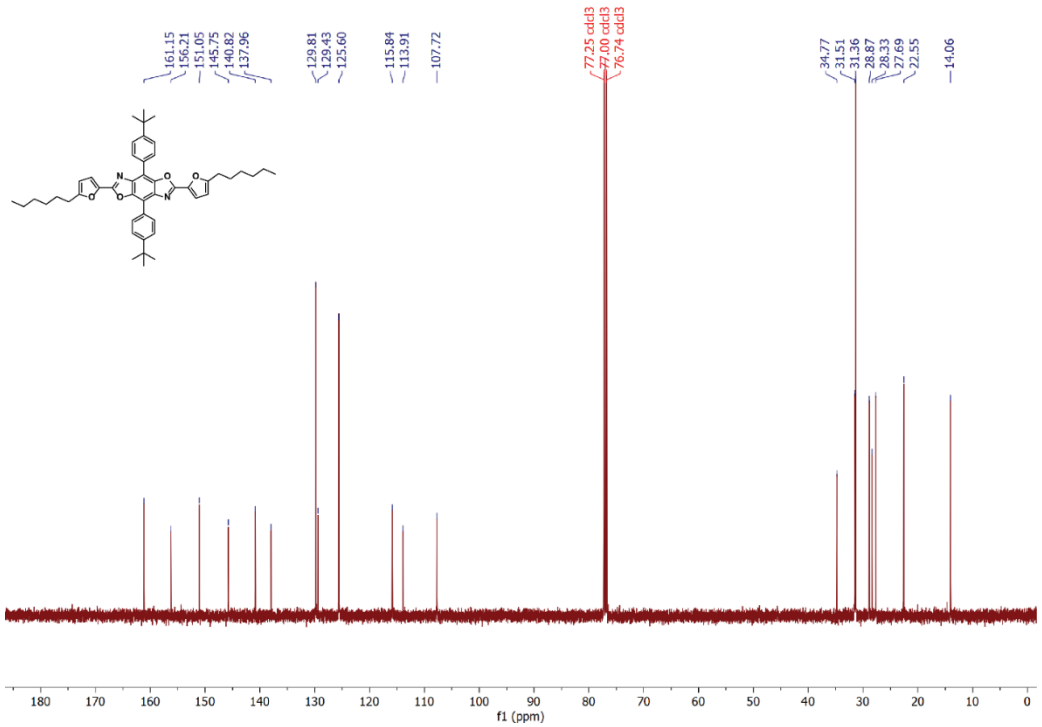


Figure S14. ^{13}C NMR of **FP**

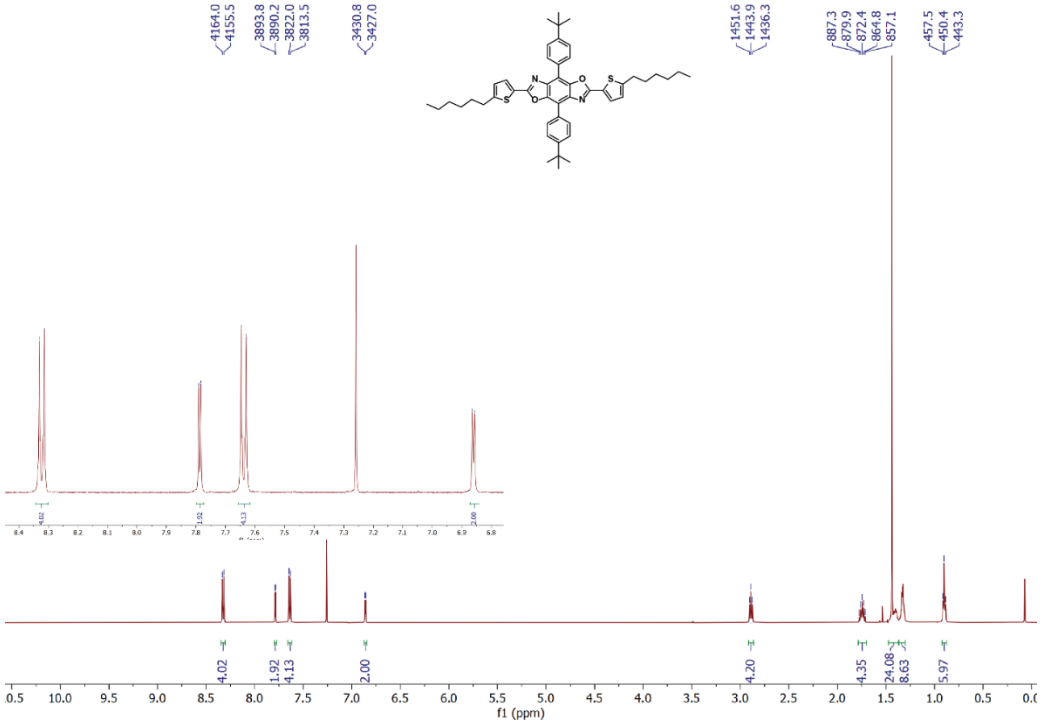


Figure S15. ^{1}H NMR of **TP**

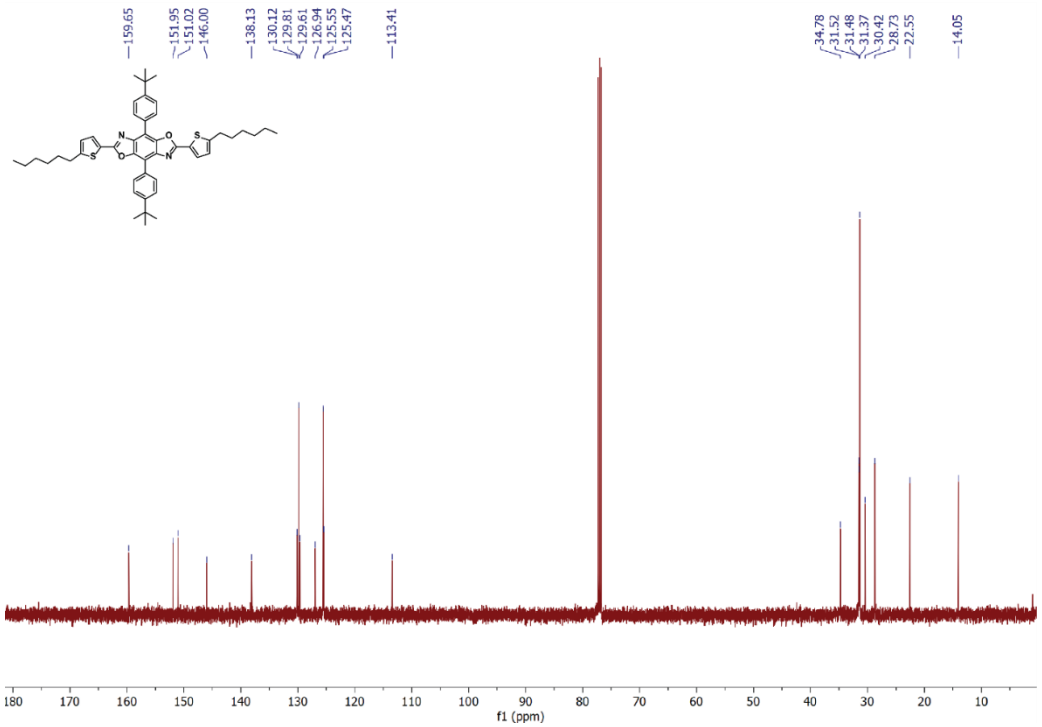


Figure S16. ^{13}C NMR of **TP**

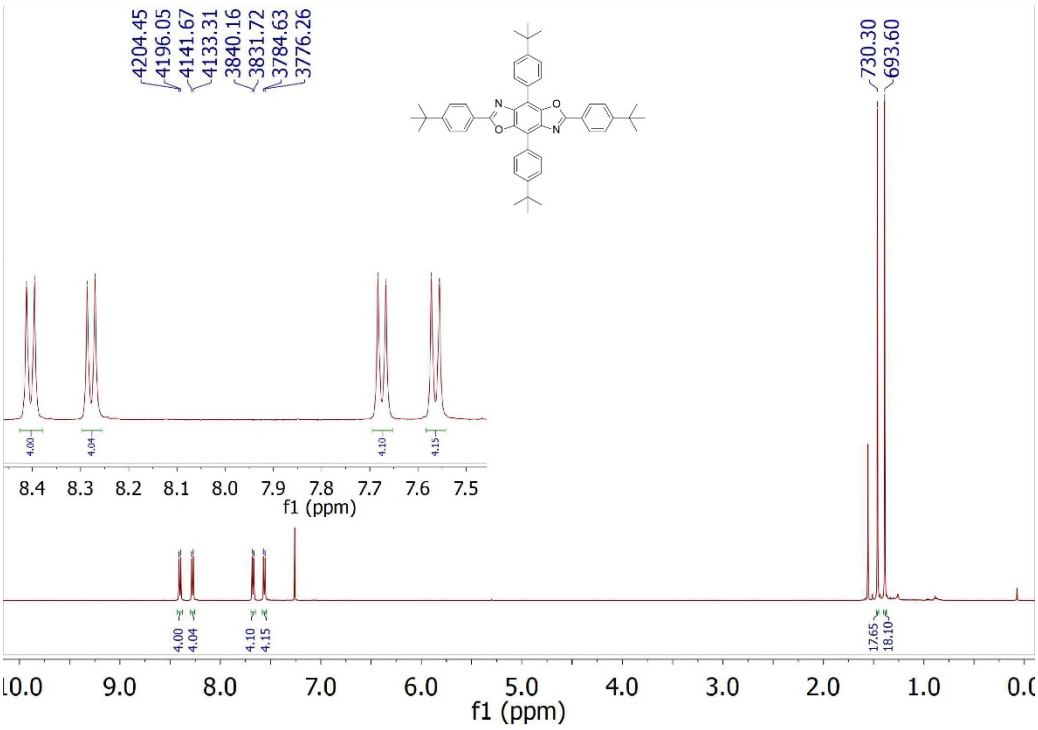


Figure S17. ^{1}H NMR of **PP**

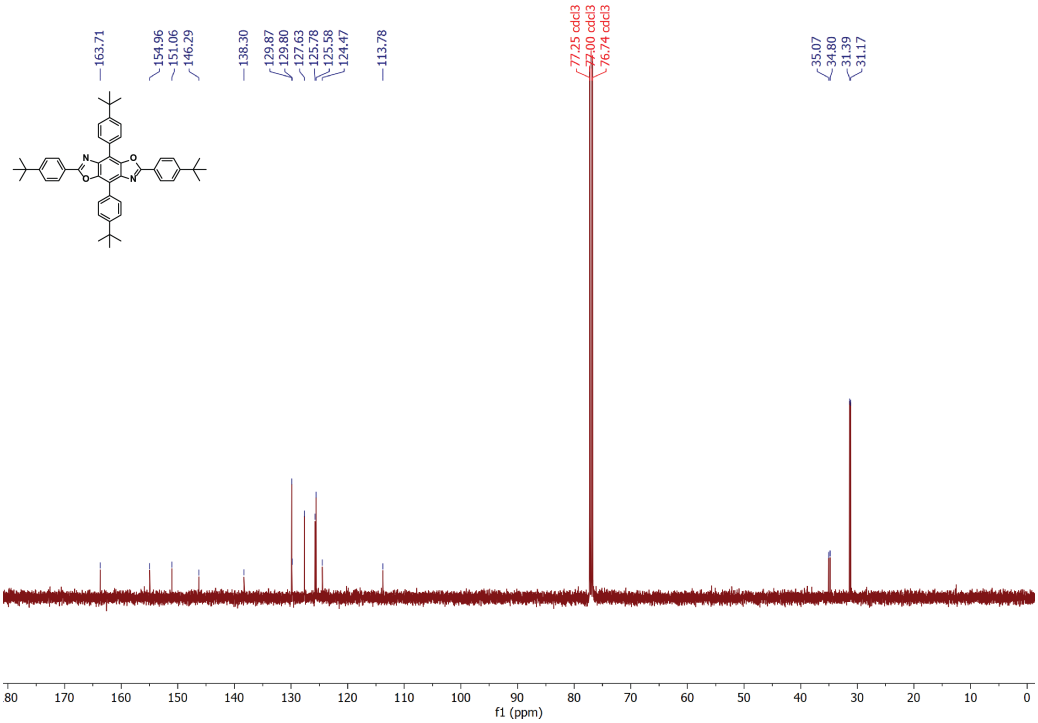


Figure S18. ^{13}C NMR of **PP**

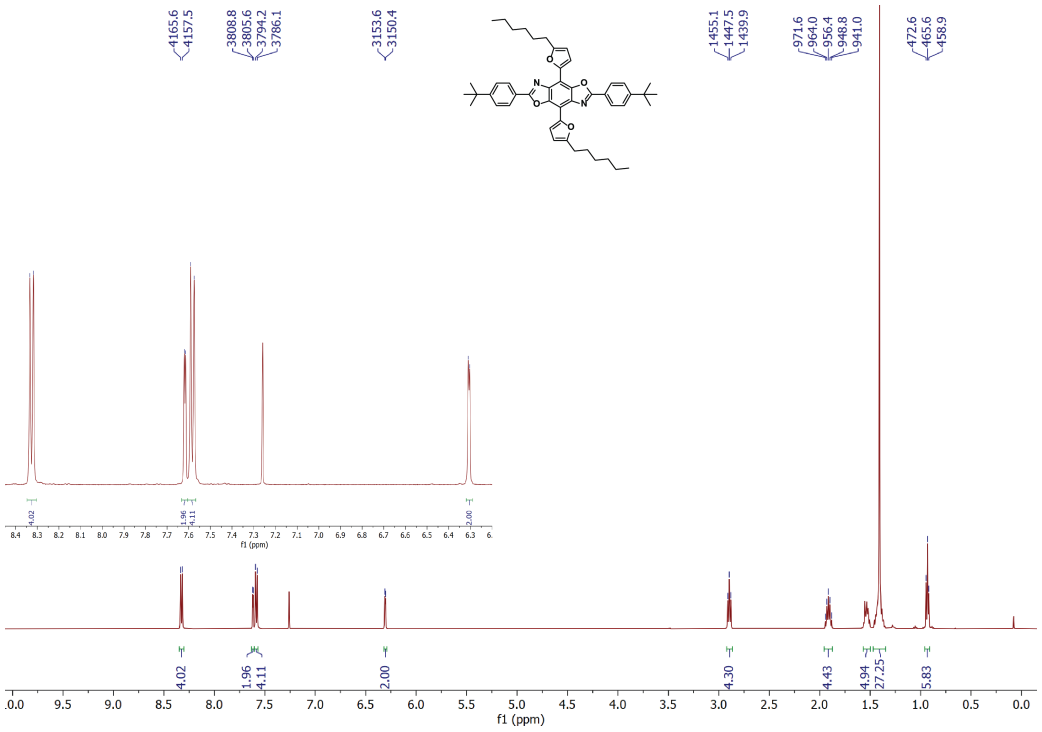


Figure S19. ^{1}H NMR of **PF**

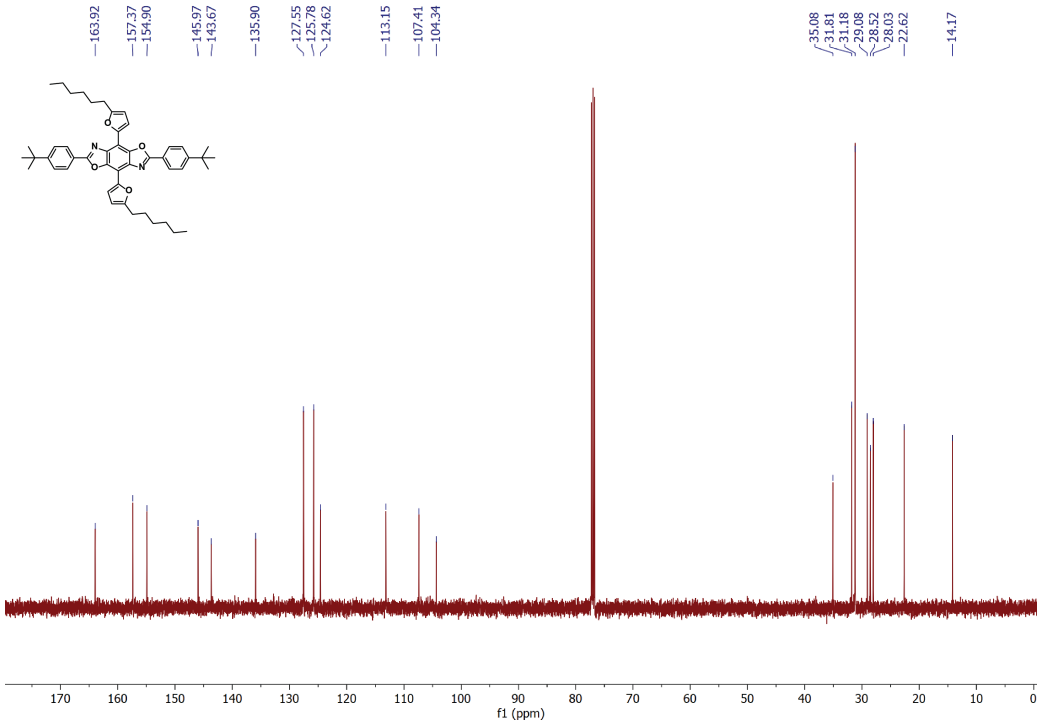


Figure S20. ^{13}C NMR of **PF**

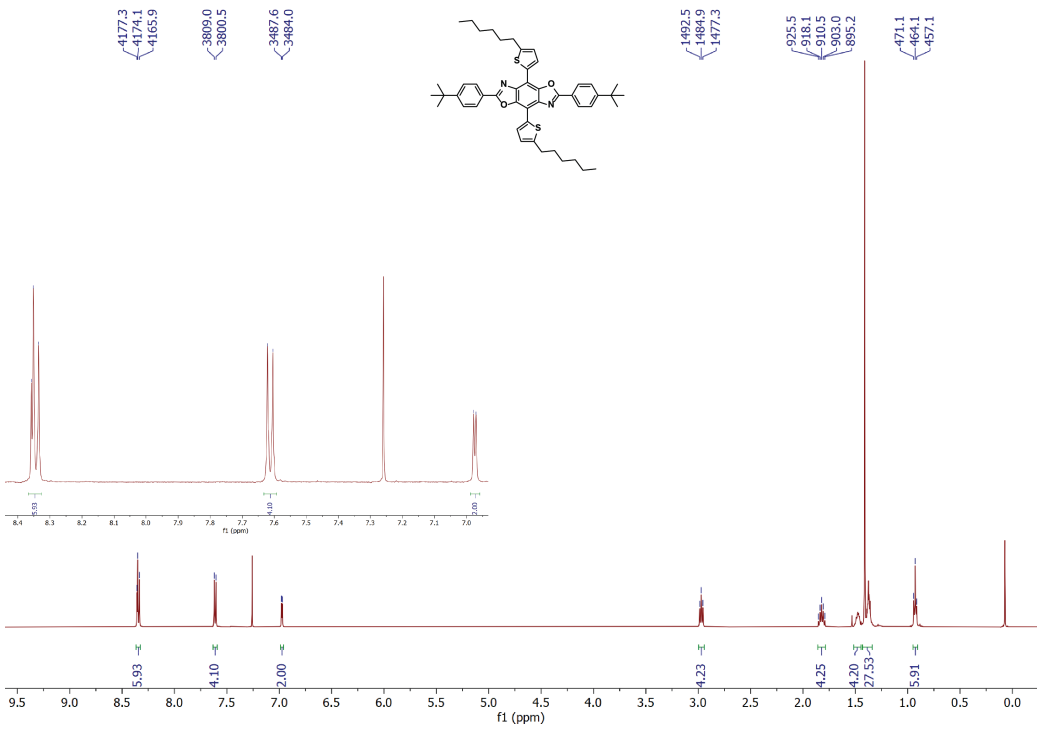


Figure S21. ^{1}H NMR of **PT**

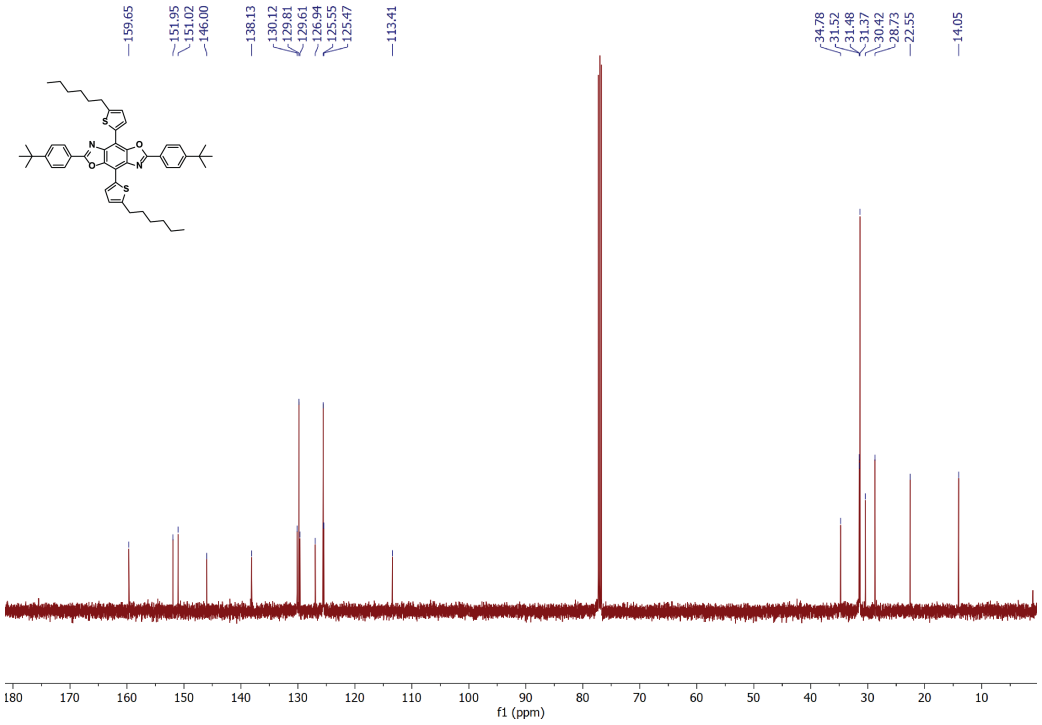


Figure S22. ^{13}C NMR of **PT**

Atomic Force Microscopy (AFM) Images

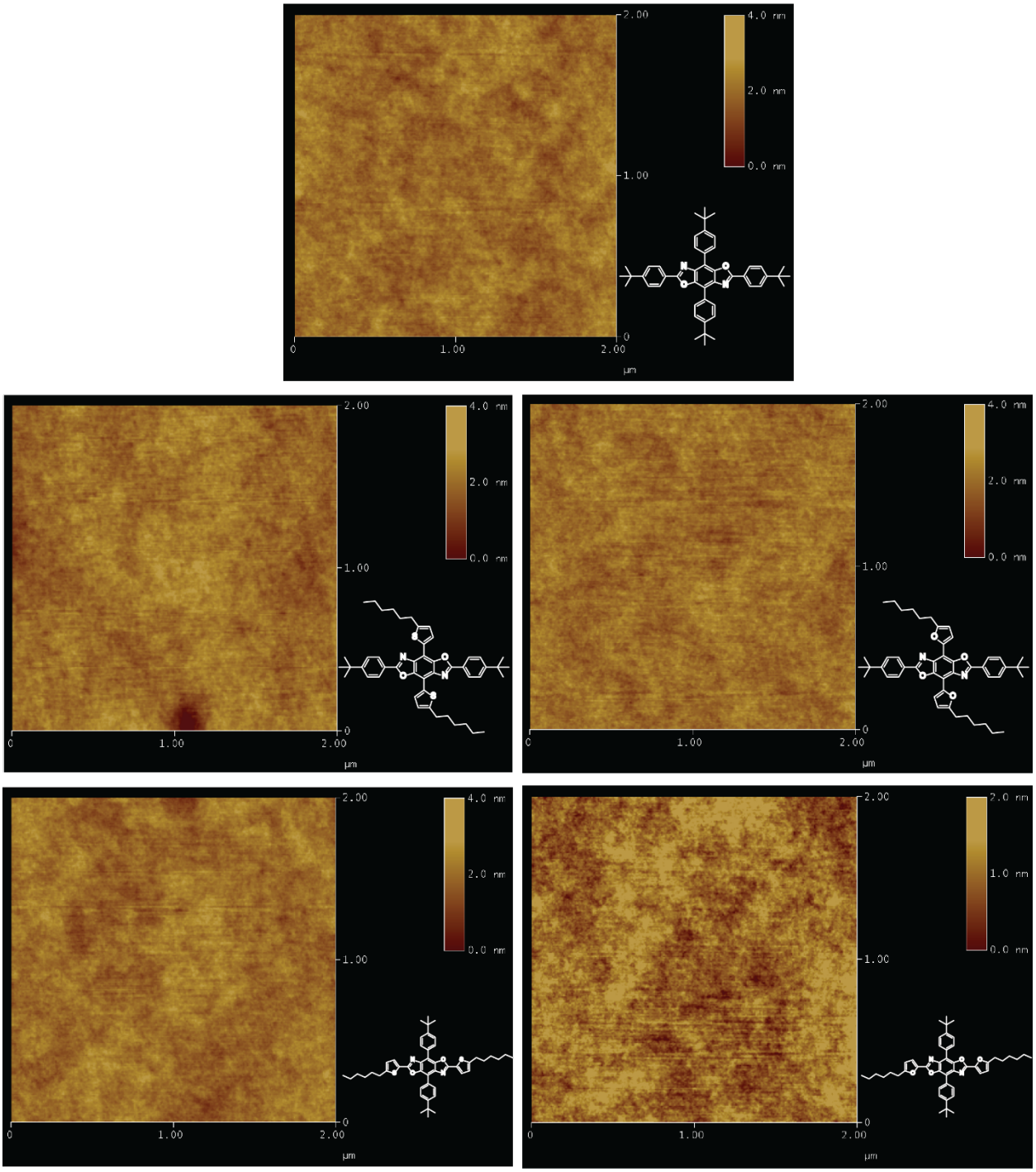


Figure S23. AFM Images of **PP** (top), **PT** (middle-left), **PF** (middle right), **TP** (bottom left), and **FP** (bottom right).

Additional Spectra

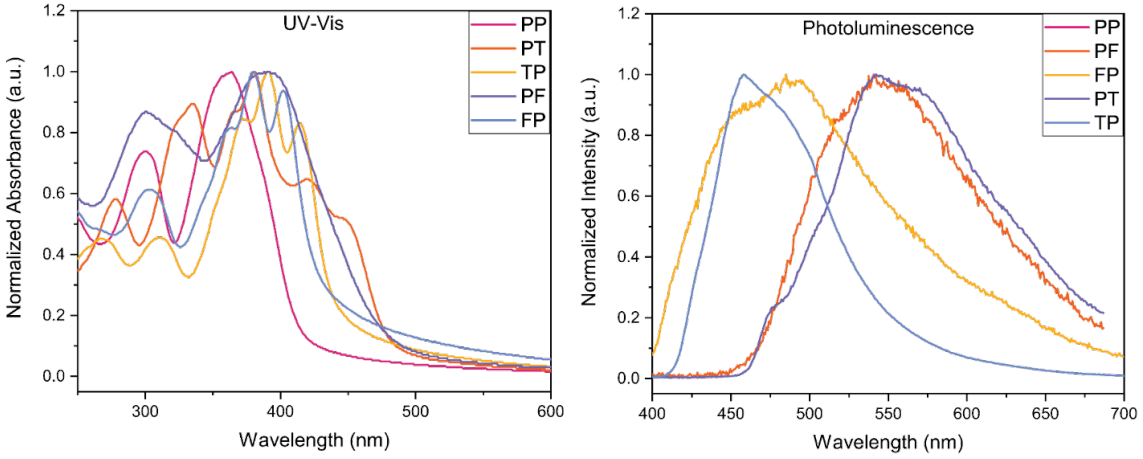


Figure S24. UV-Vis (left) and PL (right) spectra for the five investigated BBOs as amorphous thin-films.

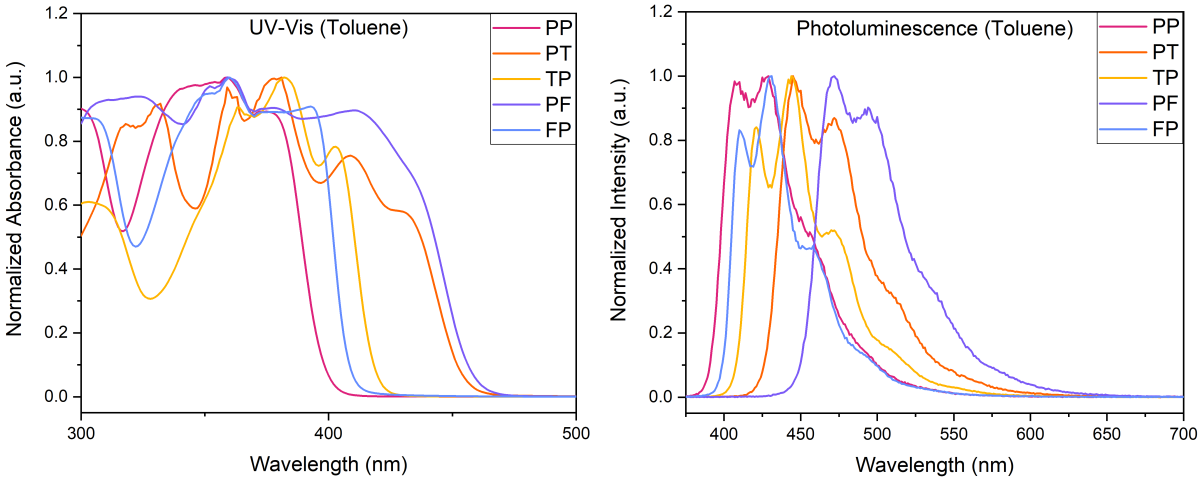


Figure S25. UV-Vis (left) and PL (right) spectra for the five investigated BBOs in toluene.

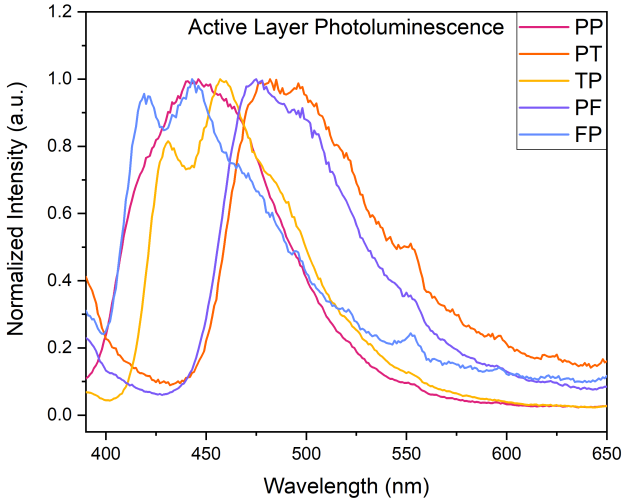


Figure S26. Photoluminescence spectra of the active layers spin-coated on quartz slides.

Cyclic Voltammograms

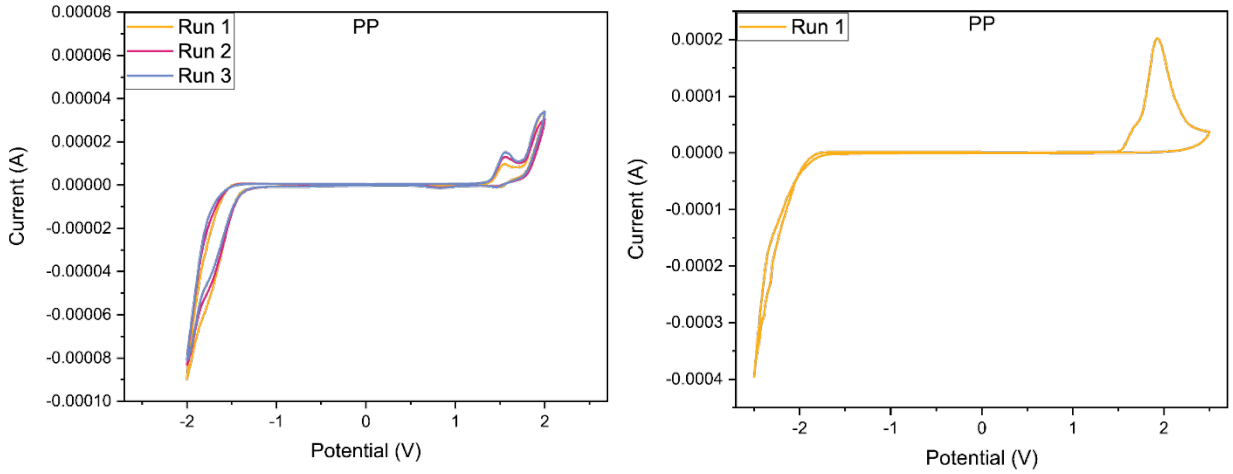


Figure S27. Cyclic voltammograms of PP in dichloromethane (left) and film (right).

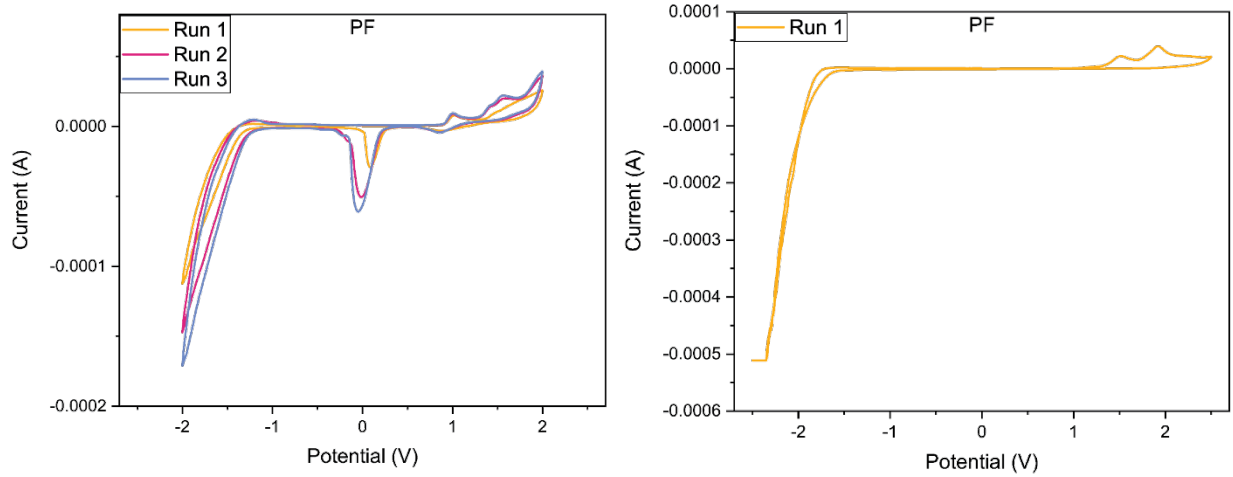


Figure S28. Cyclic voltammograms of PF in dichloromethane (left) and film (right).

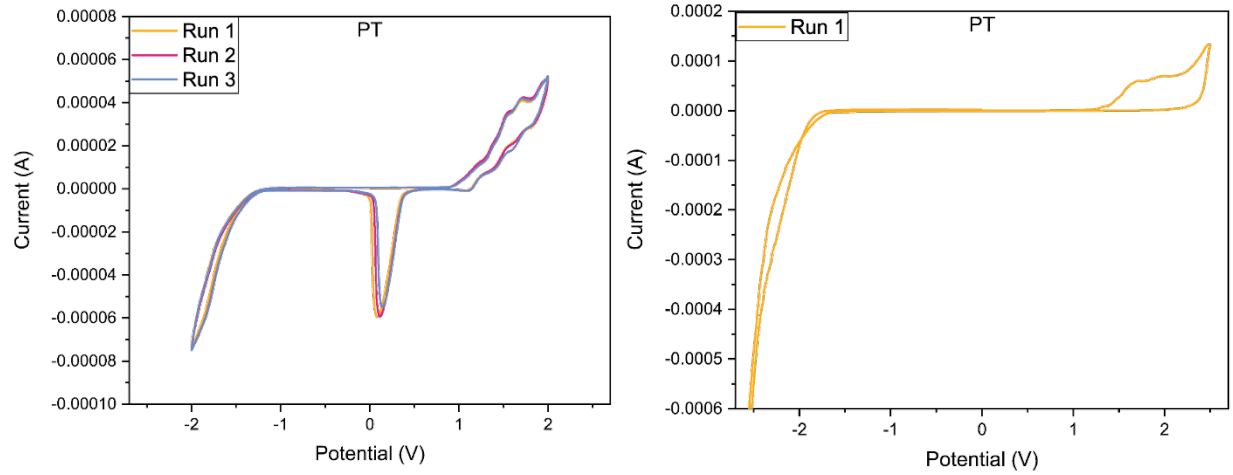


Figure S29. Cyclic voltammograms of PT in dichloromethane (left) and film (right).

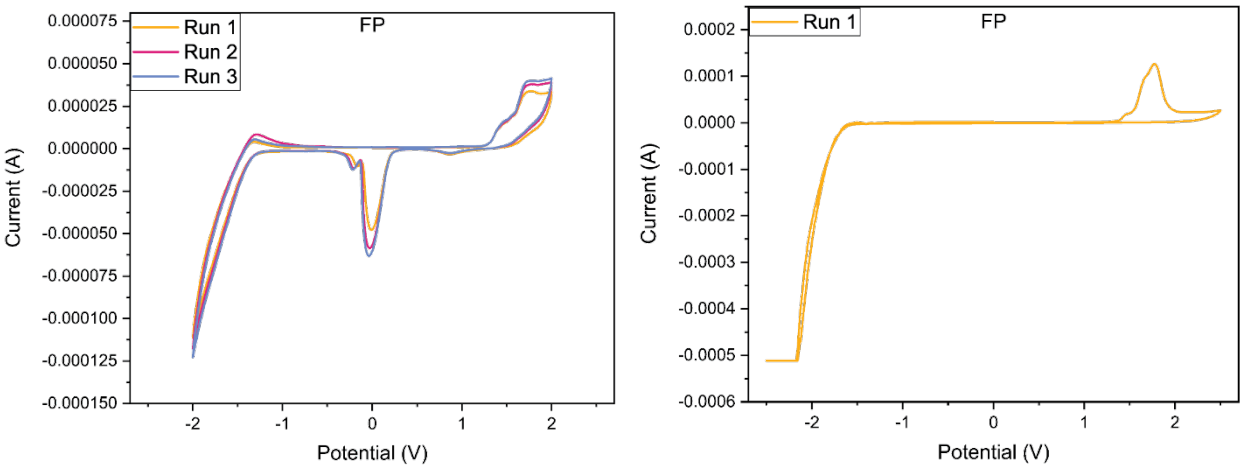


Figure S30. Cyclic voltammograms of FP in dichloromethane (left) and film (right).

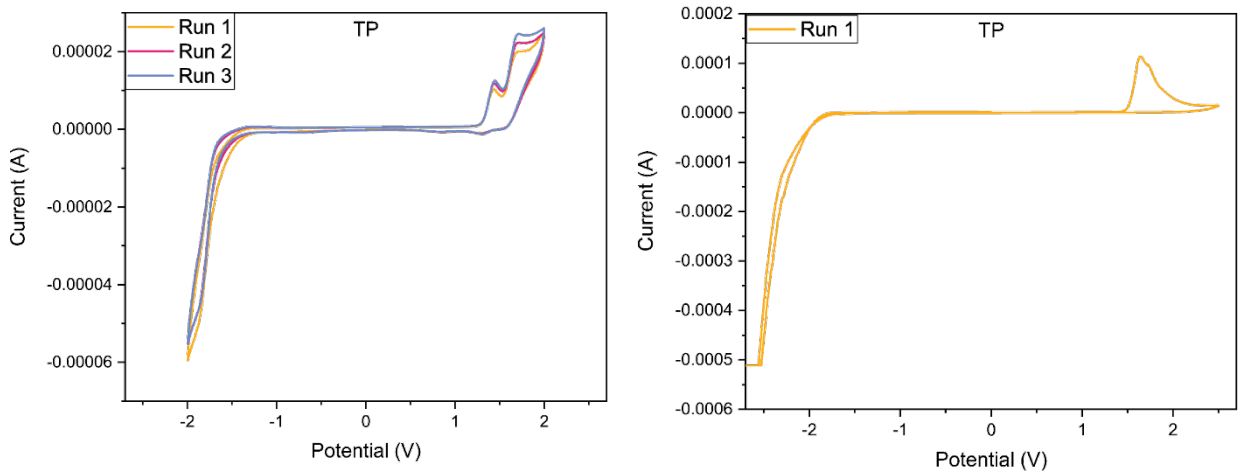


Figure S31. Cyclic voltammograms of TP in dichloromethane (left) and film (right).

JVL Characteristics

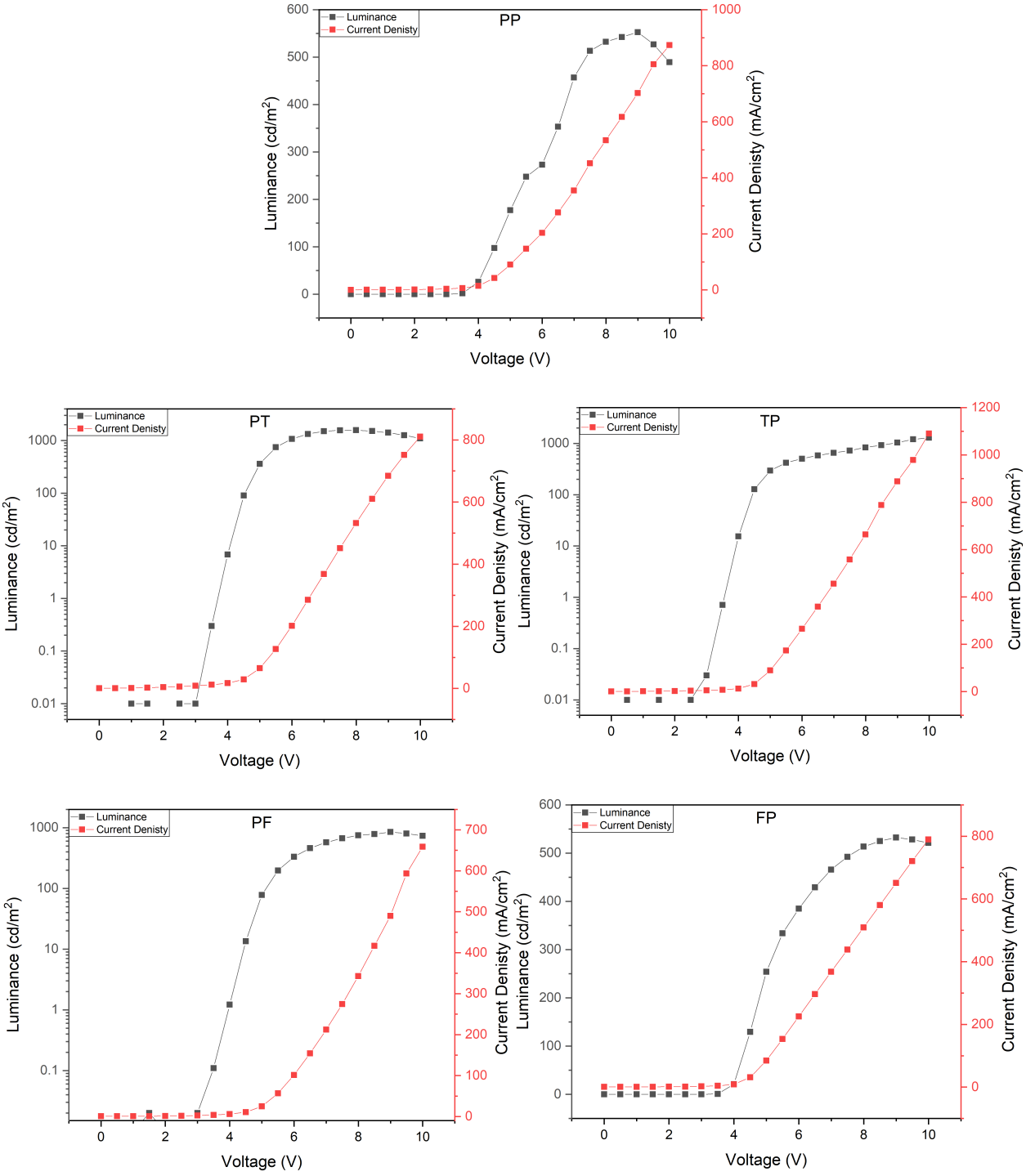


Figure S32. JVL Characteristics of the 5 BBO devices.

DFT/TDDFT Gaussian Setups

DFT Gaussian Setups

Gas Phase

opt freq b3lyp midix geom=connectivity b972

Population Example

shc scrf=(cpcm,solvent=chloroform) pop=regular geom=connectivity b972

TDDFT Gaussian Setup

td=(nstates=20)/shc scrf=(cpcm,solvent=chloroform) geom=connectivity b972

FF

Cartesian Coordinates

C	-1.18525	0.64711	0.
C	-0.07443	1.50182	0.
C	1.13998	0.77095	0.
C	1.18525	-0.64711	0.
C	0.07443	-1.50182	0.
C	-1.13998	-0.77095	0.
O	2.53194	-1.00455	0.
O	-2.53194	1.00455	0.
N	2.44779	1.2645	0.
N	-2.44779	-1.2645	0.
C	3.22809	0.21066	0.
C	-3.22809	-0.21066	0.
C	0.11254	-2.94294	0.
C	-0.87903	-3.9077	0.
C	-0.22206	-5.18263	0.00002
H	-1.94614	-3.69968	0.00001
C	1.12933	-4.93787	-0.00002
H	-0.70227	-6.15945	0.00004
H	2.01373	-5.56812	-0.00004
C	-0.11254	2.94294	0.

C	0.87903	3.9077	0.
C	0.22206	5.18263	0.00002
H	1.94614	3.69968	0.00001
C	-1.12933	4.93787	-0.00002
H	0.70227	6.15945	0.00004
H	-2.01373	5.56812	-0.00004
C	4.65451	0.11649	0.
C	5.50871	-0.96808	0.
C	6.8416	-0.44015	0.00003
H	5.20552	-2.01282	0.00001
C	6.72719	0.92976	-0.00002
H	7.76733	-1.01217	0.00006
H	7.44013	1.74889	-0.00004
C	-4.65451	-0.11649	0.
C	-5.50871	0.96808	-0.00001
C	-6.8416	0.44015	0.00002
H	-5.20552	2.01282	-0.00002
C	-6.72719	-0.92976	-0.00002
H	-7.76733	1.01217	0.00004
H	-7.44013	-1.74889	-0.00002
O	1.35589	-3.57484	-0.00001
O	-1.35589	3.57484	0.
O	-5.39439	-1.28853	0.00001
O	5.39439	1.28853	-0.00001

Energy Levels

Alpha occ. eigenvalues -- -19.21363 -19.21363 -19.21204 -19.21203 -19.19423

Alpha occ. eigenvalues -- -19.19422 -14.33738 -14.33737 -10.29385 -10.29384

Alpha occ. eigenvalues -- -10.25898 -10.25898 -10.25851 -10.25839 -10.24909

Alpha occ. eigenvalues -- -10.24909 -10.24124 -10.24113 -10.23190 -10.23179

Alpha occ. eigenvalues -- -10.23082 -10.23082 -10.22050 -10.22040 -10.20060

Alpha occ. eigenvalues -- -10.20060 -10.19662 -10.19662 -10.17883 -10.17883

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Alpha occ. eigenvalues -- -0.49807 -0.48747 -0.47836 -0.47388 -0.47170

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Alpha virt. eigenvalues -- 1.07590 1.08772 1.09346 1.09933 1.11571

Alpha virt. eigenvalues -- 1.12810 1.14595 1.15184 1.17507 1.19241

Alpha virt. eigenvalues -- 1.20637 1.21390 1.23435 1.23963 1.25399

Alpha virt. eigenvalues -- 1.25893 1.29052 1.31431 1.32800 1.33351

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Alpha virt. eigenvalues -- 1.70754 1.72836 1.74906 1.76833 1.77733

Alpha virt. eigenvalues -- 1.80235 1.88481 1.92889

Lowest 15 Excited States

Excited state	Energy (eV)	Wavelength (nm)	f
1	2.78	445.6	0.3726
2	3.39	365.6	0.8635
3	3.49	355.6	0.0000
4	3.70	335.4	0.0000
5	3.98	311.5	0.9722
6	4.26	291.0	0.0000
7	4.51	274.6	0.1191
8	4.54	272.8	0.0000
9	4.65	266.5	0.2559
10	4.67	265.7	0.0012
11	4.75	261.2	0.0000
12	4.78	259.1	0.0088
13	4.84	256.2	0.0000
14	4.87	254.7	0.0838
15	4.89	253.5	0.0000

Table S1. First 15 excitation energies, wavelength, and oscillator strengths for compound **FF**.

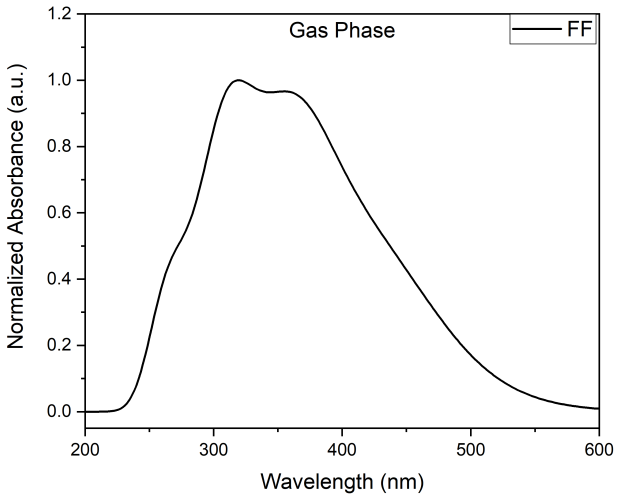

Figure S33. Simulated UV-Vis spectrum for compound **FF**.

Geometric Images

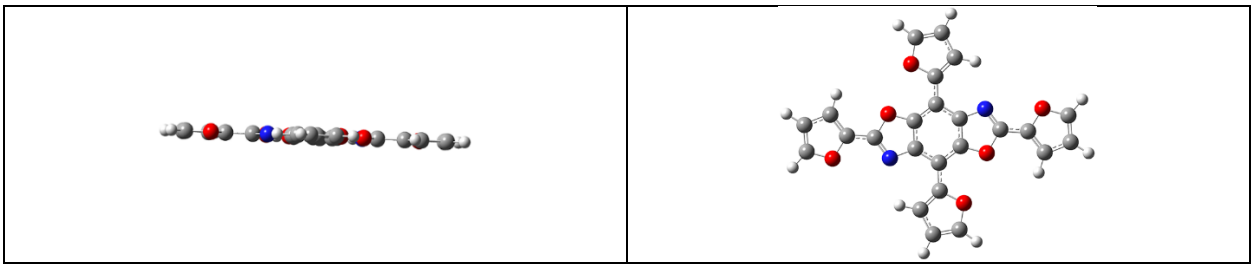

Figure S34. Geometric Images of compound **FF**.

FP

Cartesian Coordinates

C	-1.23438	-0.50872	-0.00002
C	-0.2453	-1.50613	0.00001
C	1.04265	-0.90381	0.00002
C	1.23438	0.5087	0.00002
C	0.2453	1.5061	0.
C	-1.04264	0.90379	-0.00003
O	2.61596	0.72057	0.00005
O	-2.61596	-0.72056	-0.00005
N	2.30333	-1.51567	0.00004
N	-2.30331	1.51568	-0.00007
C	3.18708	-0.54907	0.00006
C	-3.18707	0.54909	-0.00008
C	0.50952	2.96295	0.
C	-0.55601	3.89686	-0.00022
C	1.83198	3.47405	0.00021
C	-0.30797	5.27387	-0.00022
H	-1.58247	3.5285	-0.00037
C	2.07136	4.85293	0.00022
H	2.68114	2.79163	0.00038

C	1.00571	5.76334	0.
H	-1.15288	5.96982	-0.00039
H	3.10413	5.2153	0.00039
H	1.19675	6.84104	0.
C	-0.50953	-2.96298	0.00001
C	-1.83198	-3.47409	0.00027
C	0.556	-3.89691	-0.00025
C	-2.07138	-4.85296	0.00027
H	-2.68114	-2.79166	0.00047
C	0.30795	-5.27391	-0.00025
H	1.58246	-3.52855	-0.00043
C	-1.00574	-5.76338	0.00001
H	-3.10415	-5.21532	0.00048
H	1.15286	-5.96987	-0.00045
H	-1.19679	-6.84108	0.00001
C	-4.61366	0.65671	-0.0001
C	-5.45839	1.74771	-0.00015
C	-6.79587	1.23181	-0.00015
H	-5.14777	2.7901	-0.00017
C	-6.69576	-0.13912	-0.00011
H	-7.71585	1.81301	-0.00018
H	-7.41667	-0.95124	-0.00009
C	4.61367	-0.65667	0.00009
C	5.45841	-1.74767	0.00012
C	6.79588	-1.23176	0.00014
H	5.1478	-2.79006	0.00012
C	6.69576	0.13917	0.00012
H	7.71587	-1.81295	0.00016
H	7.41667	0.9513	0.00013

O	-5.36577	-0.50991	-0.00008
O	5.36577	0.50995	0.00009

Energy Levels

Alpha occ. eigenvalues -- -19.21906 -19.21906 -19.21726 -19.21726 -14.34074

Alpha occ. eigenvalues -- -14.34073 -10.29908 -10.29907 -10.26374 -10.26374

Alpha occ. eigenvalues -- -10.25893 -10.25880 -10.25314 -10.25314 -10.23455

Alpha occ. eigenvalues -- -10.23444 -10.21783 -10.21772 -10.20471 -10.20471

Alpha occ. eigenvalues -- -10.20051 -10.20051 -10.19361 -10.19348 -10.17358

Alpha occ. eigenvalues -- -10.17358 -10.17104 -10.17104 -10.17072 -10.17071

Alpha occ. eigenvalues -- -10.16885 -10.16884 -10.16583 -10.16583 -1.15434

Alpha occ. eigenvalues -- -1.15357 -1.13821 -1.13799 -0.95664 -0.95650

Alpha occ. eigenvalues -- -0.89184 -0.85933 -0.85101 -0.83303 -0.83027

Alpha occ. eigenvalues -- -0.82206 -0.80250 -0.80134 -0.75634 -0.75161

Alpha occ. eigenvalues -- -0.74085 -0.73944 -0.72515 -0.69896 -0.66553

Alpha occ. eigenvalues -- -0.64371 -0.64353 -0.63300 -0.62379 -0.61483

Alpha occ. eigenvalues -- -0.60570 -0.59712 -0.58543 -0.58521 -0.58206

Alpha occ. eigenvalues -- -0.56850 -0.56355 -0.56092 -0.52760 -0.51911

Alpha occ. eigenvalues -- -0.51500 -0.51234 -0.50352 -0.49759 -0.48376

Alpha occ. eigenvalues -- -0.47584 -0.47474 -0.47163 -0.46887 -0.46769

Alpha occ. eigenvalues -- -0.44714 -0.44476 -0.44031 -0.43816 -0.43537

Alpha occ. eigenvalues -- -0.43304 -0.43200 -0.42721 -0.42301 -0.42144

Alpha occ. eigenvalues -- -0.40849 -0.40123 -0.39551 -0.39404 -0.39392

Alpha occ. eigenvalues -- -0.39268 -0.36104 -0.35889 -0.35875 -0.35531

Alpha occ. eigenvalues -- -0.35091 -0.33775 -0.33744 -0.31551 -0.31203

Alpha occ. eigenvalues -- -0.30183 -0.29824 -0.29368 -0.29273 -0.27313

Alpha occ. eigenvalues -- -0.25496 -0.25494 -0.25267 -0.23412 -0.21371

Alpha virt. eigenvalues -- -0.09501 -0.06010 -0.04840 -0.00628 -0.00607

Alpha virt. eigenvalues -- -0.00280 0.00595 0.01760 0.02034 0.04727

Alpha virt. eigenvalues -- 0.06418 0.06475 0.07677 0.08067 0.08210

Alpha virt. eigenvalues -- 0.08320 0.08787 0.08819 0.10021 0.10596

Alpha virt. eigenvalues -- 0.10615 0.11104 0.11898 0.12354 0.12510

Alpha virt. eigenvalues -- 0.13048 0.13974 0.14401 0.14904 0.15029

Alpha virt. eigenvalues -- 0.16232 0.16496 0.17803 0.18703 0.18791

Alpha virt. eigenvalues -- 0.19829 0.19991 0.21166 0.21176 0.22021

Alpha virt. eigenvalues -- 0.22592 0.23254 0.23365 0.24069 0.26567

Alpha virt. eigenvalues -- 0.26667 0.27929 0.28024 0.28121 0.28725

Alpha virt. eigenvalues -- 0.29216 0.30092 0.30749 0.31129 0.31645

Alpha virt. eigenvalues -- 0.32565 0.32632 0.33380 0.33562 0.33779

Alpha virt. eigenvalues -- 0.34634 0.34888 0.35353 0.35805 0.36293

Alpha virt. eigenvalues -- 0.37266 0.38859 0.39394 0.39558 0.40984

Alpha virt. eigenvalues -- 0.41067 0.41750 0.42890 0.43157 0.44110

Alpha virt. eigenvalues -- 0.44125 0.44690 0.44784 0.44885 0.45257

Alpha virt. eigenvalues -- 0.45325 0.45745 0.46519 0.47017 0.47230

Alpha virt. eigenvalues -- 0.47476 0.47836 0.48024 0.48253 0.48772

Alpha virt. eigenvalues -- 0.49440 0.49729 0.49875 0.50199 0.50426

Alpha virt. eigenvalues -- 0.51136 0.51507 0.52092 0.52188 0.52310

Alpha virt. eigenvalues -- 0.52878 0.53572 0.54033 0.54277 0.54645

Alpha virt. eigenvalues -- 0.55256 0.55613 0.56440 0.56914 0.57365

Alpha virt. eigenvalues -- 0.57966 0.58805 0.58807 0.59444 0.60091

Alpha virt. eigenvalues -- 0.60285 0.61931 0.62012 0.62233 0.63001

Alpha virt. eigenvalues -- 0.64512 0.64637 0.64657 0.65872 0.66367

Alpha virt. eigenvalues -- 0.67491 0.67683 0.68167 0.68666 0.69559

Alpha virt. eigenvalues -- 0.69789 0.69832 0.70422 0.70463 0.70783

Alpha virt. eigenvalues -- 0.70983 0.70996 0.71835 0.71932 0.71978

Alpha virt. eigenvalues -- 0.72222 0.72616 0.73622 0.73941 0.74010

Alpha virt. eigenvalues -- 0.75122 0.75424 0.76532 0.76579 0.77586

Alpha virt. eigenvalues -- 0.78271 0.78818 0.79032 0.79475 0.79908

Alpha virt. eigenvalues -- 0.80320 0.81241 0.81566 0.82080 0.82130

Alpha virt. eigenvalues -- 0.83020 0.83977 0.85184 0.85281 0.87604

Alpha virt. eigenvalues -- 0.88517 0.89735 0.91393 0.91515 0.92768

Alpha virt. eigenvalues -- 0.93459 0.93614 0.96149 0.97742 0.99299

Alpha virt. eigenvalues -- 1.00341 1.00457 1.00498 1.02664 1.03962

Alpha virt. eigenvalues -- 1.04709 1.06719 1.07771 1.07821 1.09856

Alpha virt. eigenvalues -- 1.09947 1.10562 1.12404 1.12907 1.13400

Alpha virt. eigenvalues -- 1.16069 1.17158 1.19421 1.20178 1.20204

Alpha virt. eigenvalues -- 1.20730 1.24274 1.26424 1.27263 1.29946

Alpha virt. eigenvalues -- 1.32058 1.32461 1.32758 1.33907 1.34407

Alpha virt. eigenvalues -- 1.35256 1.35639 1.39591 1.43144 1.46536

Alpha virt. eigenvalues -- 1.48396 1.49474 1.51475 1.55205 1.56347

Alpha virt. eigenvalues -- 1.58786 1.60363 1.69883 1.70463 1.75769

Alpha virt. eigenvalues -- 1.80735 1.84186 1.91934

Lowest 15 Excited States

Excited state	Energy (eV)	Wavelength (nm)	f
1	2.96	418.2	0.4437
2	3.42	362.2	0.8305
3	3.67	338.2	0.0000
4	3.84	322.9	0.0000
5	3.85	322.2	0.0451
6	3.88	319.2	0.0000
7	4.12	300.4	0.8686
8	4.29	288.8	0.0000
9	4.54	273.3	0.0010
10	4.58	270.4	0.0000
11	4.60	269.6	0.1646
12	4.67	265.6	0.0000
13	4.79	258.8	0.1298
14	4.81	257.9	0.0000
15	4.81	257.6	0.0461

Table S2. First 15 excitation energies, wavelength, and oscillator strengths for compound **FP**.

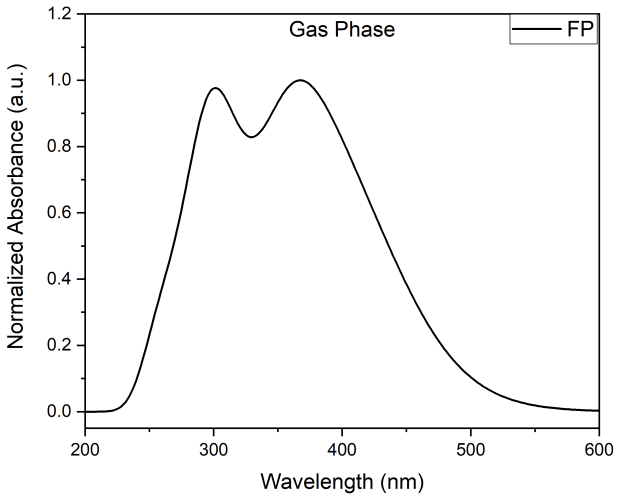

Figure S35. Simulated UV-Vis spectrum for compound **FP**.

Geometric Images

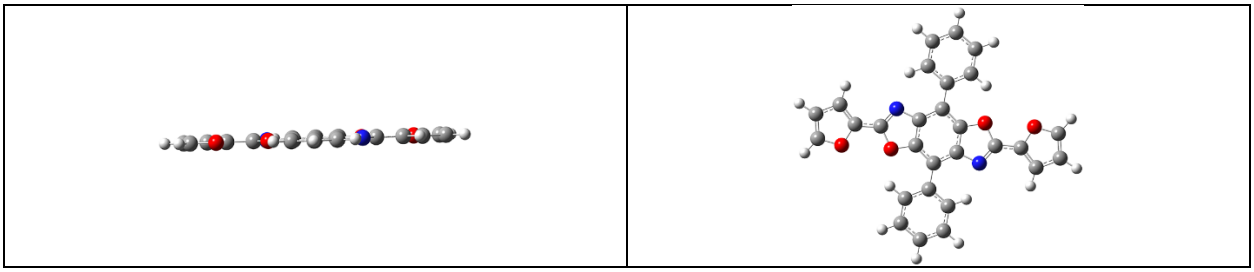

Figure S36. Geometric Images of compound **FP**.

FT

Cartesian Coordinates

C	-1.22713	-0.52725	-0.00008
C	-0.21624	-1.49901	-0.00011
C	1.06292	-0.88128	-0.00002
C	1.22713	0.52725	0.0001
C	0.21624	1.49901	0.00013
C	-1.06292	0.88128	0.00003
O	2.59864	0.77367	0.00016

O	-2.59864	-0.77367	-0.00016
N	2.32828	-1.47758	-0.00001
N	-2.32828	1.47758	0.00002
C	3.1955	-0.49558	0.00009
C	-3.1955	0.49558	-0.00009
C	0.42418	2.93112	0.00024
C	-0.54206	3.92233	0.00028
S	2.07819	3.66879	0.00036
C	-0.01422	5.25071	0.00036
H	-1.60505	3.67359	0.00023
C	1.35807	5.29426	0.00039
H	-0.63991	6.14613	0.00039
H	2.00845	6.16823	0.00044
C	-0.42418	-2.93112	-0.0002
C	0.54206	-3.92233	-0.00014
S	-2.07819	-3.66879	-0.00015
C	0.01422	-5.25071	-0.0005
H	1.60505	-3.67359	0.00001
C	-1.35807	-5.29426	-0.00084
H	0.63991	-6.14613	-0.00064
H	-2.00845	-6.16823	-0.00123
C	4.6245	-0.52108	0.00015
C	5.56905	0.48615	0.00026
C	6.85132	-0.15457	0.00027
H	5.35968	1.55372	0.00033
C	6.61959	-1.50955	0.00015
H	7.82263	0.33598	0.00035
H	7.25951	-2.38693	0.00011
C	-4.6245	0.52108	-0.00015

C	-5.56905	-0.48615	-0.00027
C	-6.85132	0.15457	-0.00027
H	-5.35968	-1.55372	-0.00034
C	-6.61959	1.50955	-0.00017
H	-7.82263	-0.33598	-0.00034
H	-7.25951	2.38693	-0.00014
O	-5.26109	1.75242	-0.0001
O	5.26109	-1.75242	0.00007

Energy Levels

Alpha occ. eigenvalues -- -88.85349 -88.85349 -19.21833 -19.21832 -19.21612

Alpha occ. eigenvalues -- -19.21612 -14.34142 -14.34142 -10.29886 -10.29885

Alpha occ. eigenvalues -- -10.26199 -10.26199 -10.26061 -10.26049 -10.25151

Alpha occ. eigenvalues -- -10.25151 -10.23546 -10.23536 -10.22456 -10.22446

Alpha occ. eigenvalues -- -10.22215 -10.22202 -10.20502 -10.20502 -10.20347

Alpha occ. eigenvalues -- -10.20347 -10.19879 -10.19879 -10.18111 -10.18111

Alpha occ. eigenvalues -- -10.17667 -10.17667 -7.98040 -7.98040 -5.94459

Alpha occ. eigenvalues -- -5.94459 -5.94017 -5.94017 -5.93526 -5.93526

Alpha occ. eigenvalues -- -1.15227 -1.15130 -1.13800 -1.13791 -0.95795

Alpha occ. eigenvalues -- -0.95774 -0.90253 -0.89020 -0.87738 -0.83465

Alpha occ. eigenvalues -- -0.82978 -0.81879 -0.80955 -0.80030 -0.75230

Alpha occ. eigenvalues -- -0.74792 -0.74168 -0.73950 -0.71202 -0.69860

Alpha occ. eigenvalues -- -0.66471 -0.64308 -0.64177 -0.63501 -0.62056

Alpha occ. eigenvalues -- -0.59828 -0.58529 -0.58403 -0.57033 -0.56756

Alpha occ. eigenvalues -- -0.56400 -0.56269 -0.54771 -0.54298 -0.52006

Alpha occ. eigenvalues -- -0.51639 -0.51352 -0.51269 -0.50219 -0.48928

Alpha occ. eigenvalues -- -0.47516 -0.47378 -0.46838 -0.46773 -0.45732

Alpha occ. eigenvalues -- -0.44276 -0.43999 -0.43582 -0.43163 -0.43135

Alpha occ. eigenvalues -- -0.42288 -0.40981 -0.40466 -0.40335 -0.40232

Alpha occ. eigenvalues -- -0.39532 -0.39375 -0.39269 -0.38717 -0.37885

Alpha occ. eigenvalues -- -0.36914 -0.36330 -0.34967 -0.34672 -0.34231

Alpha occ. eigenvalues -- -0.31403 -0.31076 -0.30274 -0.30140 -0.29731

Alpha occ. eigenvalues -- -0.29511 -0.27074 -0.26083 -0.26078 -0.24671

Alpha occ. eigenvalues -- -0.23299 -0.20626

Alpha virt. eigenvalues -- -0.09766 -0.05962 -0.05464 -0.02099 0.00026

Alpha virt. eigenvalues -- 0.01893 0.02093 0.03146 0.03665 0.03759

Alpha virt. eigenvalues -- 0.05933 0.07343 0.07362 0.07897 0.08246

Alpha virt. eigenvalues -- 0.08306 0.08467 0.08629 0.08647 0.09013

Alpha virt. eigenvalues -- 0.09046 0.09410 0.10387 0.11157 0.12203

Alpha virt. eigenvalues -- 0.12277 0.12598 0.14341 0.14592 0.15032

Alpha virt. eigenvalues -- 0.15987 0.16166 0.17068 0.17809 0.18480

Alpha virt. eigenvalues -- 0.18924 0.19125 0.20378 0.22909 0.23475

Alpha virt. eigenvalues -- 0.25342 0.25460 0.27273 0.27985 0.28497

Alpha virt. eigenvalues -- 0.28934 0.29085 0.29889 0.29946 0.30361

Alpha virt. eigenvalues -- 0.30708 0.32627 0.33200 0.33370 0.34046

Alpha virt. eigenvalues -- 0.34366 0.34621 0.35494 0.37659 0.37842

Alpha virt. eigenvalues -- 0.39102 0.39335 0.40425 0.40669 0.41819

Alpha virt. eigenvalues -- 0.42015 0.42173 0.42418 0.43041 0.43089

Alpha virt. eigenvalues -- 0.43711 0.43893 0.44521 0.44998 0.45316

Alpha virt. eigenvalues -- 0.45873 0.46448 0.46584 0.47930 0.48058

Alpha virt. eigenvalues -- 0.48228 0.48394 0.48862 0.49050 0.49904

Alpha virt. eigenvalues -- 0.50708 0.50715 0.51333 0.51748 0.51791

Alpha virt. eigenvalues -- 0.53153 0.53184 0.53504 0.53871 0.54366

Alpha virt. eigenvalues -- 0.54456 0.55014 0.55770 0.56051 0.57217

Alpha virt. eigenvalues -- 0.57227 0.57599 0.57795 0.58474 0.58589

Alpha virt. eigenvalues -- 0.60020 0.60342 0.61753 0.61878 0.63435

Alpha virt. eigenvalues -- 0.63505 0.65278 0.65320 0.66096 0.67044

Alpha virt. eigenvalues -- 0.67073 0.67181 0.67213 0.67395 0.69077

Alpha virt. eigenvalues -- 0.69252 0.69891 0.70334 0.70478 0.71575

Alpha virt. eigenvalues -- 0.71636 0.71817 0.71991 0.72266 0.73556

Alpha virt. eigenvalues -- 0.74523 0.74709 0.75219 0.75437 0.75564

Alpha virt. eigenvalues -- 0.75851 0.76378 0.76926 0.77246 0.77948

Alpha virt. eigenvalues -- 0.78165 0.78235 0.79984 0.80285 0.80384

Alpha virt. eigenvalues -- 0.81345 0.81904 0.82573 0.84036 0.84232

Alpha virt. eigenvalues -- 0.84894 0.88278 0.88550 0.92716 0.93119

Alpha virt. eigenvalues -- 0.93147 0.94319 0.95675 0.96525 0.98356

Alpha virt. eigenvalues -- 1.01720 1.03458 1.03687 1.04121 1.04254

Alpha virt. eigenvalues -- 1.04505 1.06018 1.06118 1.08300 1.09969

Alpha virt. eigenvalues -- 1.10462 1.10611 1.12087 1.14397 1.14700

Alpha virt. eigenvalues -- 1.16854 1.17019 1.19568 1.19585 1.21100

Alpha virt. eigenvalues -- 1.21891 1.22753 1.24629 1.28102 1.28505

Alpha virt. eigenvalues -- 1.31101 1.31176 1.32838 1.34928 1.37186

Alpha virt. eigenvalues -- 1.40032 1.40845 1.44773 1.49513 1.52437

Alpha virt. eigenvalues -- 1.55026 1.55589 1.71726 1.73390 1.74617

Alpha virt. eigenvalues -- 1.78885 1.83313 1.88841

Lowest 15 Excited States

Excited state	Energy (eV)	Wavelength (nm)	f
1	2.74	452.0	0.4173
2	3.32	373.2	0.7405
3	3.47	357.6	0.0000
4	3.64	240.2	0.0000
5	3.81	325.5	0.7822
6	3.95	313.8	0.0000
7	3.96	312.9	0.1130
8	4.22	293.7	0.0000
9	4.40	281.6	0.2186
10	4.42	280.3	0.0000
11	4.58	270.6	0.0012
12	4.63	267.6	0.0000
13	4.64	267.1	0.2343
14	4.68	264.9	0.0000

15	4.79	259.1	0.0376

Table S3. First 15 excitation energies, wavelength, and oscillator strengths for compound **FT**.

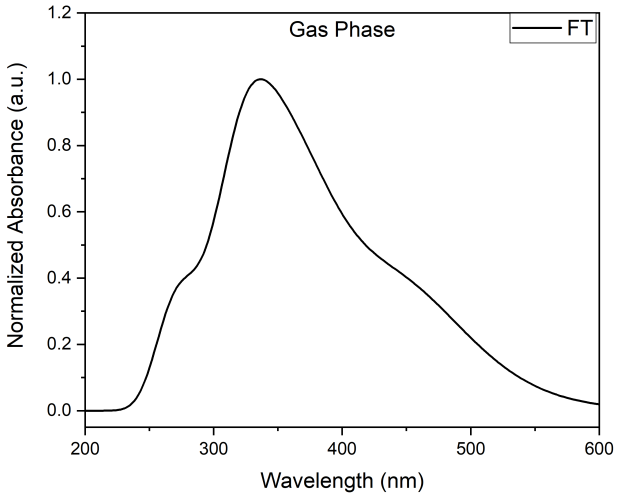

Figure S37. Simulated UV-Vis spectrum for compound **FT**.

Geometric Images

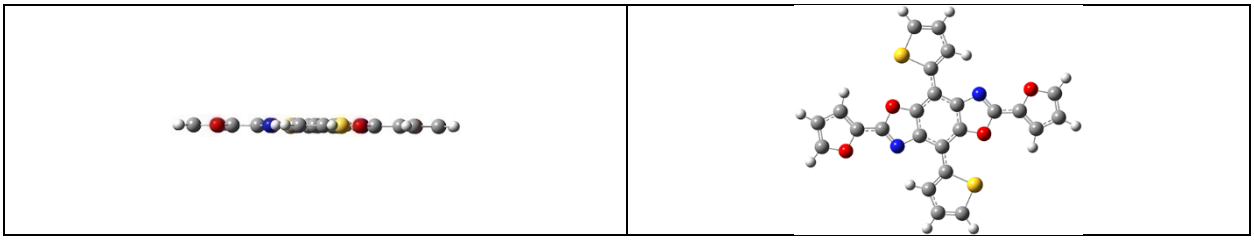

Figure S38. Geometric Images of compound **FT**.

PF

Cartesian Coordinates

C	-1.19734	0.62104	0.
C	-0.10475	1.49948	0.00001
C	1.12552	0.79586	0.
C	1.19734	-0.62104	0.
C	0.10475	-1.49948	-0.00001

C	-1.12552	-0.79586	0.
O	2.54868	-0.95162	0.
O	-2.54868	0.95162	0.00001
N	2.42669	1.30799	0.00001
N	-2.42669	-1.30799	0.
C	3.23188	0.27056	0.
C	-3.23188	-0.27056	0.
C	-4.68238	-0.23453	0.
C	-5.3692	0.99745	0.
C	-5.41078	-1.44242	0.
C	-6.76847	1.01554	0.
H	-4.79543	1.9279	0.
C	-6.80846	-1.41532	0.
H	-4.86417	-2.38927	0.
C	-7.49103	-0.18761	0.
H	-7.29818	1.97279	0.
H	-7.3699	-2.35429	0.
H	-8.5852	-0.1696	0.
C	4.68238	0.23453	0.
C	5.3692	-0.99745	-0.00001
C	5.41078	1.44242	0.
C	6.76847	-1.01554	-0.00001
H	4.79543	-1.9279	-0.00002
C	6.80846	1.41532	0.
H	4.86417	2.38927	0.00001
C	7.49103	0.18761	-0.00001
H	7.29818	-1.97279	-0.00002
H	7.3699	2.35429	0.00001
H	8.5852	0.1696	-0.00001

C	0.18144	-2.93944	-0.00001
C	-0.78234	-3.93168	-0.00001
C	-0.09146	-5.18855	-0.00002
H	-1.85431	-3.75365	-0.00001
C	1.25254	-4.90683	-0.00002
H	-0.54442	-6.17831	-0.00003
H	2.15414	-5.51215	-0.00002
C	-0.18144	2.93944	0.00001
C	0.78234	3.93168	0.00002
C	0.09146	5.18855	0.00002
H	1.85431	3.75365	0.00002
C	-1.25254	4.90683	0.00002
H	0.54442	6.17831	0.00002
H	-2.15414	5.51215	0.00002
O	-1.44105	3.53788	0.00002
O	1.44105	-3.53788	-0.00001

Energy Levels

Alpha occ. eigenvalues -- -19.21004 -19.21003 -19.19591 -19.19591 -14.33631

Alpha occ. eigenvalues -- -14.33631 -10.28738 -10.28738 -10.25789 -10.25777

Alpha occ. eigenvalues -- -10.24313 -10.24302 -10.23234 -10.23234 -10.23188

Alpha occ. eigenvalues -- -10.23178 -10.22095 -10.22086 -10.20797 -10.20796

Alpha occ. eigenvalues -- -10.19185 -10.19185 -10.19170 -10.19170 -10.19147

Alpha occ. eigenvalues -- -10.19147 -10.18935 -10.18935 -10.18918 -10.18918

Alpha occ. eigenvalues -- -10.18078 -10.18078 -10.17771 -10.17771 -1.14500

Alpha occ. eigenvalues -- -1.14386 -1.11630 -1.11625 -0.95163 -0.95121

Alpha occ. eigenvalues -- -0.89373 -0.87832 -0.87105 -0.82255 -0.80924

Alpha occ. eigenvalues -- -0.80757 -0.80255 -0.78822 -0.76578 -0.76120

Alpha occ. eigenvalues -- -0.76101 -0.74336 -0.72968 -0.69059 -0.66162

Alpha occ. eigenvalues -- -0.64934 -0.64315 -0.62968 -0.61772 -0.61475

Alpha occ. eigenvalues -- -0.60550 -0.59684 -0.59389 -0.57989 -0.56005

Alpha occ. eigenvalues -- -0.55976 -0.55779 -0.54445 -0.54197 -0.53235

Alpha occ. eigenvalues -- -0.51172 -0.50442 -0.48849 -0.48769 -0.48333

Alpha occ. eigenvalues -- -0.47977 -0.47403 -0.47062 -0.46458 -0.46146

Alpha occ. eigenvalues -- -0.45864 -0.45611 -0.44669 -0.44389 -0.44104

Alpha occ. eigenvalues -- -0.44082 -0.42055 -0.41808 -0.41387 -0.41282

Alpha occ. eigenvalues -- -0.40686 -0.40142 -0.39338 -0.39283 -0.37480

Alpha occ. eigenvalues -- -0.37406 -0.37212 -0.37046 -0.36912 -0.36819

Alpha occ. eigenvalues -- -0.36129 -0.35994 -0.34131 -0.30550 -0.30043

Alpha occ. eigenvalues -- -0.29724 -0.29567 -0.29151 -0.28862 -0.27606

Alpha occ. eigenvalues -- -0.27421 -0.27416 -0.24742 -0.23613 -0.20470

Alpha virt. eigenvalues -- -0.09229 -0.05644 -0.04781 -0.02183 -0.02140

Alpha virt. eigenvalues -- -0.00192 0.00477 0.03113 0.03952 0.05055

Alpha virt. eigenvalues -- 0.06015 0.06026 0.06298 0.08411 0.08439

Alpha virt. eigenvalues -- 0.09488 0.09640 0.09921 0.10300 0.10633

Alpha virt. eigenvalues -- 0.10871 0.10875 0.11928 0.12055 0.13191

Alpha virt. eigenvalues -- 0.13218 0.14018 0.14214 0.15012 0.15080

Alpha virt. eigenvalues -- 0.15874 0.16676 0.16711 0.17836 0.18467

Alpha virt. eigenvalues -- 0.18590 0.18616 0.20234 0.20256 0.20505

Alpha virt. eigenvalues -- 0.22807 0.23018 0.24859 0.26239 0.26244

Alpha virt. eigenvalues -- 0.27367 0.27779 0.27898 0.28984 0.29379

Alpha virt. eigenvalues -- 0.29613 0.30083 0.30299 0.30513 0.31031

Alpha virt. eigenvalues -- 0.31294 0.31448 0.31921 0.32630 0.32896

Alpha virt. eigenvalues -- 0.33632 0.36357 0.37149 0.37193 0.37821

Alpha virt. eigenvalues -- 0.38224 0.38471 0.39601 0.40793 0.41147

Alpha virt. eigenvalues -- 0.41388 0.41861 0.42201 0.43183 0.43211

Alpha virt. eigenvalues -- 0.43366 0.43519 0.43762 0.44718 0.45170

Alpha virt. eigenvalues -- 0.45317 0.45460 0.45921 0.46251 0.47029

Alpha virt. eigenvalues -- 0.47757 0.47936 0.48258 0.48320 0.48447

Alpha virt. eigenvalues -- 0.49066 0.49124 0.49290 0.49579 0.50251

Alpha virt. eigenvalues -- 0.50416 0.51037 0.51378 0.51804 0.52675

Alpha virt. eigenvalues -- 0.53588 0.54129 0.54217 0.54262 0.54466

Alpha virt. eigenvalues -- 0.55037 0.55741 0.56146 0.56905 0.57642

Alpha virt. eigenvalues -- 0.58541 0.59480 0.59533 0.59645 0.59826

Alpha virt. eigenvalues -- 0.59841 0.59870 0.61805 0.63378 0.63785

Alpha virt. eigenvalues -- 0.64092 0.65489 0.65958 0.66893 0.67097

Alpha virt. eigenvalues -- 0.67286 0.67678 0.67888 0.67893 0.68553

Alpha virt. eigenvalues -- 0.68978 0.68991 0.69093 0.69550 0.69589

Alpha virt. eigenvalues -- 0.69850 0.70656 0.71227 0.71261 0.71803

Alpha virt. eigenvalues -- 0.72183 0.72337 0.72583 0.73767 0.74012

Alpha virt. eigenvalues -- 0.74701 0.75130 0.75260 0.75862 0.76460

Alpha virt. eigenvalues -- 0.76745 0.77953 0.78234 0.78914 0.79041

Alpha virt. eigenvalues -- 0.79430 0.80509 0.80916 0.82000 0.82089

Alpha virt. eigenvalues -- 0.82719 0.84640 0.85158 0.85835 0.86475

Alpha virt. eigenvalues -- 0.87453 0.89218 0.90150 0.90821 0.93244

Alpha virt. eigenvalues -- 0.93865 0.93942 0.95415 0.96494 0.99179

Alpha virt. eigenvalues -- 1.00538 1.03586 1.03957 1.04499 1.05307

Alpha virt. eigenvalues -- 1.05759 1.06131 1.06146 1.08144 1.08678

Alpha virt. eigenvalues -- 1.09002 1.09062 1.09987 1.10576 1.13026

Alpha virt. eigenvalues -- 1.13365 1.14085 1.14170 1.15931 1.18369

Alpha virt. eigenvalues -- 1.21160 1.22276 1.25062 1.25706 1.27800

Alpha virt. eigenvalues -- 1.28794 1.29519 1.30856 1.31086 1.32998

Alpha virt. eigenvalues -- 1.33563 1.35097 1.39428 1.40575 1.42178

Alpha virt. eigenvalues -- 1.45227 1.51055 1.53017 1.55017 1.55989

Alpha virt. eigenvalues -- 1.59428 1.62463 1.72618 1.74514 1.76775

Alpha virt. eigenvalues -- 1.79866 1.88122 1.93312

Lowest 15 Excited States

Excited state	Energy (eV)	Wavelength (nm)	f
1	2.83	437.4	0.3848
2	3.50	354.1	0.8343
3	3.53	351.4	0.0000
4	3.78	327.7	0.0000
5	4.00	310.3	0.9429
6	4.43	280.1	0.0000
7	4.43	279.9	0.0232
8	4.46	278.2	0.0000
9	4.57	271.4	0.0645
10	4.58	270.7	0.0000
11	4.63	267.9	0.1282
12	4.67	265.7	0.0000
13	4.71	263.4	0.0012
14	4.73	262.3	0.1897
15	4.79	259.0	0.0000

Table S4. First 15 excitation energies, wavelength, and oscillator strengths for compound **PF**.

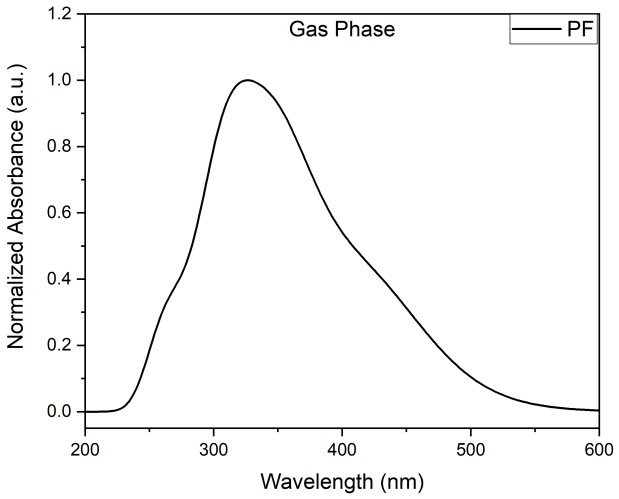

Figure S39. Simulated UV-Vis spectrum for compound **PF**.

Geometric Images

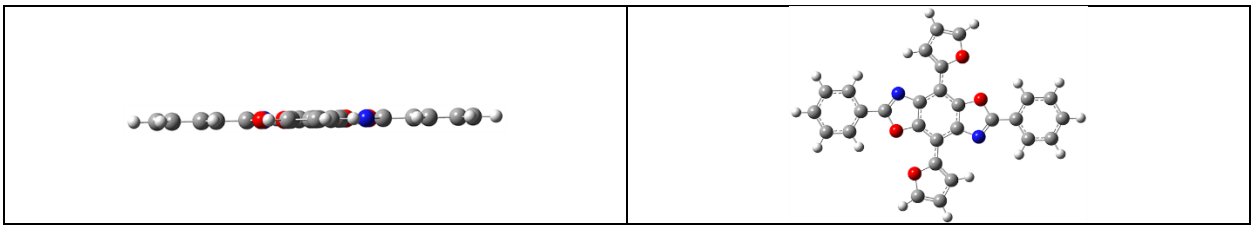

Figure S40. Geometric Images of compound **PF**.

PP

Cartesian Coordinates

C	-1.188	-0.62056	0.02494
C	-0.10401	-1.50896	0.02251
C	1.12344	-0.80031	0.01421
C	1.18803	0.62062	0.02482
C	0.10404	1.50902	0.02241
C	-1.12342	0.80037	0.01412
O	2.54309	0.95786	0.01355
O	-2.54304	-0.95784	0.01376
N	2.43167	-1.30044	-0.00266
N	-2.43167	1.30045	-0.00277
C	3.2325	-0.26369	-0.00479
C	-3.23247	0.26368	-0.00475
C	-4.68366	0.23367	-0.02007
C	-5.39919	1.44889	0.02709
C	-5.38488	-0.98799	-0.08367
C	-6.7969	1.43797	0.01133
H	-4.84078	2.38742	0.07912
C	-6.78436	-0.99031	-0.09862
H	-4.82649	-1.92666	-0.12635
C	-7.49341	0.21973	-0.05117
H	-7.34747	2.38258	0.04928

H	-7.32433	-1.94042	-0.14935
H	-8.5876	0.21431	-0.06309
C	0.22623	2.98142	0.02558
C	-0.79651	3.79696	-0.51145
C	1.37074	3.61322	0.56569
C	-0.67144	5.19112	-0.51507
H	-1.69529	3.32874	-0.91549
C	1.48728	5.00808	0.56573
H	2.16948	3.00728	0.99704
C	0.46941	5.80492	0.0221
H	-1.4735	5.80193	-0.94105
H	2.37908	5.47448	0.99596
H	0.5635	6.89528	0.01957
C	4.68369	-0.23373	-0.02008
C	5.39917	-1.44896	0.02754
C	5.38495	0.98789	-0.08408
C	6.79688	-1.4381	0.01182
H	4.84072	-2.38745	0.07988
C	6.78443	0.99015	-0.09899
H	4.82659	1.92656	-0.12709
C	7.49343	-0.2199	-0.0511
H	7.34742	-2.3827	0.05015
H	7.32443	1.94022	-0.15002
H	8.58762	-0.21452	-0.06297
C	-0.22623	-2.98135	0.02562
C	0.79632	-3.79685	-0.51182
C	-1.37059	-3.61316	0.566
C	0.67121	-5.19101	-0.51557
H	1.69498	-3.32861	-0.9161

C	-1.48719	-5.00802	0.56591
H	-2.16918	-3.00724	0.99767
C	-0.4695	-5.80482	0.02187
H	1.47314	-5.8018	-0.94182
H	-2.37885	-5.47445	0.99638
H	-0.56364	-6.89518	0.01922

Energy Levels

Alpha occ. eigenvalues -- -19.21336 -19.21336 -14.33680 -14.33679 -10.28949

Alpha occ. eigenvalues -- -10.28948 -10.25702 -10.25692 -10.23180 -10.23171

Alpha occ. eigenvalues -- -10.21630 -10.21620 -10.21040 -10.21040 -10.19628

Alpha occ. eigenvalues -- -10.19616 -10.19481 -10.19481 -10.19352 -10.19352

Alpha occ. eigenvalues -- -10.19317 -10.19316 -10.19150 -10.19150 -10.19101

Alpha occ. eigenvalues -- -10.19101 -10.17771 -10.17771 -10.17675 -10.17675

Alpha occ. eigenvalues -- -10.17633 -10.17632 -10.17536 -10.17536 -10.17309

Alpha occ. eigenvalues -- -10.17308 -1.14526 -1.14421 -0.95269 -0.95260

Alpha occ. eigenvalues -- -0.89556 -0.88031 -0.87440 -0.86421 -0.85385

Alpha occ. eigenvalues -- -0.80891 -0.80364 -0.78790 -0.76336 -0.76305

Alpha occ. eigenvalues -- -0.75912 -0.74860 -0.74642 -0.74192 -0.72715

Alpha occ. eigenvalues -- -0.69126 -0.66232 -0.64636 -0.64389 -0.63190

Alpha occ. eigenvalues -- -0.61854 -0.61495 -0.60760 -0.60686 -0.59800

Alpha occ. eigenvalues -- -0.58746 -0.58351 -0.56512 -0.55929 -0.54452

Alpha occ. eigenvalues -- -0.53143 -0.51978 -0.51366 -0.50433 -0.49247

Alpha occ. eigenvalues -- -0.49026 -0.48573 -0.48447 -0.47461 -0.47287

Alpha occ. eigenvalues -- -0.46831 -0.46604 -0.45896 -0.45004 -0.44407

Alpha occ. eigenvalues -- -0.44341 -0.44118 -0.44042 -0.43673 -0.43515

Alpha occ. eigenvalues -- -0.42688 -0.42622 -0.40918 -0.40585 -0.39776

Alpha occ. eigenvalues -- -0.39646 -0.38683 -0.38394 -0.37683 -0.37550

Alpha occ. eigenvalues -- -0.36519 -0.36408 -0.36257 -0.36131 -0.35870

Alpha occ. eigenvalues -- -0.35503 -0.34620 -0.34403 -0.34205 -0.30395

Alpha occ. eigenvalues -- -0.29919 -0.29380 -0.29113 -0.27831 -0.27633

Alpha occ. eigenvalues -- -0.27621 -0.25997 -0.25942 -0.25795 -0.23884

Alpha occ. eigenvalues -- -0.21838

Alpha virt. eigenvalues -- -0.09102 -0.05826 -0.04802 -0.02413 -0.02367

Alpha virt. eigenvalues -- -0.01014 -0.00960 -0.00792 0.00420 0.02851

Alpha virt. eigenvalues -- 0.03850 0.05487 0.05616 0.06063 0.07155

Alpha virt. eigenvalues -- 0.07265 0.09252 0.09364 0.09589 0.09729

Alpha virt. eigenvalues -- 0.11242 0.11359 0.11970 0.12361 0.12930

Alpha virt. eigenvalues -- 0.13004 0.13726 0.14215 0.14646 0.14803

Alpha virt. eigenvalues -- 0.14937 0.15241 0.15335 0.15691 0.16371

Alpha virt. eigenvalues -- 0.17422 0.17873 0.18282 0.18491 0.19931

Alpha virt. eigenvalues -- 0.19971 0.20687 0.22441 0.23946 0.24135

Alpha virt. eigenvalues -- 0.25486 0.25968 0.26162 0.27475 0.27485

Alpha virt. eigenvalues -- 0.27821 0.28101 0.28681 0.28725 0.29257

Alpha virt. eigenvalues -- 0.29470 0.29593 0.29981 0.30261 0.30622

Alpha virt. eigenvalues -- 0.31365 0.31447 0.31899 0.32237 0.32665

Alpha virt. eigenvalues -- 0.32825 0.33554 0.34427 0.34889 0.36550

Alpha virt. eigenvalues -- 0.37052 0.37662 0.38932 0.40041 0.40276

Alpha virt. eigenvalues -- 0.40564 0.41005 0.42643 0.42761 0.42995

Alpha virt. eigenvalues -- 0.43185 0.43285 0.43758 0.43777 0.44272

Alpha virt. eigenvalues -- 0.44426 0.44803 0.45172 0.45404 0.45597

Alpha virt. eigenvalues -- 0.46116 0.46331 0.47012 0.47061 0.47409

Alpha virt. eigenvalues -- 0.47543 0.48081 0.48677 0.48718 0.48975

Alpha virt. eigenvalues -- 0.49463 0.49778 0.49864 0.50408 0.50451

Alpha virt. eigenvalues -- 0.50620 0.51023 0.51627 0.51991 0.52294

Alpha virt. eigenvalues -- 0.53768 0.53988 0.54062 0.54101 0.54396

Alpha virt. eigenvalues -- 0.55048 0.55597 0.55782 0.57111 0.58416

Alpha virt. eigenvalues -- 0.58438 0.58770 0.58888 0.59134 0.59211

Alpha virt. eigenvalues --	0.59999	0.60198	0.60434	0.61601	0.61784
Alpha virt. eigenvalues --	0.62995	0.63133	0.64699	0.65399	0.65933
Alpha virt. eigenvalues --	0.66191	0.67054	0.67239	0.67389	0.67579
Alpha virt. eigenvalues --	0.67749	0.67929	0.68114	0.68846	0.69264
Alpha virt. eigenvalues --	0.69561	0.69732	0.69780	0.69897	0.70142
Alpha virt. eigenvalues --	0.70762	0.70886	0.71339	0.71770	0.71815
Alpha virt. eigenvalues --	0.72253	0.72324	0.72849	0.73121	0.73327
Alpha virt. eigenvalues --	0.74900	0.75034	0.75859	0.76110	0.76218
Alpha virt. eigenvalues --	0.76387	0.76969	0.77019	0.77632	0.78012
Alpha virt. eigenvalues --	0.78171	0.78680	0.79461	0.79489	0.80372
Alpha virt. eigenvalues --	0.80515	0.81450	0.81451	0.82537	0.82699
Alpha virt. eigenvalues --	0.83750	0.84026	0.84352	0.84620	0.84948
Alpha virt. eigenvalues --	0.85613	0.85875	0.88896	0.91839	0.92157
Alpha virt. eigenvalues --	0.92947	0.93882	0.94549	0.94889	0.95517
Alpha virt. eigenvalues --	0.97466	0.98686	0.99578	1.03012	1.03279
Alpha virt. eigenvalues --	1.05730	1.06133	1.07350	1.07974	1.09402
Alpha virt. eigenvalues --	1.09766	1.11331	1.11977	1.12704	1.13176
Alpha virt. eigenvalues --	1.13408	1.14207	1.14873	1.16550	1.17556
Alpha virt. eigenvalues --	1.19220	1.21152	1.22720	1.23199	1.23986
Alpha virt. eigenvalues --	1.24844	1.25669	1.28343	1.28432	1.30615
Alpha virt. eigenvalues --	1.30685	1.33145	1.33454	1.34779	1.36101
Alpha virt. eigenvalues --	1.39308	1.41850	1.44951	1.46738	1.51143
Alpha virt. eigenvalues --	1.54897	1.55689	1.58534	1.59073	1.72539
Alpha virt. eigenvalues --	1.79117	1.81887	1.88372		

Lowest 15 Excited States

Excited state	Energy (eV)	Wavelength (nm)	f
1	3.17	390.6	0.4602
2	3.59	345.0	0.8523
3	3.86	321.4	0.0000

4	4.06	305.4	0.0247
5	4.06	305.2	0.0004
6	4.09	303.4	0.0011
7	4.23	293.5	0.7983
8	4.47	277.0	0.0000
9	4.51	274.8	0.0180
10	4.52	274.3	0.0001
11	4.65	266.7	0.0011
12	4.71	263.1	0.1606
13	4.76	260.7	0.0000
14	4.76	260.7	0.0017
15	4.86	255.1	0.0167

Table S5. First 15 excitation energies, wavelength, and oscillator strengths for compound **PP**.

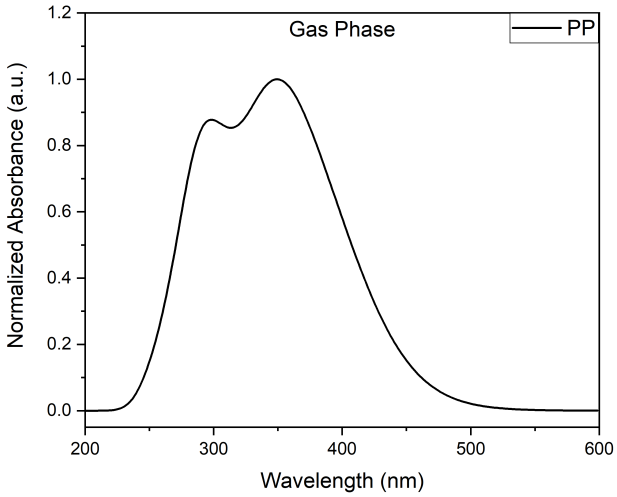

Figure S41. Simulated UV-Vis spectrum for compound **PP**.

Geometric Images

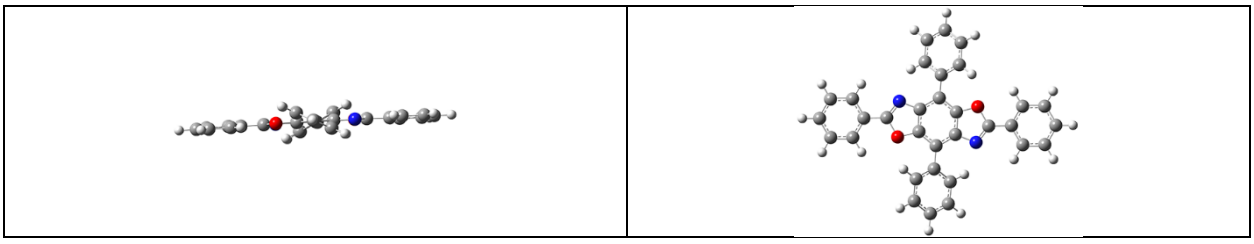

Figure S42. Geometric Images of compound **PP**.

PT

Cartesian Coordinates

C	1.21975	0.54336	0.00005
C	0.1949	1.50114	0.00001
C	-1.07621	0.86727	-0.00003
C	-1.21975	-0.54336	-0.00004
C	-0.1949	-1.50114	0.
C	1.07621	-0.86727	0.00005
O	-2.58589	-0.80875	-0.00008
O	2.58589	0.80875	0.0001
N	-2.35325	1.43919	-0.00007
N	2.35325	-1.43919	0.0001
C	-3.21154	0.44692	-0.00012
C	3.21154	-0.44692	0.00011
C	4.66182	-0.48929	0.00015
C	5.42039	0.69974	0.00017
C	5.31871	-1.73808	0.00018
C	6.81832	0.63558	0.00021
H	4.90701	1.66465	0.00014
C	6.71536	-1.79316	0.00023
H	4.71792	-2.65146	0.00017
C	7.46899	-0.60776	0.00024
H	7.40284	1.5603	0.00022
H	7.22046	-2.76355	0.00025
H	8.56229	-0.65399	0.00028
C	-4.66182	0.48929	-0.00018
C	-5.42039	-0.69974	-0.00022
C	-5.31871	1.73808	-0.0002
C	-6.81832	-0.63558	-0.00027

H	-4.90701	-1.66465	-0.0002
C	-6.71536	1.79316	-0.00025
H	-4.71792	2.65146	-0.00017
C	-7.46899	0.60776	-0.00029
H	-7.40284	-1.5603	-0.0003
H	-7.22046	2.76355	-0.00027
H	-8.56229	0.65399	-0.00034
C	-0.3879	-2.93567	0.
C	0.58775	-3.91725	0.00003
S	-2.03327	-3.69179	-0.00006
C	0.07502	-5.2515	0.00003
H	1.64721	-3.65608	0.00007
C	-1.29668	-5.30957	-0.00001
H	0.70992	-6.14044	0.00006
H	-1.93792	-6.19027	-0.00002
C	0.3879	2.93567	0.00003
C	-0.58775	3.91725	0.00002
S	2.03327	3.69179	0.00015
C	-0.07502	5.2515	-0.00004
H	-1.64721	3.65608	0.
C	1.29668	5.30957	-0.00008
H	-0.70992	6.14044	-0.0001
H	1.93792	6.19027	-0.00015

Energy Levels

Alpha occ. eigenvalues -- -88.85493 -88.85492 -19.21635 -19.21634 -14.34021

Alpha occ. eigenvalues -- -14.34020 -10.29235 -10.29234 -10.25994 -10.25982

Alpha occ. eigenvalues -- -10.23525 -10.23515 -10.22490 -10.22478 -10.22362

Alpha occ. eigenvalues -- -10.22350 -10.21096 -10.21096 -10.20630 -10.20630

Alpha occ. eigenvalues -- -10.19423 -10.19423 -10.19419 -10.19419 -10.19377

Alpha occ. eigenvalues -- -10.19377 -10.19136 -10.19136 -10.19122 -10.19122

Alpha occ. eigenvalues -- -10.18291 -10.18290 -10.17896 -10.17896 -7.98176

Alpha occ. eigenvalues -- -7.98176 -5.94595 -5.94595 -5.94153 -5.94153

Alpha occ. eigenvalues -- -5.93662 -5.93662 -1.14946 -1.14836 -0.95591

Alpha occ. eigenvalues -- -0.95552 -0.90434 -0.89165 -0.88391 -0.88076

Alpha occ. eigenvalues -- -0.87000 -0.81232 -0.80772 -0.78887 -0.76354

Alpha occ. eigenvalues -- -0.76316 -0.74902 -0.74853 -0.74327 -0.73985

Alpha occ. eigenvalues -- -0.71314 -0.69231 -0.66420 -0.64528 -0.64251

Alpha occ. eigenvalues -- -0.63207 -0.61647 -0.60633 -0.60059 -0.58500

Alpha occ. eigenvalues -- -0.57666 -0.56411 -0.56187 -0.55439 -0.54289

Alpha occ. eigenvalues -- -0.54103 -0.52213 -0.51499 -0.51290 -0.50760

Alpha occ. eigenvalues -- -0.49226 -0.49019 -0.48485 -0.47385 -0.47119

Alpha occ. eigenvalues -- -0.46144 -0.45834 -0.44849 -0.44696 -0.44332

Alpha occ. eigenvalues -- -0.44226 -0.43734 -0.42045 -0.41174 -0.41174

Alpha occ. eigenvalues -- -0.40585 -0.40582 -0.39501 -0.39379 -0.39058

Alpha occ. eigenvalues -- -0.38941 -0.38067 -0.37608 -0.37547 -0.36739

Alpha occ. eigenvalues -- -0.36395 -0.36300 -0.36229 -0.34765 -0.34537

Alpha occ. eigenvalues -- -0.34337 -0.30632 -0.30208 -0.29813 -0.29603

Alpha occ. eigenvalues -- -0.27853 -0.27639 -0.27633 -0.26242 -0.26233

Alpha occ. eigenvalues -- -0.25041 -0.23892 -0.20743

Alpha virt. eigenvalues -- -0.09717 -0.05981 -0.05520 -0.02409 -0.02399

Alpha virt. eigenvalues -- -0.02171 0.00166 0.02187 0.03625 0.03629

Alpha virt. eigenvalues -- 0.03709 0.04808 0.05784 0.06111 0.06161

Alpha virt. eigenvalues -- 0.07980 0.08127 0.08192 0.08419 0.09049

Alpha virt. eigenvalues -- 0.09714 0.09758 0.10241 0.11098 0.11984

Alpha virt. eigenvalues -- 0.12424 0.12908 0.13769 0.14178 0.14260

Alpha virt. eigenvalues -- 0.14751 0.14830 0.15915 0.15943 0.16300

Alpha virt. eigenvalues -- 0.17832 0.18207 0.19397 0.20488 0.21006

Alpha virt. eigenvalues -- 0.22308 0.22809 0.25443 0.25995 0.26056

Alpha virt. eigenvalues -- 0.26991 0.27412 0.27675 0.28241 0.28496

Alpha virt. eigenvalues -- 0.28888 0.29245 0.29515 0.30080 0.30265

Alpha virt. eigenvalues -- 0.30746 0.31094 0.31664 0.31698 0.32893

Alpha virt. eigenvalues -- 0.33496 0.34559 0.34781 0.36651 0.37131

Alpha virt. eigenvalues -- 0.37600 0.38071 0.39972 0.40074 0.41243

Alpha virt. eigenvalues -- 0.41462 0.41950 0.42571 0.42788 0.42865

Alpha virt. eigenvalues -- 0.43027 0.43234 0.43440 0.44183 0.44784

Alpha virt. eigenvalues -- 0.44887 0.45394 0.45544 0.45747 0.45905

Alpha virt. eigenvalues -- 0.46215 0.47904 0.47922 0.48050 0.48560

Alpha virt. eigenvalues -- 0.48601 0.48842 0.48887 0.49008 0.49661

Alpha virt. eigenvalues -- 0.50122 0.50764 0.51220 0.51777 0.51947

Alpha virt. eigenvalues -- 0.52698 0.53728 0.53901 0.54009 0.54204

Alpha virt. eigenvalues -- 0.54403 0.55682 0.56410 0.56598 0.57119

Alpha virt. eigenvalues -- 0.57593 0.57595 0.58197 0.58460 0.58639

Alpha virt. eigenvalues -- 0.59246 0.59310 0.59507 0.59539 0.61954

Alpha virt. eigenvalues -- 0.63162 0.63257 0.63859 0.66141 0.66542

Alpha virt. eigenvalues -- 0.66718 0.66903 0.66929 0.67027 0.67386

Alpha virt. eigenvalues -- 0.67418 0.67881 0.67991 0.68087 0.69287

Alpha virt. eigenvalues -- 0.69643 0.70220 0.70445 0.70671 0.71139

Alpha virt. eigenvalues -- 0.71396 0.71743 0.71757 0.71945 0.72310

Alpha virt. eigenvalues -- 0.73110 0.73431 0.73459 0.74419 0.75383

Alpha virt. eigenvalues -- 0.75952 0.76184 0.76331 0.76376 0.76727

Alpha virt. eigenvalues -- 0.76937 0.77478 0.78151 0.78159 0.78286

Alpha virt. eigenvalues -- 0.79486 0.79893 0.80439 0.81385 0.82629

Alpha virt. eigenvalues -- 0.83529 0.83978 0.85054 0.85665 0.86274

Alpha virt. eigenvalues -- 0.86407 0.88461 0.89584 0.89959 0.91538

Alpha virt. eigenvalues -- 0.94315 0.94506 0.95155 0.95552 0.96766

Alpha virt. eigenvalues -- 0.97294 1.00562 1.04081 1.04094 1.04780

Alpha virt. eigenvalues --	1.05998	1.08343	1.08914	1.09209	1.09263
Alpha virt. eigenvalues --	1.11037	1.11897	1.11906	1.13324	1.14044
Alpha virt. eigenvalues --	1.16619	1.16818	1.18507	1.18959	1.21271
Alpha virt. eigenvalues --	1.23866	1.25851	1.26803	1.28934	1.30450
Alpha virt. eigenvalues --	1.30498	1.30908	1.32226	1.32343	1.33184
Alpha virt. eigenvalues --	1.37270	1.37860	1.41698	1.41800	1.45643
Alpha virt. eigenvalues --	1.50287	1.53274	1.56312	1.57612	1.72015
Alpha virt. eigenvalues --	1.78312	1.81831	1.89304		

Lowest 15 Excited States

Excited state	Energy (eV)	Wavelength (nm)	f
1	2.79	444.6	0.4326
2	3.43	361.3	0.7013
3	3.51	353.3	0.0000
4	3.72	333.0	0.0000
5	3.83	324.1	0.7664
6	4.01	309.1	0.0000
7	4.02	308.1	0.1108
8	4.38	283.1	0.0000
9	4.38	283.0	0.0242
10	4.42	280.4	0.0000
11	4.49	276.2	0.0000
12	4.52	274.3	0.2894
13	4.58	270.8	0.0025
14	4.59	270.3	0.0000
15	4.62	268.3	0.0012

Table S6. First 15 excitation energies, wavelength, and oscillator strengths for compound **PT**.

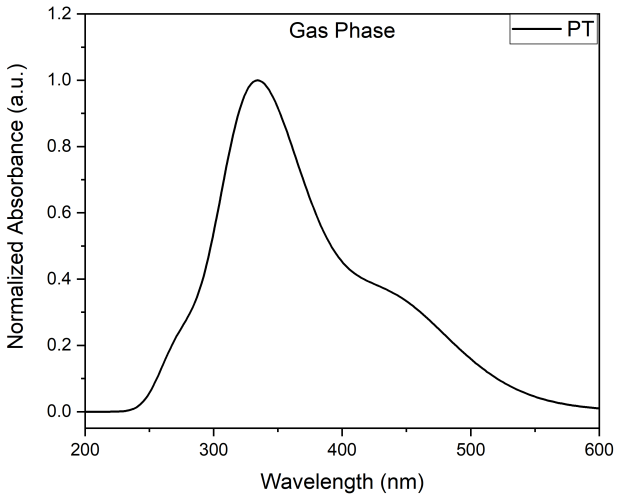

Figure S43. Simulated UV-Vis spectrum for compound **PT**.

Geometric Images

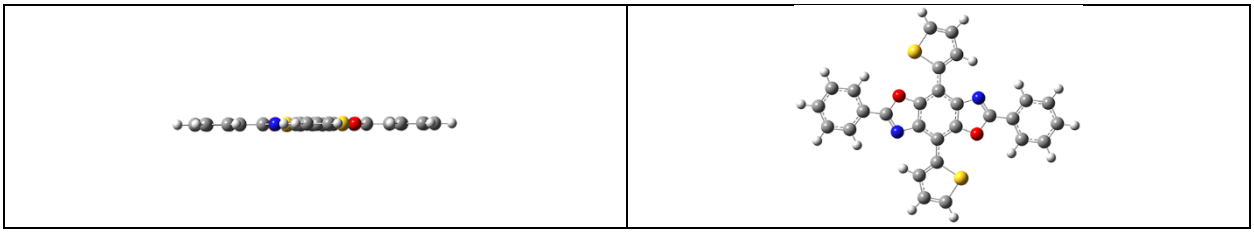

Figure S44. Geometric Images of compound **PT**.

TF

Cartesian Coordinates

C	1.14477	0.71519	0.
C	-0.01408	1.50335	0.
C	-1.18429	0.7033	0.
C	-1.14477	-0.71519	0.
C	0.01408	-1.50335	0.
C	1.18429	-0.7033	0.
O	-2.46742	-1.15275	0.
O	2.46742	1.15275	0.

N	-2.51955	1.11438	0.
N	2.51955	-1.11438	0.
C	-3.23921	0.01564	0.
C	3.23921	-0.01564	0.
C	0.05708	-2.94447	0.
C	1.1002	-3.85303	-0.00005
C	0.51533	-5.1626	0.00024
H	2.1539	-3.58678	-0.00005
C	-0.84748	-4.99309	-0.00016
H	1.04898	-6.11129	0.00046
H	-1.69557	-5.67136	-0.00027
C	-0.05708	2.94447	0.
C	-1.1002	3.85303	-0.00005
C	-0.51533	5.1626	0.00025
H	-2.1539	3.58678	-0.00006
C	0.84748	4.99309	-0.00016
H	-1.04898	6.11129	0.00046
H	1.69557	5.67136	-0.00027
C	-4.65851	-0.14301	0.
C	-5.37826	-1.32126	-0.00002
C	-6.79333	-1.11722	0.00002
H	-4.88782	-2.29688	-0.00003
C	-7.14897	0.21058	0.00008
H	-7.52261	-1.93013	0.00004
H	-8.14915	0.64228	0.00013
C	4.65851	0.14301	0.
C	5.37826	1.32126	-0.00002
C	6.79333	1.11722	0.00002
H	4.88782	2.29688	-0.00003

C	7.14897	-0.21058	0.00008
H	7.52261	1.93013	0.00004
H	8.14915	-0.64228	0.00013
S	5.7335	-1.28848	-0.00002
S	-5.7335	1.28848	-0.00002
O	-1.149	-3.64463	-0.00009
O	1.149	3.64463	-0.00009

Energy Levels

Alpha occ. eigenvalues -- -88.87136 -88.87136 -19.21188 -19.21188 -19.19540

Alpha occ. eigenvalues -- -19.19540 -14.33830 -14.33829 -10.29502 -10.29501

Alpha occ. eigenvalues -- -10.25924 -10.25912 -10.24262 -10.24250 -10.23520

Alpha occ. eigenvalues -- -10.23520 -10.23320 -10.23310 -10.23192 -10.23191

Alpha occ. eigenvalues -- -10.22279 -10.22279 -10.22144 -10.22135 -10.20199

Alpha occ. eigenvalues -- -10.20198 -10.19854 -10.19854 -10.18008 -10.18007

Alpha occ. eigenvalues -- -10.17674 -10.17674 -7.99860 -7.99860 -5.96273

Alpha occ. eigenvalues -- -5.96273 -5.95831 -5.95831 -5.95341 -5.95341

Alpha occ. eigenvalues -- -1.14675 -1.14564 -1.11588 -1.11582 -0.95479

Alpha occ. eigenvalues -- -0.95452 -0.91255 -0.90970 -0.88611 -0.82310

Alpha occ. eigenvalues -- -0.81033 -0.80699 -0.80218 -0.78401 -0.76331

Alpha occ. eigenvalues -- -0.76121 -0.76104 -0.73416 -0.72899 -0.68576

Alpha occ. eigenvalues -- -0.66023 -0.64907 -0.63479 -0.61491 -0.60686

Alpha occ. eigenvalues -- -0.60378 -0.58046 -0.57855 -0.57239 -0.56787

Alpha occ. eigenvalues -- -0.55942 -0.55486 -0.54427 -0.54366 -0.53822

Alpha occ. eigenvalues -- -0.53215 -0.50653 -0.49847 -0.49069 -0.48119

Alpha occ. eigenvalues -- -0.47242 -0.46824 -0.46116 -0.45868 -0.45153

Alpha occ. eigenvalues -- -0.44323 -0.42691 -0.42643 -0.42041 -0.41758

Alpha occ. eigenvalues -- -0.41405 -0.41337 -0.41169 -0.41077 -0.40712

Alpha occ. eigenvalues -- -0.40502 -0.40471 -0.39295 -0.37548 -0.37082

Alpha occ. eigenvalues -- -0.37061 -0.36767 -0.36538 -0.36498 -0.34343

Alpha occ. eigenvalues -- -0.30436 -0.30260 -0.29932 -0.29553 -0.29083

Alpha occ. eigenvalues -- -0.28823 -0.27816 -0.27782 -0.26956 -0.24477

Alpha occ. eigenvalues -- -0.23097 -0.20434

Alpha virt. eigenvalues -- -0.09717 -0.06717 -0.05231 -0.00422 -0.00284

Alpha virt. eigenvalues -- 0.01782 0.02180 0.02262 0.02623 0.03631

Alpha virt. eigenvalues -- 0.05747 0.06452 0.06954 0.07111 0.07327

Alpha virt. eigenvalues -- 0.07991 0.08121 0.08921 0.09095 0.10052

Alpha virt. eigenvalues -- 0.10404 0.10853 0.10855 0.11038 0.12243

Alpha virt. eigenvalues -- 0.13022 0.13165 0.13829 0.14836 0.16071

Alpha virt. eigenvalues -- 0.16469 0.16839 0.17171 0.17980 0.18478

Alpha virt. eigenvalues -- 0.18497 0.19516 0.20500 0.22757 0.23971

Alpha virt. eigenvalues -- 0.24662 0.26364 0.26728 0.27592 0.28468

Alpha virt. eigenvalues -- 0.28517 0.29339 0.30000 0.30034 0.31009

Alpha virt. eigenvalues -- 0.31521 0.32059 0.32272 0.33138 0.33368

Alpha virt. eigenvalues -- 0.36441 0.36824 0.37072 0.37874 0.38198

Alpha virt. eigenvalues -- 0.38425 0.38606 0.39540 0.40123 0.40669

Alpha virt. eigenvalues -- 0.41155 0.41685 0.42319 0.42730 0.42993

Alpha virt. eigenvalues -- 0.43189 0.43499 0.44825 0.45025 0.45847

Alpha virt. eigenvalues -- 0.45898 0.46741 0.46849 0.47066 0.47950

Alpha virt. eigenvalues -- 0.48351 0.48481 0.48796 0.48915 0.49869

Alpha virt. eigenvalues -- 0.50469 0.50714 0.51399 0.51432 0.52097

Alpha virt. eigenvalues -- 0.53044 0.53151 0.53524 0.53585 0.54459

Alpha virt. eigenvalues -- 0.55294 0.55646 0.55883 0.55933 0.57267

Alpha virt. eigenvalues -- 0.57287 0.57891 0.58457 0.59113 0.59340

Alpha virt. eigenvalues -- 0.60128 0.60128 0.61363 0.62315 0.62534

Alpha virt. eigenvalues -- 0.63190 0.64859 0.65628 0.66139 0.66292

Alpha virt. eigenvalues -- 0.66955 0.67011 0.68094 0.68206 0.68796

Alpha virt. eigenvalues -- 0.69743 0.69755 0.69808 0.70418 0.70744

Alpha virt. eigenvalues -- 0.71650 0.72050 0.72106 0.72698 0.73034

Alpha virt. eigenvalues -- 0.73659 0.73787 0.74456 0.74913 0.75504

Alpha virt. eigenvalues -- 0.75820 0.76020 0.77022 0.77416 0.77851

Alpha virt. eigenvalues -- 0.78365 0.78718 0.78990 0.79305 0.80449

Alpha virt. eigenvalues -- 0.80778 0.81182 0.83526 0.84145 0.85359

Alpha virt. eigenvalues -- 0.85537 0.87975 0.89670 0.89911 0.89946

Alpha virt. eigenvalues -- 0.93450 0.94759 0.95929 0.97633 0.99470

Alpha virt. eigenvalues -- 1.02440 1.02444 1.03916 1.04475 1.05067

Alpha virt. eigenvalues -- 1.05481 1.06103 1.06776 1.07201 1.07505

Alpha virt. eigenvalues -- 1.09372 1.09459 1.11083 1.11662 1.12645

Alpha virt. eigenvalues -- 1.14812 1.15957 1.19112 1.19728 1.20909

Alpha virt. eigenvalues -- 1.21039 1.23061 1.23498 1.26370 1.27212

Alpha virt. eigenvalues -- 1.28830 1.31049 1.32703 1.33574 1.38110

Alpha virt. eigenvalues -- 1.39825 1.41444 1.44585 1.50789 1.53387

Alpha virt. eigenvalues -- 1.58843 1.61219 1.72008 1.73876 1.76181

Alpha virt. eigenvalues -- 1.78949 1.87642 1.92790

Lowest 15 Excited States

Excited state	Energy (eV)	Wavelength (nm)	f
1	2.66	465.7	0.3082
2	3.24	382/3	0.0000
3	3.30	375.5	0.9369
4	3.61	343.8	0.0000
5	3.89	318.6	0.9054
6	4.07	304.3	0.0000
7	4.36	284.1	0.0076
8	4.37	283.4	0.0000
9	4.41	281.0	0.2553
10	4.51	274.8	0.0674
11	4.54	272.9	0.0000
12	4.65	266.5	0.0010
13	4.72	262.9	0.0000
14	4.73	260.0	0.0000
15	4.77	260.0	0.0000

Table S7. First 15 excitation energies, wavelength, and oscillator strengths for compound **TF**.

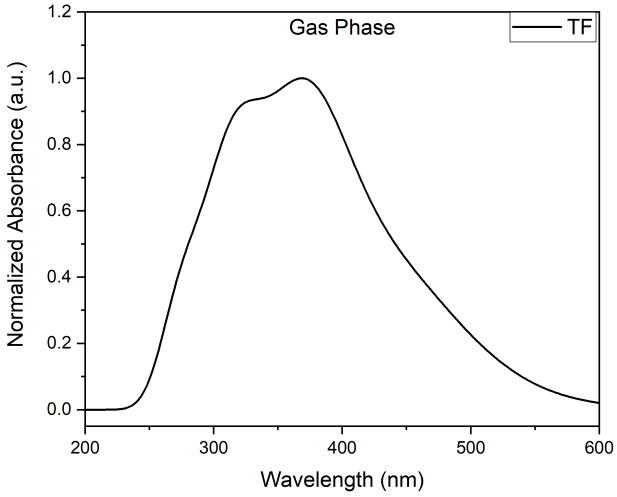

Figure S45. Simulated UV-Vis spectrum for compound **TF**.

Geometric Images

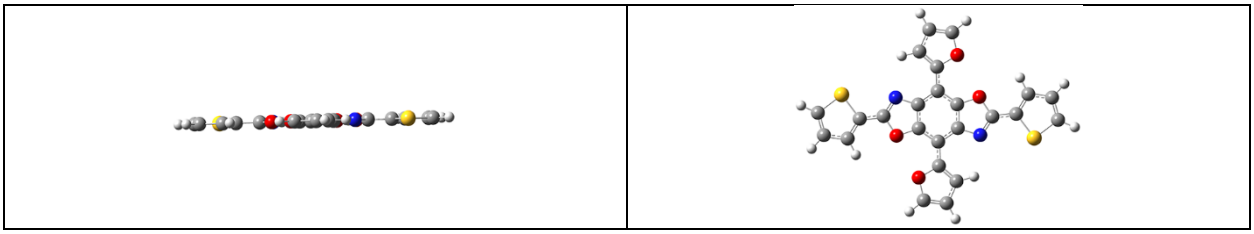

Figure S46. Geometric Images of compound **TF**.

TP

Cartesian Coordinates

C	-1.12232	-0.73189	0.03027
C	0.04046	-1.51477	0.02999
C	1.19411	-0.68951	0.01985
C	1.12232	0.73189	0.03027
C	-0.04046	1.51477	0.02999
C	-1.19411	0.68951	0.01985

O	2.44038	1.19833	0.01506
O	-2.44038	-1.19833	0.01506
N	2.54269	-1.0635	-0.00205
N	-2.54269	1.0635	-0.00205
C	3.23896	0.04624	-0.00752
C	-3.23896	-0.04624	-0.00752
C	-0.06081	2.99249	0.03592
C	-1.18564	3.70758	-0.43807
C	1.045	3.73248	0.51772
C	-1.19556	5.1072	-0.43855
H	-2.05854	3.15714	-0.79153
C	1.02643	5.13187	0.52066
H	1.9213	3.20765	0.90096
C	-0.09148	5.82795	0.03884
H	-2.07626	5.6374	-0.81401
H	1.89149	5.68123	0.90519
H	-0.1033	6.92232	0.0389
C	0.06081	-2.99249	0.03592
C	-1.045	-3.73248	0.51772
C	1.18564	-3.70758	-0.43808
C	-1.02643	-5.13187	0.52066
H	-1.9213	-3.20765	0.90096
C	1.19556	-5.1072	-0.43855
H	2.05854	-3.15714	-0.79153
C	0.09148	-5.82795	0.03884
H	-1.89149	-5.68123	0.90519
H	2.07626	-5.6374	-0.81401
H	0.1033	-6.92232	0.0389
C	-4.65606	-0.22661	-0.03329

C	-5.36672	-1.40962	-0.07772
S	-5.74364	1.19577	-0.01466
C	-6.78335	-1.21702	-0.09703
H	-4.87408	-2.38377	-0.10058
C	-7.14949	0.1075	-0.06838
H	-7.5054	-2.03555	-0.1322
H	-8.15311	0.53116	-0.07448
C	4.65606	0.22661	-0.03329
C	5.36672	1.40962	-0.07772
S	5.74364	-1.19577	-0.01466
C	6.78335	1.21702	-0.09703
H	4.87408	2.38377	-0.10058
C	7.14949	-0.1075	-0.06838
H	7.5054	2.03555	-0.1322
H	8.15311	-0.53116	-0.07448

Energy Levels

Alpha occ. eigenvalues -- -88.87332 -88.87332 -19.21582 -19.21581 -14.33937

Alpha occ. eigenvalues -- -14.33936 -10.29774 -10.29773 -10.25895 -10.25884

Alpha occ. eigenvalues -- -10.23802 -10.23802 -10.23382 -10.23372 -10.22466

Alpha occ. eigenvalues -- -10.22466 -10.21753 -10.21742 -10.20540 -10.20540

Alpha occ. eigenvalues -- -10.20073 -10.20073 -10.19607 -10.19594 -10.17698

Alpha occ. eigenvalues -- -10.17698 -10.17601 -10.17601 -10.17560 -10.17559

Alpha occ. eigenvalues -- -10.17411 -10.17411 -10.17138 -10.17137 -8.00057

Alpha occ. eigenvalues -- -8.00057 -5.96470 -5.96470 -5.96025 -5.96025

Alpha occ. eigenvalues -- -5.95537 -5.95537 -1.14796 -1.14693 -0.95647

Alpha occ. eigenvalues -- -0.95624 -0.91462 -0.91194 -0.88882 -0.86357

Alpha occ. eigenvalues -- -0.85405 -0.81086 -0.80387 -0.78258 -0.76378

Alpha occ. eigenvalues -- -0.76334 -0.75760 -0.74601 -0.74548 -0.73440

Alpha occ. eigenvalues -- -0.72692 -0.68715 -0.66130 -0.64586 -0.63540

Alpha occ. eigenvalues -- -0.61764 -0.61189 -0.60265 -0.59480 -0.58418

Alpha occ. eigenvalues -- -0.58292 -0.57570 -0.57062 -0.55726 -0.54755

Alpha occ. eigenvalues -- -0.54115 -0.53096 -0.51921 -0.50714 -0.50021

Alpha occ. eigenvalues -- -0.49380 -0.48675 -0.48085 -0.46954 -0.45970

Alpha occ. eigenvalues -- -0.45474 -0.44597 -0.44023 -0.43741 -0.43550

Alpha occ. eigenvalues -- -0.42857 -0.42826 -0.42587 -0.42566 -0.41571

Alpha occ. eigenvalues -- -0.41540 -0.40936 -0.40785 -0.40699 -0.39876

Alpha occ. eigenvalues -- -0.38886 -0.38754 -0.36763 -0.36756 -0.36383

Alpha occ. eigenvalues -- -0.36128 -0.35934 -0.35606 -0.34506 -0.34470

Alpha occ. eigenvalues -- -0.34327 -0.30244 -0.30088 -0.29528 -0.29254

Alpha occ. eigenvalues -- -0.28040 -0.28001 -0.27343 -0.25903 -0.25862

Alpha occ. eigenvalues -- -0.25424 -0.23480 -0.21718

Alpha virt. eigenvalues -- -0.09746 -0.06941 -0.05223 -0.01118 -0.01029

Alpha virt. eigenvalues -- -0.00708 -0.00275 0.01507 0.01999 0.02055

Alpha virt. eigenvalues -- 0.02184 0.04237 0.05998 0.06171 0.06568

Alpha virt. eigenvalues -- 0.06774 0.07527 0.07700 0.07784 0.08058

Alpha virt. eigenvalues -- 0.09616 0.09697 0.10930 0.11969 0.12518

Alpha virt. eigenvalues -- 0.12765 0.12862 0.12924 0.13726 0.14630

Alpha virt. eigenvalues -- 0.15433 0.15856 0.16836 0.16936 0.17467

Alpha virt. eigenvalues -- 0.18222 0.18505 0.19205 0.19993 0.20827

Alpha virt. eigenvalues -- 0.23398 0.23704 0.23852 0.25641 0.26403

Alpha virt. eigenvalues -- 0.26568 0.27410 0.27612 0.28218 0.28380

Alpha virt. eigenvalues -- 0.29069 0.29367 0.29753 0.30472 0.30547

Alpha virt. eigenvalues -- 0.30867 0.31265 0.32504 0.32792 0.32825

Alpha virt. eigenvalues -- 0.33551 0.34312 0.34566 0.37011 0.37424

Alpha virt. eigenvalues -- 0.37985 0.38123 0.38669 0.39440 0.40473

Alpha virt. eigenvalues -- 0.40579 0.40795 0.41527 0.42381 0.42519

Alpha virt. eigenvalues -- 0.43206 0.44167 0.44208 0.44460 0.44528

Alpha virt. eigenvalues -- 0.45029 0.45601 0.45692 0.46314 0.46376

Alpha virt. eigenvalues -- 0.46533 0.47230 0.47330 0.47583 0.47962

Alpha virt. eigenvalues -- 0.48854 0.48921 0.49823 0.49825 0.50494

Alpha virt. eigenvalues -- 0.50660 0.50946 0.51059 0.51749 0.51878

Alpha virt. eigenvalues -- 0.52654 0.53045 0.53700 0.54250 0.54892

Alpha virt. eigenvalues -- 0.54935 0.55098 0.55477 0.56363 0.57118

Alpha virt. eigenvalues -- 0.57344 0.57728 0.58171 0.58736 0.59440

Alpha virt. eigenvalues -- 0.59674 0.60154 0.60179 0.60604 0.61025

Alpha virt. eigenvalues -- 0.62182 0.62370 0.63955 0.64682 0.65235

Alpha virt. eigenvalues -- 0.65732 0.66261 0.66767 0.67026 0.67328

Alpha virt. eigenvalues -- 0.68184 0.68372 0.68881 0.69525 0.69742

Alpha virt. eigenvalues -- 0.69873 0.70304 0.71002 0.71188 0.71564

Alpha virt. eigenvalues -- 0.71838 0.71852 0.72572 0.72845 0.73410

Alpha virt. eigenvalues -- 0.73603 0.73763 0.74242 0.74745 0.74855

Alpha virt. eigenvalues -- 0.75051 0.75819 0.76292 0.76634 0.77273

Alpha virt. eigenvalues -- 0.77451 0.77905 0.78114 0.78259 0.78637

Alpha virt. eigenvalues -- 0.80399 0.80520 0.80703 0.81288 0.82609

Alpha virt. eigenvalues -- 0.82626 0.82853 0.83369 0.84033 0.84774

Alpha virt. eigenvalues -- 0.85150 0.86618 0.87467 0.88331 0.92122

Alpha virt. eigenvalues -- 0.92931 0.93116 0.93398 0.95954 0.96557

Alpha virt. eigenvalues -- 0.97984 0.98748 1.01194 1.02302 1.05461

Alpha virt. eigenvalues -- 1.05603 1.06292 1.08129 1.08535 1.09597

Alpha virt. eigenvalues -- 1.09910 1.12317 1.12351 1.13431 1.14289

Alpha virt. eigenvalues -- 1.15237 1.16042 1.18750 1.19427 1.20149

Alpha virt. eigenvalues -- 1.22151 1.22202 1.23200 1.23724 1.25251

Alpha virt. eigenvalues -- 1.25734 1.26955 1.28741 1.31687 1.32050

Alpha virt. eigenvalues -- 1.33997 1.35396 1.37992 1.41876 1.44891

Alpha virt. eigenvalues -- 1.46546 1.51148 1.57623 1.58444 1.72125

Alpha virt. eigenvalues -- 1.78072 1.81179 1.87888

Lowest 15 Excited States

Excited state	Energy (eV)	Wavelength (nm)	f
1	2.97	417.2	0.4087
2	3.36	268.5	0.8928
3	3.55	349.5	0.0000
4	3.85	322.3	0.0000
5	3.88	319.2	0.0206
6	3.90	318.1	0.0010
7	4.10	302.5	0.6998
8	4.11	301.5	0.0001
9	4.44	279.4	0.0002
10	4.51	275.1	0.1309
11	4.55	272.6	0.0009
12	4.56	282.2	0.0547
13	4.61	268.8	0.0001
14	4.62	268.1	0.2156
15	4.66	266.2	0.0068

Table S8. First 15 excitation energies, wavelength, and oscillator strengths for compound **TP**.

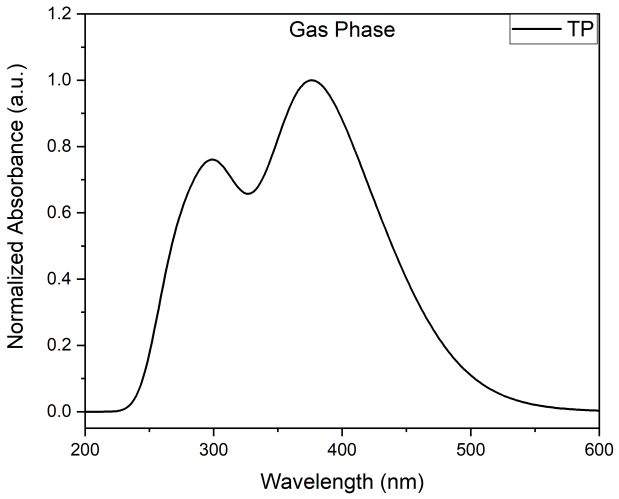

Figure S47. Simulated UV-Vis spectrum for compound **TP**.

Geometric Images

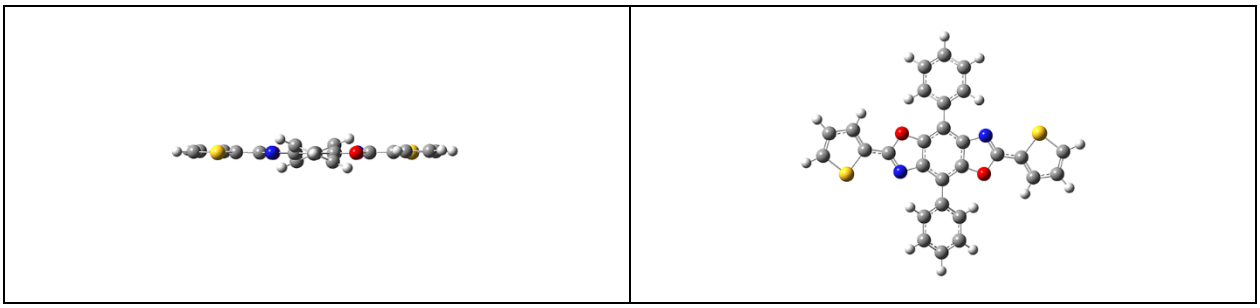

Figure S48. Geometric Images of compound **TP**.

TT

Cartesian Coordinates

C	1.16856	0.64697	0.00001
C	0.06571	1.51289	-0.00004
C	-1.14606	0.77122	-0.00005
C	-1.16856	-0.64697	-0.00001
C	-0.06571	-1.51289	0.00004
C	1.14606	-0.77122	0.00005
O	-2.50845	-1.02989	-0.00003
O	2.50845	1.02989	0.00004
N	-2.46499	1.23418	-0.00008
N	2.46499	-1.23418	0.0001
C	-3.23362	0.17059	-0.00009
C	3.23362	-0.17059	0.00008
C	-0.13138	-2.95874	0.00007
C	0.92793	-3.8497	0.00008
S	-1.70349	-3.85757	0.
C	0.53529	-5.22388	0.0002
H	1.96086	-3.49772	0.00006
C	-0.82586	-5.4036	0.00027
H	1.24694	-6.0526	0.00027
H	-1.38622	-6.33781	0.00039

C	0.13138	2.95874	-0.00007
C	-0.92793	3.8497	-0.00014
S	1.70349	3.85757	-0.0001
C	-0.53529	5.22388	-0.00009
H	-1.96086	3.49772	-0.00019
C	0.82586	5.4036	0.00002
H	-1.24694	6.0526	-0.00009
H	1.38622	6.33781	0.0001
C	-4.65831	0.07724	-0.00012
C	-5.43606	-1.06379	-0.00012
S	-5.66125	1.5606	-0.00017
C	-6.83911	-0.78941	-0.00016
H	-4.9981	-2.06411	-0.00008
C	-7.12804	0.55448	-0.00021
H	-7.60771	-1.56516	-0.00017
H	-8.10555	1.03536	-0.00026
C	4.65831	-0.07724	0.0001
C	5.43606	1.06379	0.00009
S	5.66125	-1.5606	0.00017
C	6.83911	0.78941	0.00013
H	4.9981	2.06411	0.00006
C	7.12804	-0.55448	0.00015
H	7.60771	1.56516	0.00012
H	8.10555	-1.03536	0.00018

Energy Levels

Alpha occ. eigenvalues -- -88.87370 -88.87370 -88.85453 -88.85452 -19.21814

Alpha occ. eigenvalues -- -19.21813 -14.34215 -14.34214 -10.29992 -10.29991

Alpha occ. eigenvalues -- -10.26126 -10.26113 -10.23806 -10.23806 -10.23660

Alpha occ. eigenvalues -- -10.23651 -10.22542 -10.22531 -10.22505 -10.22505

Alpha occ. eigenvalues -- -10.22331 -10.22319 -10.20597 -10.20597 -10.20481

Alpha occ. eigenvalues -- -10.20481 -10.20061 -10.20061 -10.18220 -10.18220

Alpha occ. eigenvalues -- -10.17809 -10.17808 -8.00095 -8.00095 -7.98142

Alpha occ. eigenvalues -- -7.98142 -5.96508 -5.96508 -5.96065 -5.96065

Alpha occ. eigenvalues -- -5.95574 -5.95574 -5.94561 -5.94561 -5.94120

Alpha occ. eigenvalues -- -5.94120 -5.93628 -5.93628 -1.15141 -1.15033

Alpha occ. eigenvalues -- -0.95916 -0.95868 -0.91597 -0.91221 -0.89951

Alpha occ. eigenvalues -- -0.89130 -0.87638 -0.81409 -0.80833 -0.78347

Alpha occ. eigenvalues -- -0.76378 -0.76328 -0.74728 -0.74419 -0.74280

Alpha occ. eigenvalues -- -0.73423 -0.71295 -0.68759 -0.66278 -0.64184

Alpha occ. eigenvalues -- -0.63699 -0.61071 -0.59220 -0.58359 -0.57695

Alpha occ. eigenvalues -- -0.57521 -0.56690 -0.56338 -0.55071 -0.54718

Alpha occ. eigenvalues -- -0.54146 -0.53854 -0.52143 -0.51458 -0.50991

Alpha occ. eigenvalues -- -0.49935 -0.49534 -0.47473 -0.46134 -0.45181

Alpha occ. eigenvalues -- -0.44781 -0.43702 -0.42927 -0.42840 -0.42338

Alpha occ. eigenvalues -- -0.41906 -0.41148 -0.41119 -0.41063 -0.41034

Alpha occ. eigenvalues -- -0.40477 -0.40139 -0.39560 -0.39416 -0.38857

Alpha occ. eigenvalues -- -0.37979 -0.36863 -0.36760 -0.36747 -0.36342

Alpha occ. eigenvalues -- -0.34761 -0.34760 -0.34323 -0.30483 -0.30407

Alpha occ. eigenvalues -- -0.29994 -0.29662 -0.28043 -0.28007 -0.27212

Alpha occ. eigenvalues -- -0.26192 -0.26187 -0.24777 -0.23372 -0.20715

Alpha virt. eigenvalues -- -0.10155 -0.07033 -0.05991 -0.02276 -0.00736

Alpha virt. eigenvalues -- 0.01419 0.01819 0.01922 0.01969 0.03145

Alpha virt. eigenvalues -- 0.03689 0.03725 0.05816 0.06427 0.06809

Alpha virt. eigenvalues -- 0.06935 0.06992 0.07688 0.07853 0.08251

Alpha virt. eigenvalues -- 0.08446 0.08640 0.08805 0.09205 0.10364

Alpha virt. eigenvalues -- 0.11449 0.12326 0.12940 0.13332 0.14418

Alpha virt. eigenvalues -- 0.14740 0.15444 0.16571 0.17135 0.17704

Alpha virt. eigenvalues -- 0.18654 0.18829 0.19636 0.22784 0.23347

Alpha virt. eigenvalues -- 0.24582 0.26348 0.26379 0.27022 0.27882

Alpha virt. eigenvalues -- 0.28244 0.28511 0.28904 0.29462 0.29928

Alpha virt. eigenvalues -- 0.30574 0.30886 0.31400 0.32972 0.33309

Alpha virt. eigenvalues -- 0.34227 0.34573 0.36745 0.37089 0.37575

Alpha virt. eigenvalues -- 0.37698 0.38615 0.38826 0.40526 0.40935

Alpha virt. eigenvalues -- 0.41506 0.41972 0.42151 0.42358 0.42598

Alpha virt. eigenvalues -- 0.43006 0.43027 0.43975 0.44087 0.45521

Alpha virt. eigenvalues -- 0.45616 0.46099 0.46687 0.46826 0.47155

Alpha virt. eigenvalues -- 0.47937 0.48241 0.48491 0.48659 0.48830

Alpha virt. eigenvalues -- 0.49810 0.50033 0.51132 0.51236 0.51405

Alpha virt. eigenvalues -- 0.51877 0.52553 0.53380 0.53905 0.54013

Alpha virt. eigenvalues -- 0.54052 0.55244 0.55358 0.55863 0.56579

Alpha virt. eigenvalues -- 0.56740 0.57347 0.57391 0.57782 0.58267

Alpha virt. eigenvalues -- 0.58516 0.58776 0.59828 0.59888 0.61290

Alpha virt. eigenvalues -- 0.61680 0.62329 0.62893 0.65052 0.65259

Alpha virt. eigenvalues -- 0.65776 0.66833 0.66841 0.66982 0.67098

Alpha virt. eigenvalues -- 0.67104 0.68840 0.69069 0.69178 0.70411

Alpha virt. eigenvalues -- 0.70538 0.71062 0.71396 0.71769 0.72084

Alpha virt. eigenvalues -- 0.72168 0.72583 0.73423 0.73510 0.73841

Alpha virt. eigenvalues -- 0.74417 0.75383 0.75389 0.75815 0.75848

Alpha virt. eigenvalues -- 0.76220 0.76230 0.76634 0.77664 0.77685

Alpha virt. eigenvalues -- 0.77767 0.78461 0.79782 0.80381 0.80703

Alpha virt. eigenvalues -- 0.81192 0.81472 0.82109 0.84131 0.84328

Alpha virt. eigenvalues -- 0.84674 0.85906 0.85983 0.88595 0.89467

Alpha virt. eigenvalues -- 0.91181 0.93838 0.94736 0.95562 0.96743

Alpha virt. eigenvalues -- 0.97821 1.01470 1.02916 1.04257 1.04423

Alpha virt. eigenvalues -- 1.07391 1.08404 1.08476 1.08665 1.09846

Alpha virt. eigenvalues -- 1.11959 1.13854 1.14032 1.15583 1.16431

Alpha virt. eigenvalues -- 1.16794 1.19857 1.20655 1.20869 1.21011

Alpha virt. eigenvalues -- 1.23278 1.25487 1.28190 1.28811 1.30792

Alpha virt. eigenvalues -- 1.31711 1.32721 1.35895 1.36616 1.40612

Alpha virt. eigenvalues -- 1.40775 1.46144 1.49713 1.53616 1.71158

Alpha virt. eigenvalues -- 1.77510 1.81164 1.88626

Lowest 15 Excited States

Excited state	Energy (eV)	Wavelength (nm)	*f*
1	2.63	471.1	0.3431
2	3.23	383.6	0.0000
3	3.25	382.1	0.8209
4	3.56	348.1	0.0000
5	3.72	333.0	0.7889
6	3.88	319.4	0.0000
7	3.89	318.6	0.0847
8	4.06	305.7	0.0000
9	4.27	290.6	0.1234
10	4.29	289.2	0.0000
11	4.40	282.0	0.1869
12	4.45	278.4	0.0600
13	4.48	276.8	0.0000
14	4.55	272.4	0.0000
15	4.57	271.2	0.0010

Table S9. First 15 excitation energies, wavelength, and oscillator strengths for compound **TT**.

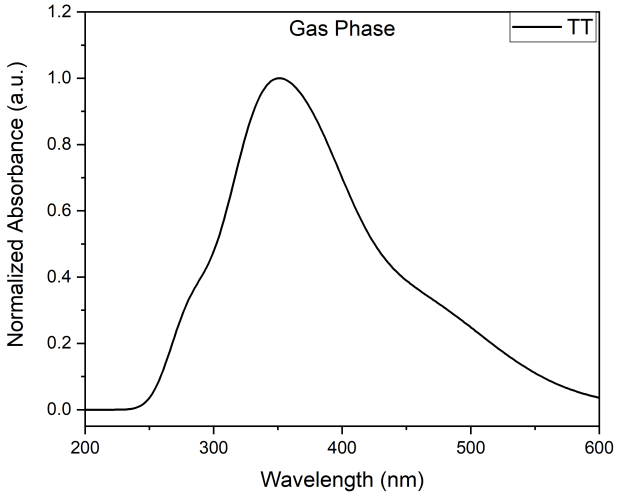

Figure S49. Simulated UV-Vis spectrum for compound **TT**.

Geometric Images

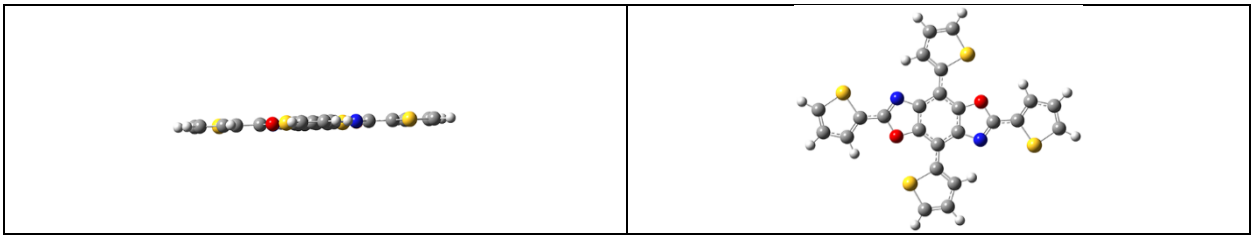

Figure S50. Geometric Images of compound **TT**.

Theoretical Overlays

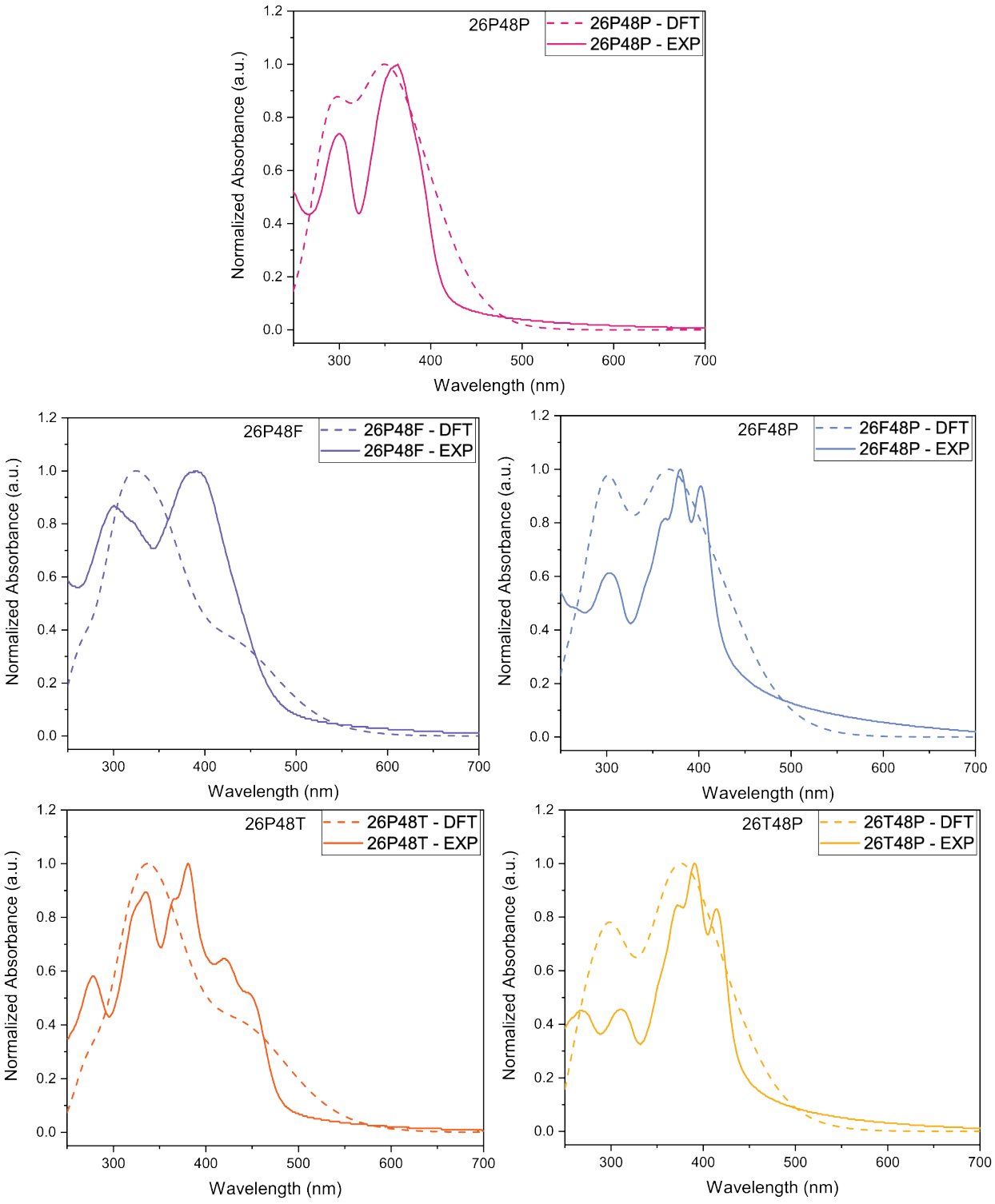

Figure S51. Overlays of DFT gas phase calculations with film-state spectra of each compound.

Triplet Energies

	Singlet E (a.u.)	Triplet E (a.u.)	S0-T1 (eV)	Band Gap (eV)	S1-T1 (eV)
PP	-1488.93	-1488.85	2.08	3.17	1.09
PF	-1484.48	-1484.41	1.80	2.92	1.11
PT	-2130.24	-2130.18	1.72	2.81	1.09
FP	-1484.46	-1484.38	2.02	2.96	0.94
TP	-2130.23	-2130.16	1.99	2.94	0.96

Table S10. S1 and T1 energies of the five BBO compounds.