PCCP

Electronic Supplementary Information

Terphenyl Backbone-Based Donor-π-Acceptor Dyads: Geometric Isomer Effects on Intramolecular Charge Transfer

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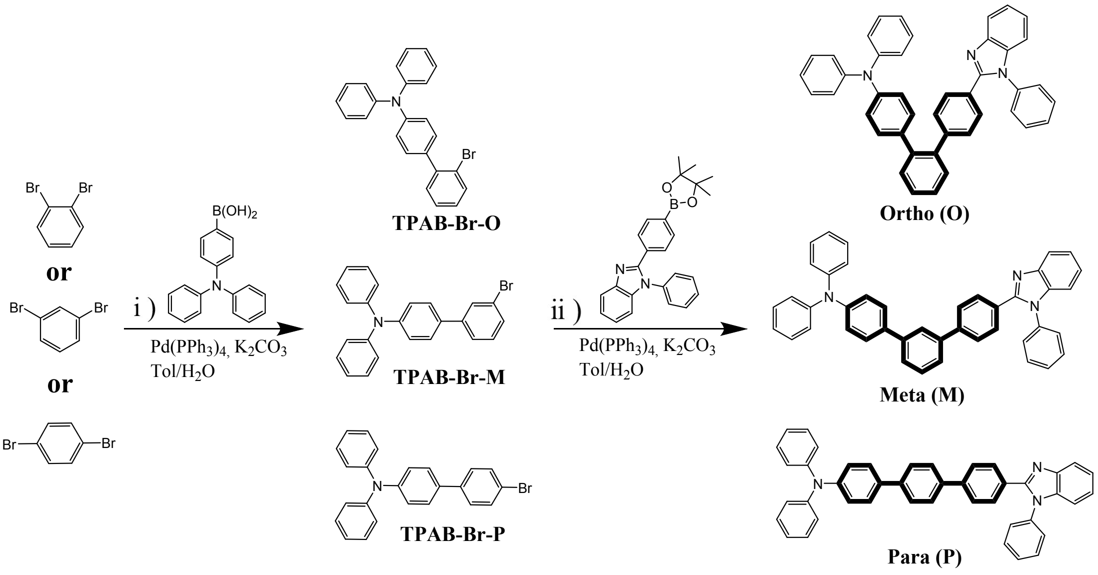

Scheme S1. Synthetic scheme for the preparation of three terphenyl backbone based donor-π–acceptor dyads (**O**, **M** and **P**).

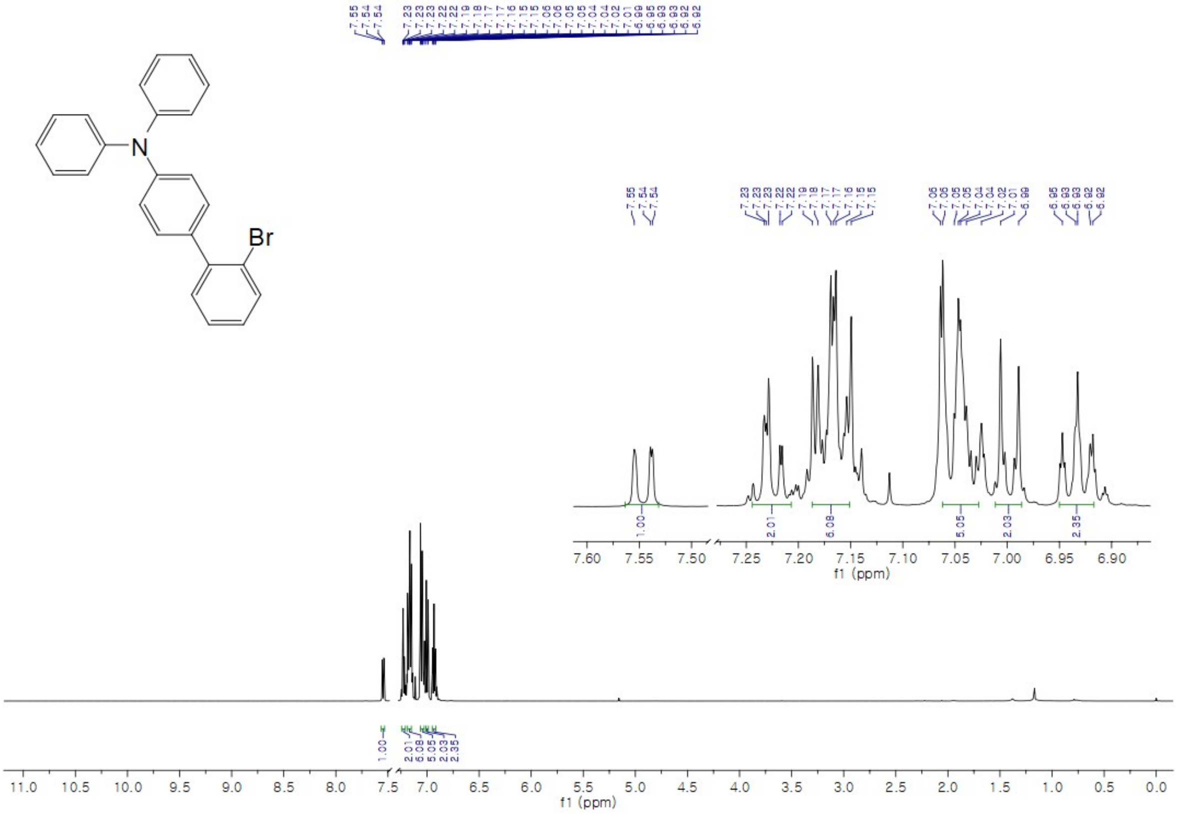

Figure S1-1. ^{1}H-NMR spectrum of **TPAB-Br-O** in $CDCl_3$ (500MHz, 293K)

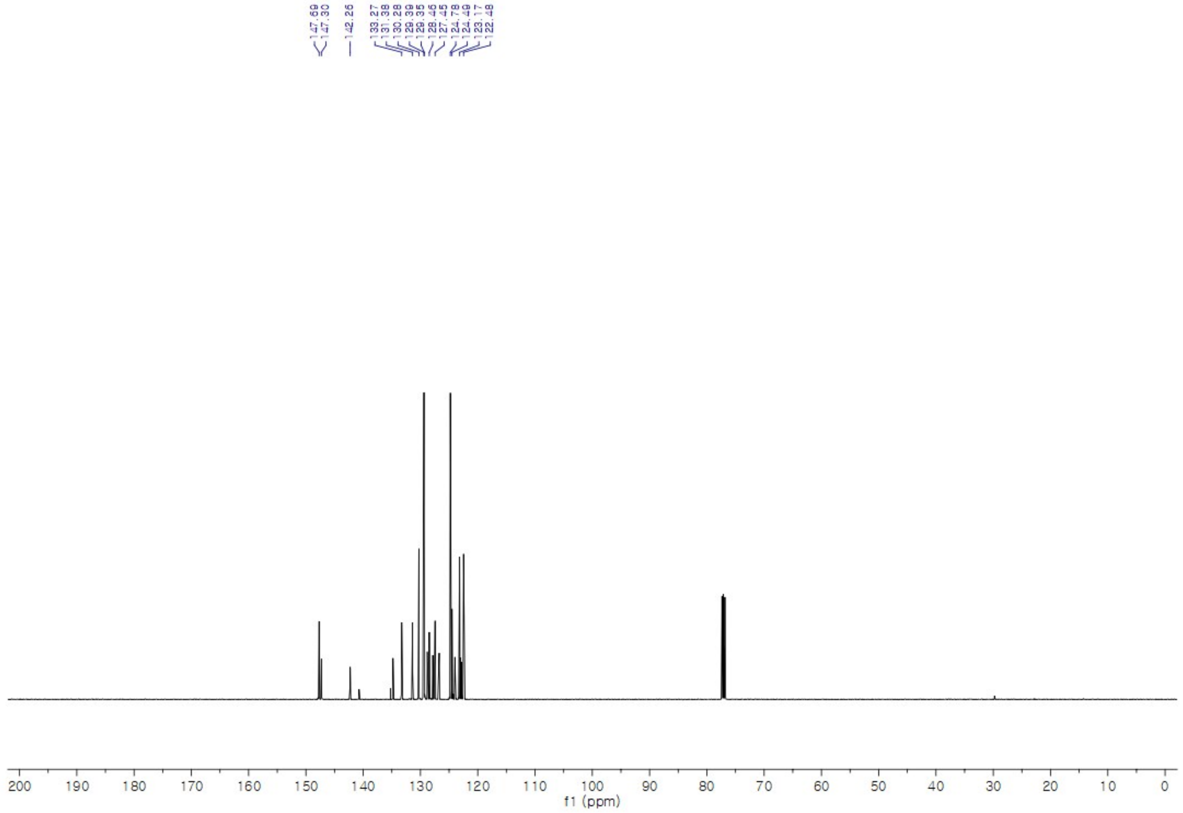

Figure S2-1. $^{13}C\{^1H\}$-NMR spectrum of **TPAB-Br-O** in $CDCl_3$ (125MHz, 293K)

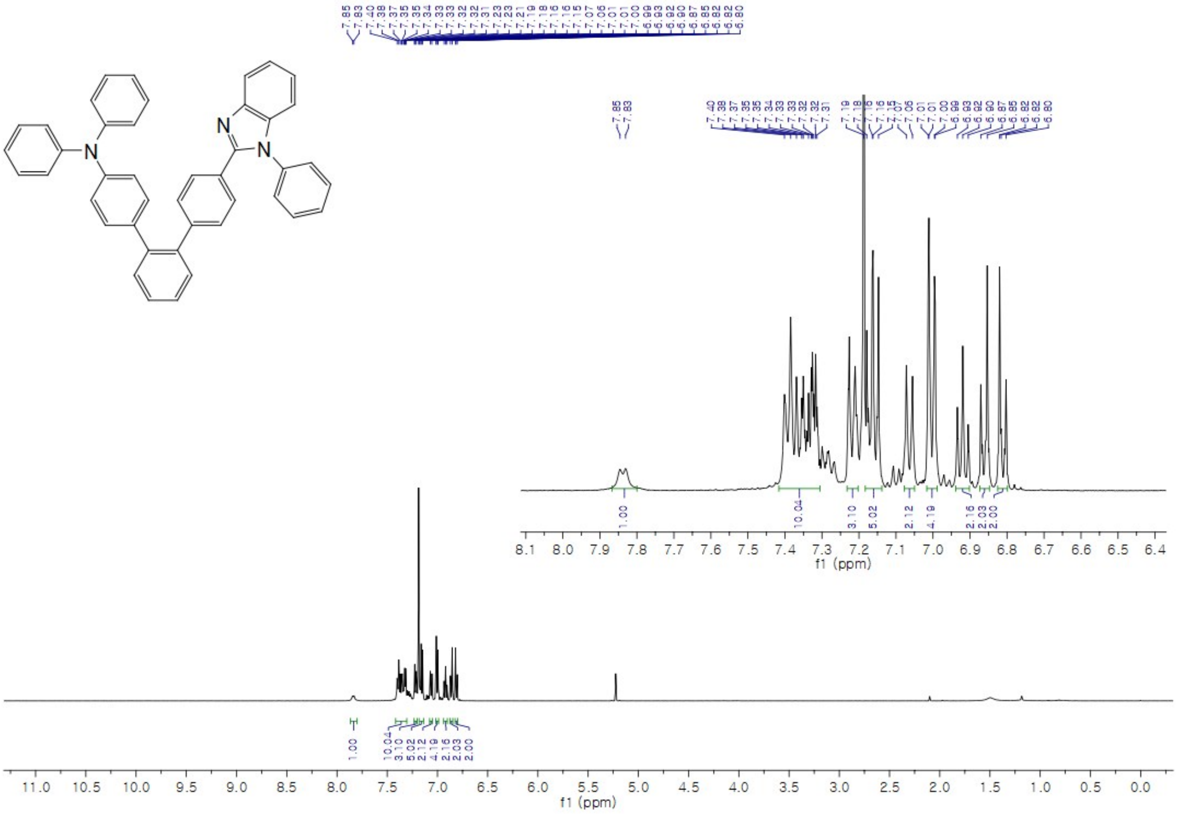

Figure S1-2. ^{1}H-NMR spectrum of **O** in $CDCl_3$ (500MHz, 293K)

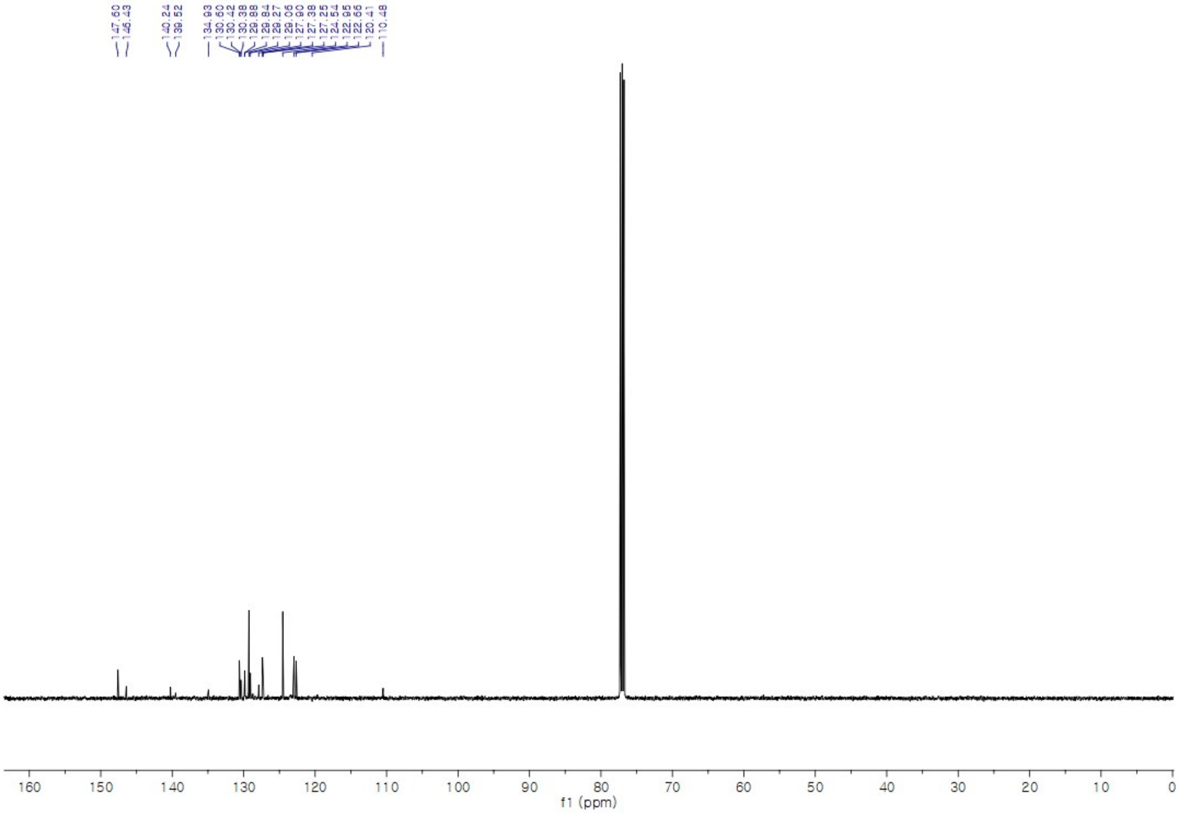

Figure S2-2. $^{13}C\{^{1}H\}$-NMR spectrum of **O** in $CDCl_3$ (125MHz, 293K)

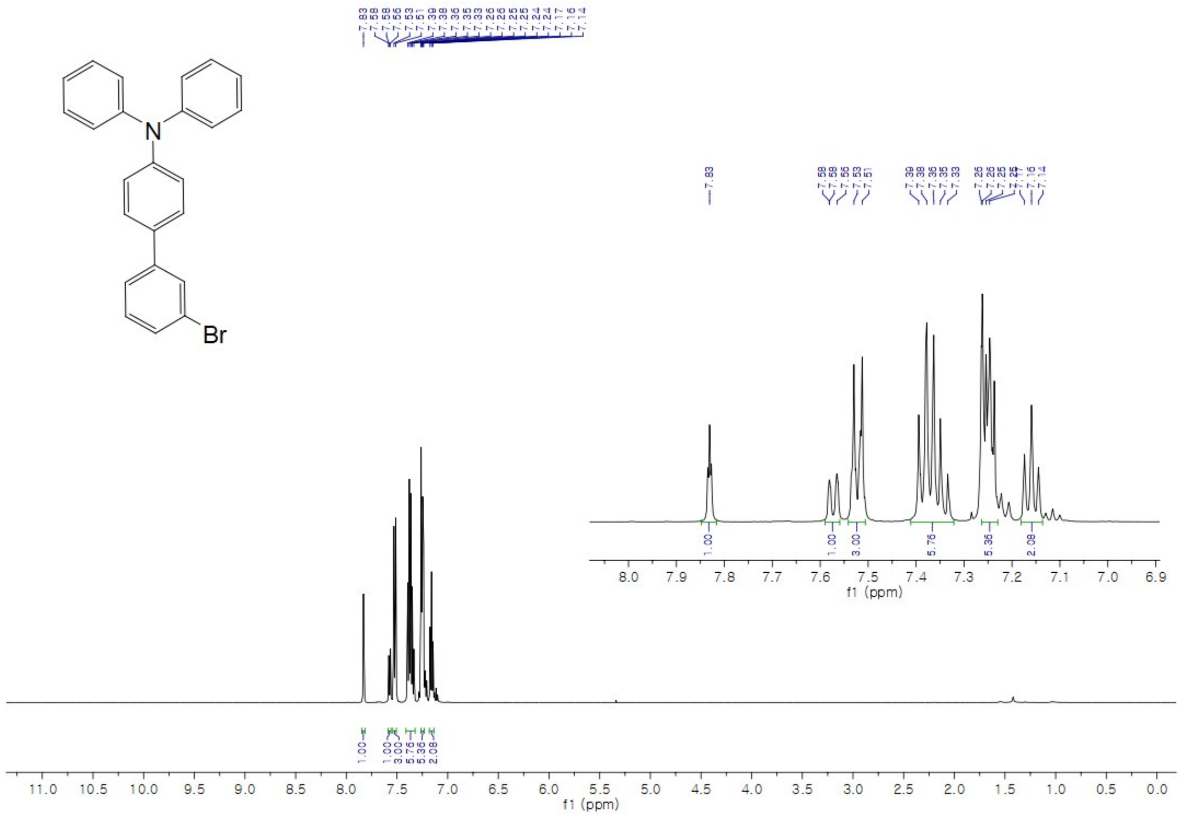

Figure S1-3. ^{1}H-NMR spectrum of **TPAB-Br-M** in $CDCl_3$ (500MHz, 293K)

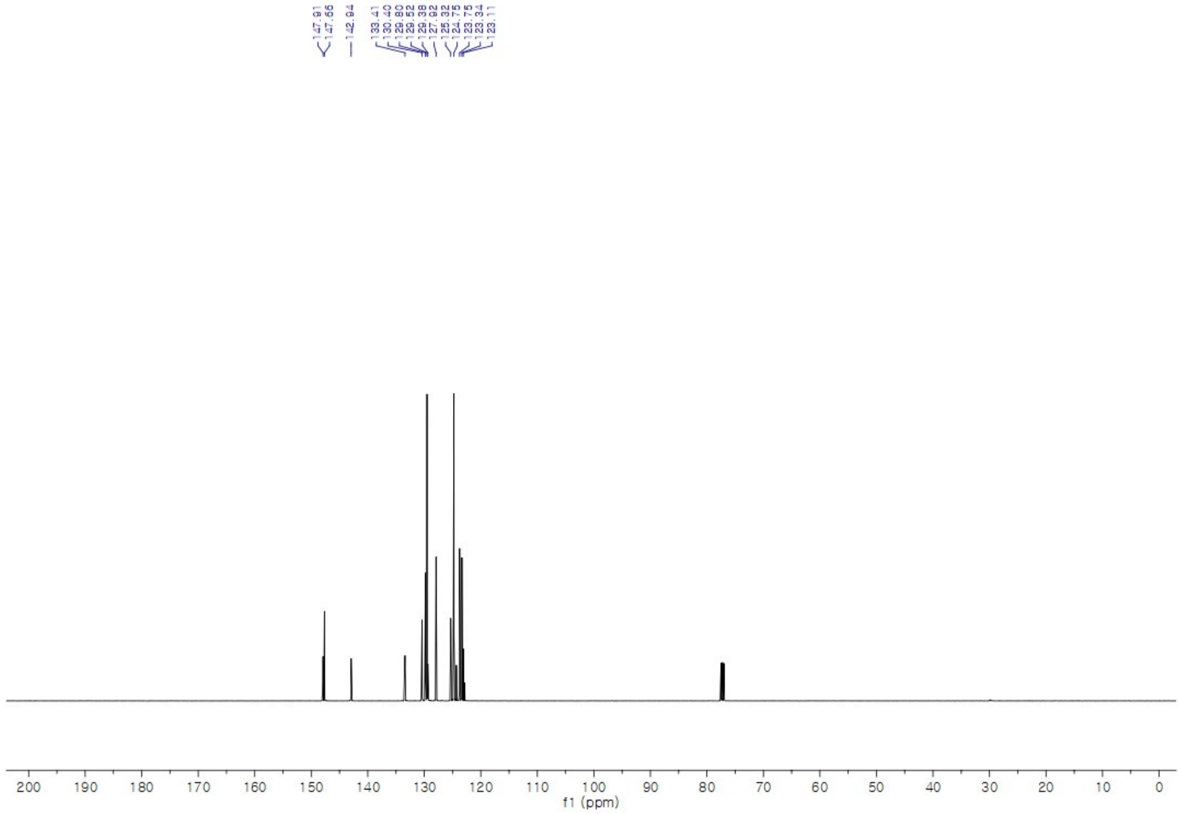

Figure S2-3. $^{13}C\{^1H\}$-NMR spectrum of **TPAB-Br-M** in $CDCl_3$ (125MHz, 293K)

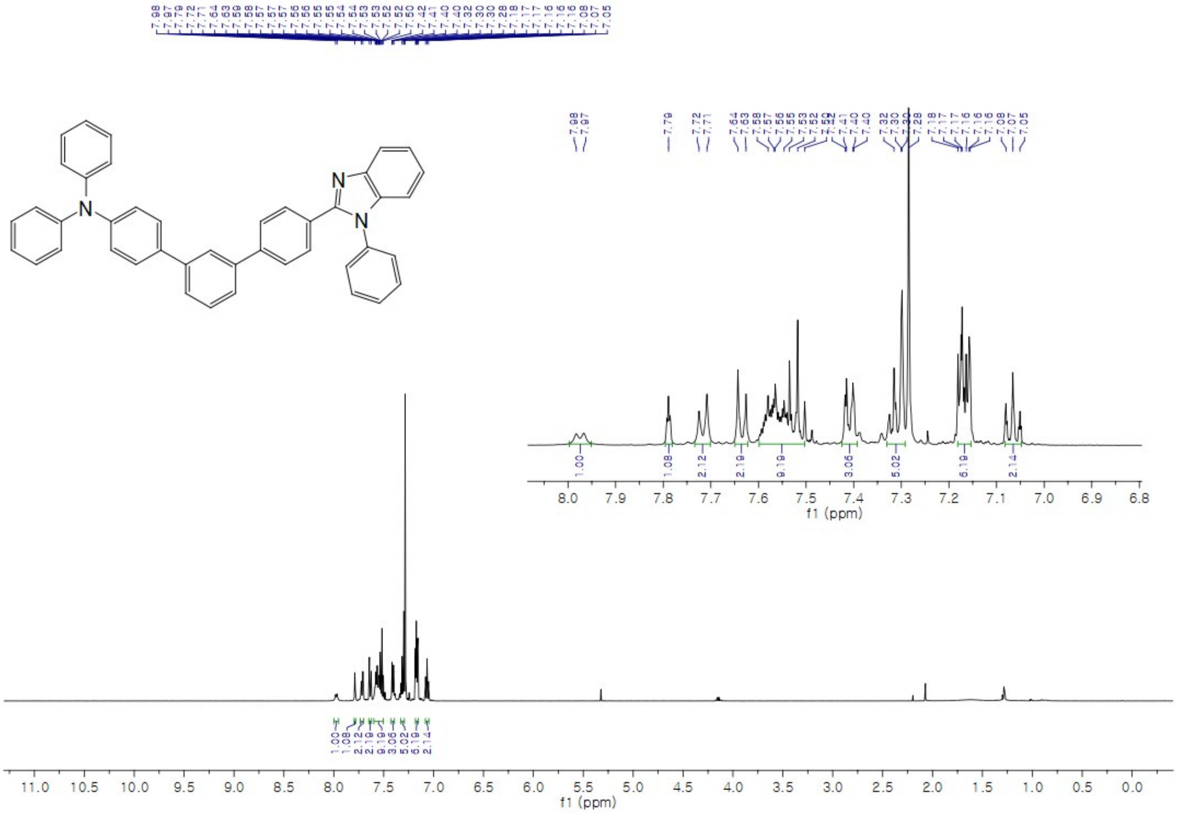

Figure S1-4. ^{1}H-NMR spectrum of **M** in $CDCl_3$ (500MHz, 293K)

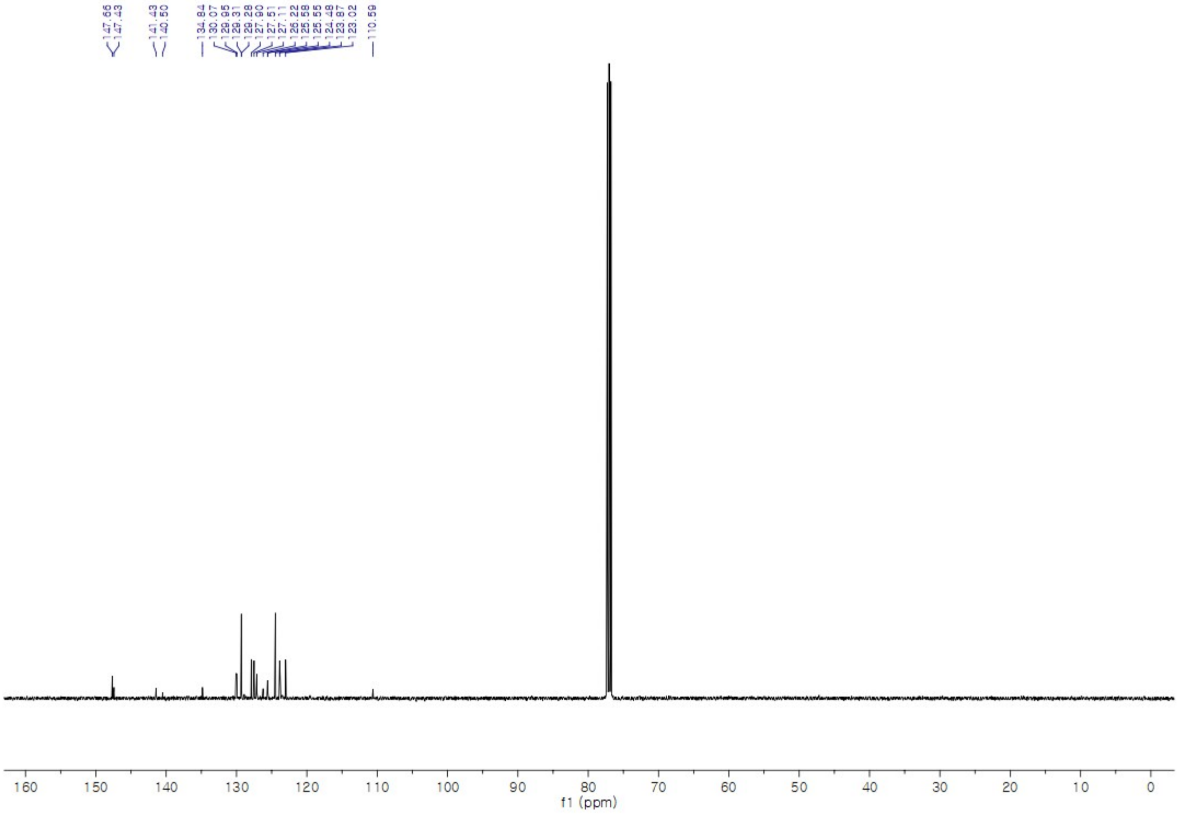

Figure S2-4. $^{13}C\{^1H\}$-NMR spectrum of **M** in $CDCl_3$ (125MHz, 293K)

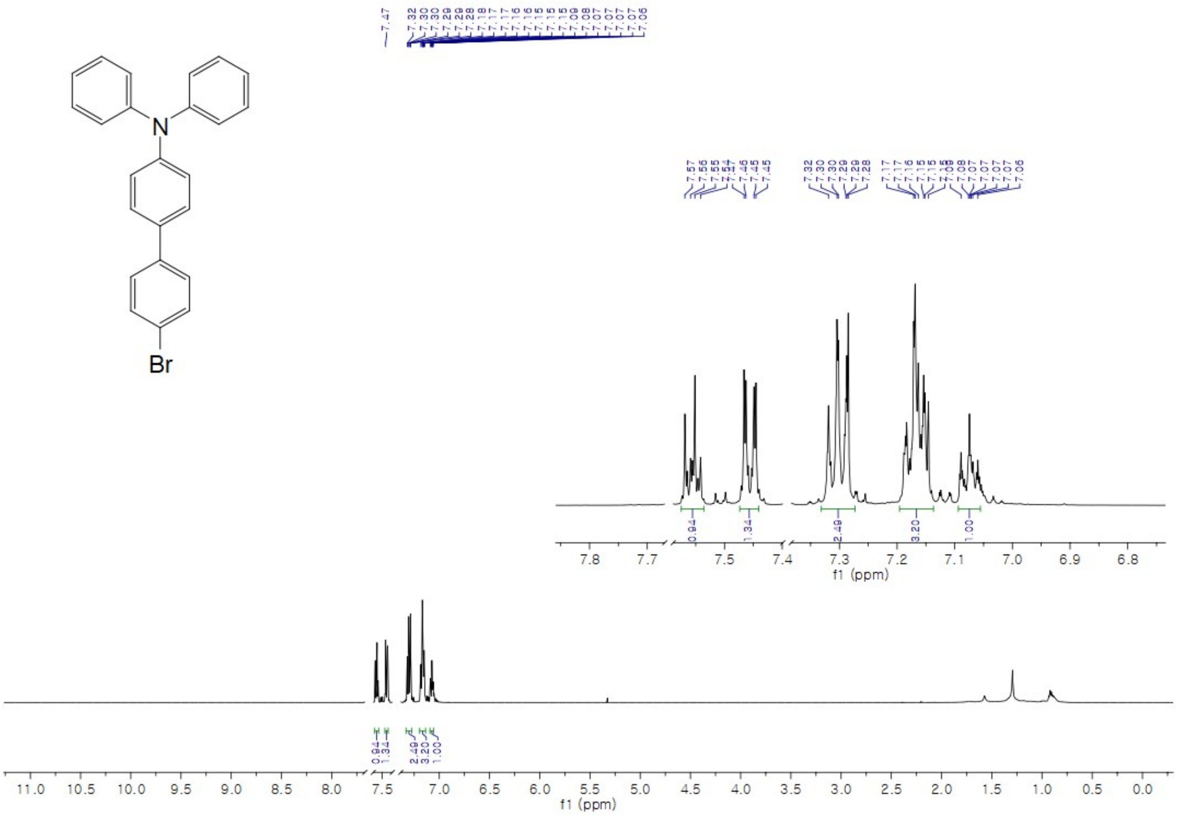

Figure S1-5. ^{1}H-NMR spectrum of **TPAB-Br-P** in $CDCl_3$ (500MHz, 293K)

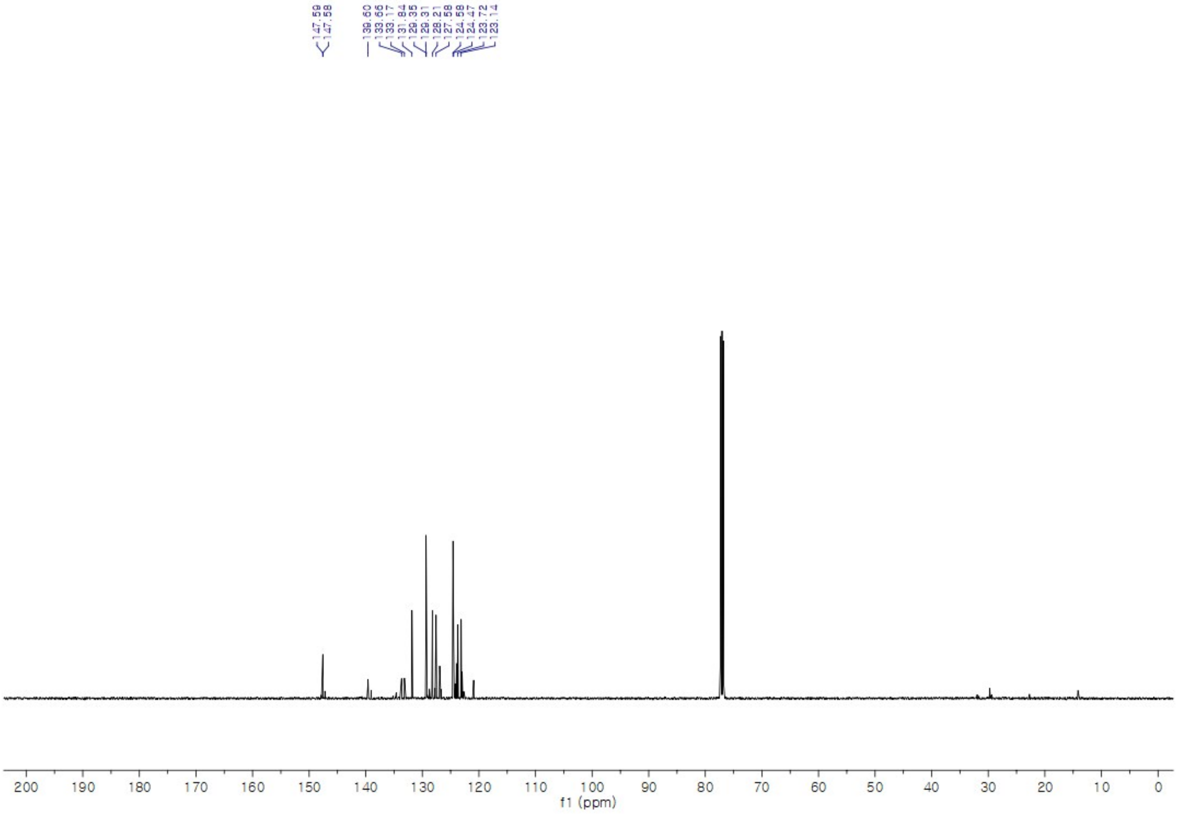

Figure S2-5. $^{13}C\{^{1}H\}$-NMR spectrum of **TPAB-Br-P** in $CDCl_3$ (125MHz, 293K)

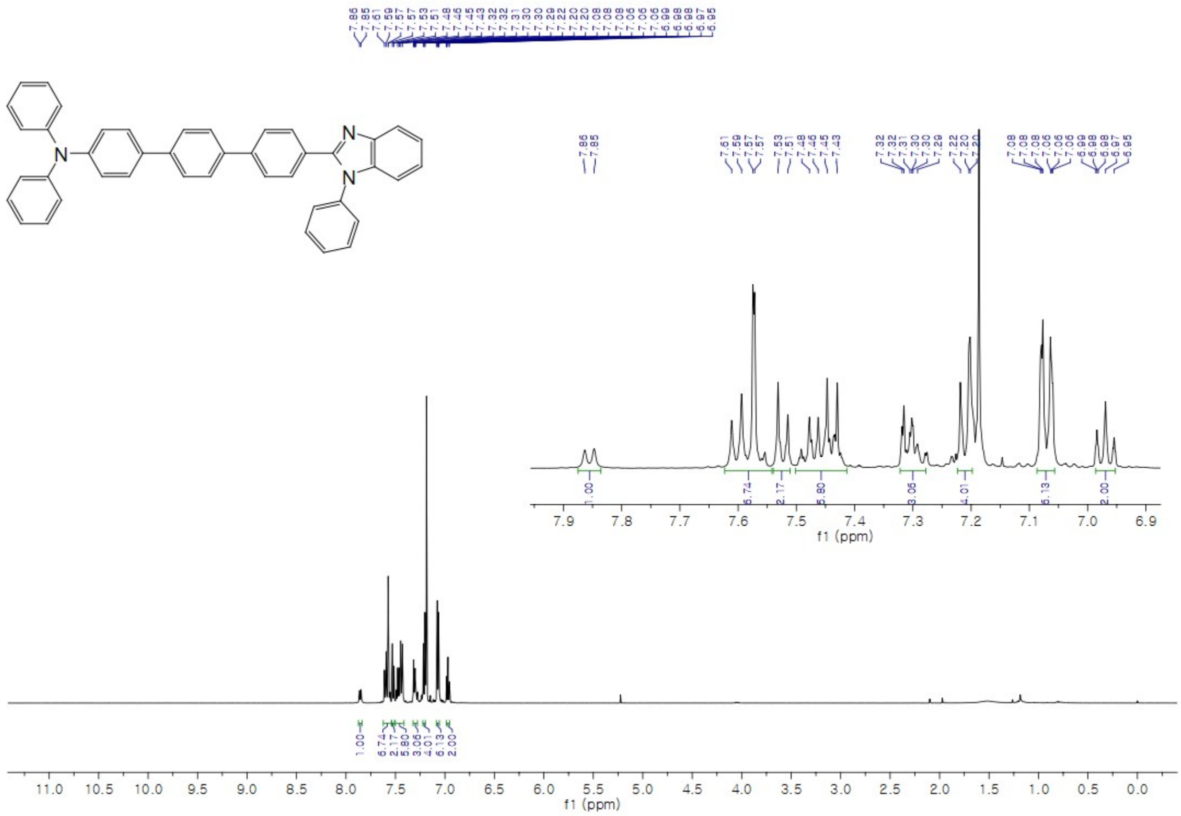

Figure S1-6. ^{1}H-NMR spectrum of **P** in $CDCl_3$ (500MHz, 293K)

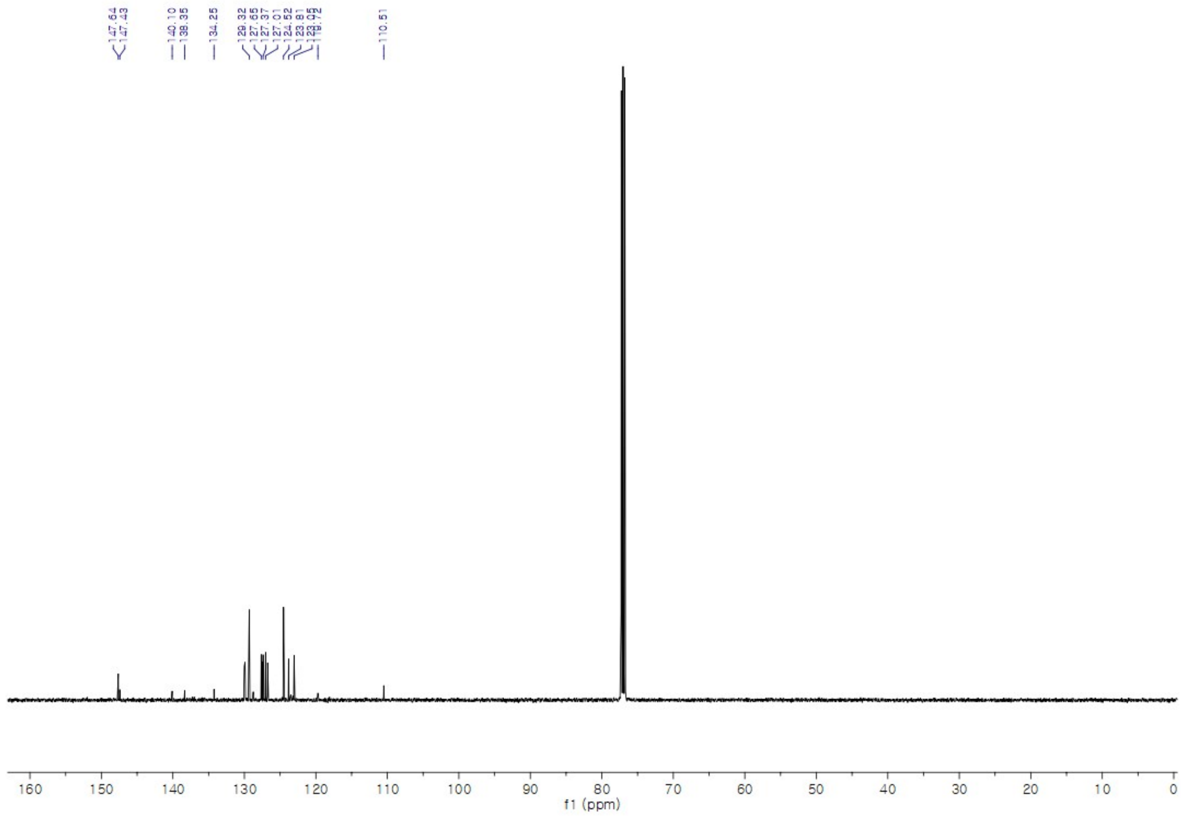

Figure S2-6. $^{13}C\{^1H\}$-NMR spectrum of **P** in $CDCl_3$ (125MHz, 293K)

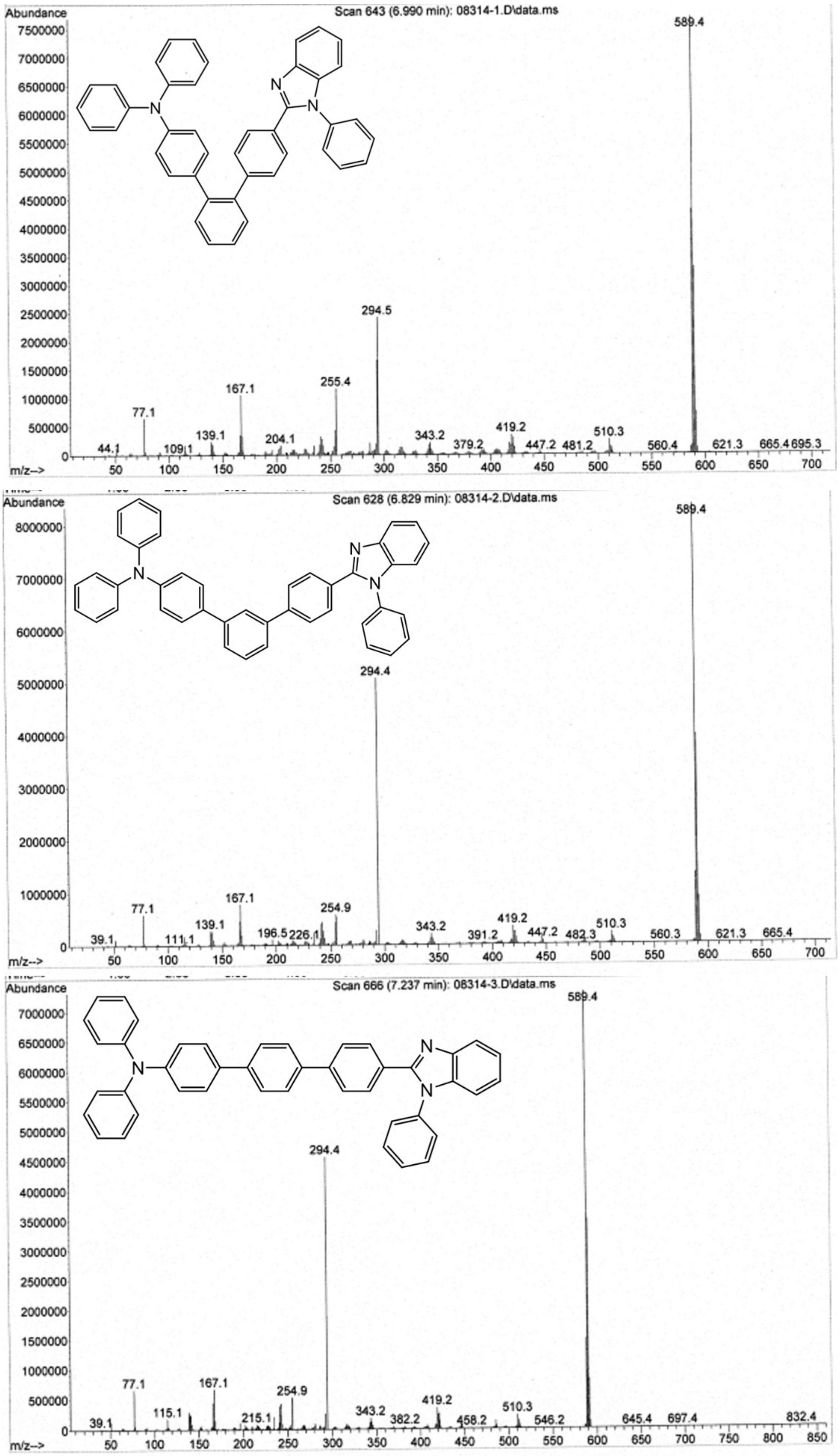

Figure S3. GC-MS data of **O**, **M**, and **P**

Table S1. Crystal data and structure refinement for **M**

	M	
Empirical formula	$C_{43}H_{31}N_3$	
Formula weight	589.74	
Crystal system, space group	Triclinic, *P*-1	
Unit cell dimensions	a = 9.7503(5) Å b = 18.6569(11) Å c = 19.6036(11) Å	α = 65.086(2)° β = 76.413(2)° γ = 80.311(2)°
Volume	3134.0(3) $Å^3$	
Z, Calculated density	4, 1.250 mg/m^3	
μ	0.073 mm^{-1}	
F(000)	1240	
Crystal size	0.26 × 0.14 × 0.1 mm	
θ range for data collection	1.98 to 28.41°	
Limiting indices	$-13 \le h \le 13$ $-24 \le k \le 24$ $-26 \le l \le 26$	
Max. and min. transmission	0.993 and 0.981	
Refinement method	SHELXL-2014/7 (Sheldrick, 2014)	
Data / restraints / parameters	15650 / 0 / 830	
Goodness-of-fit on F^2	1.052	
Final R indices [I>2σ(I)]	$R_1 = 0.052$, $wR_2 = 0.1122$	
R indices (all data)	$R_1 =0.1211$, $wR_2 = 0.1573$	
Largest diff. peak and hole	0.207 and -0.22 e. $Å^{-3}$	

Table S2. Selected bond lengths [Å], bond angles [º], and torsion angles [º] of **M**

	M	
Bond lengths [Å]	N(1)-C(22)	1.421
	C(7)-C(15)	1.387
	C(7)-C(17)	1.483
	C(14)-C(15)	1.399
	C(14)-C(49)	1.484
	C(18)-C(20)	1.385
	C(54)-C(59)	1.462
	C(55)-C(57)	1.373
Bond angles [º]	C(49)-C(14)-C(15)	119.239
	C(49)-C(14)- C(12)	122.823
	C(17)-C(7)-C(15)	119.867
	C(17)-C(7)-C(8)	121.930
Torsion angles [º]	C(12)-C(14)-C(49)-C(57)	151.817
	C(12)-C(14)-C(49)-C(50)	-29.094
	C(15)-C(14)-C(49)-C(57)	-26.555
	C(15)-C(14)-C(49)-C(50)	152.534
	C(18)-C(17)-C(7)-C(15)	-36.087
	C(18)-C(17)-C(7)-C(8)	144.719
	C(28)-C(17)-C(7)-C(15)	142.890
	C(28)-C(17)-C(7)-C(8)	-36.304

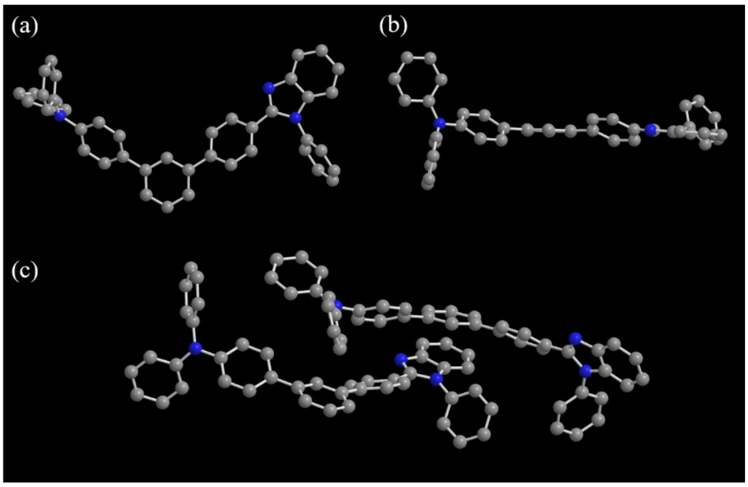

Figure S4. Single-crystal X-ray structure of **M**: (a) front view and (b) side view (c) molecular packing styles. Hydrogen atoms are omitted for clarity.

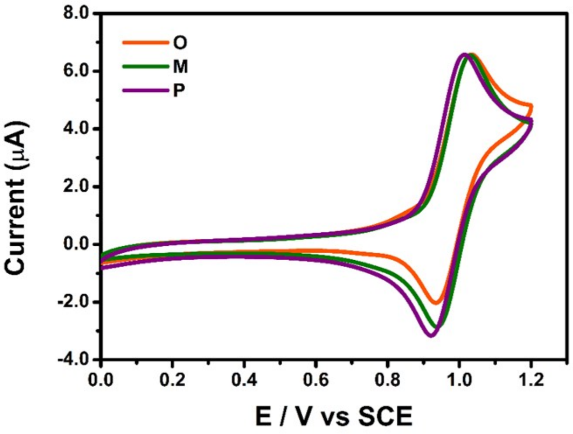

Figure S5. CV curves of **O**, **M**, and **P**. Condition: in CH_2Cl_2 solution containing 0.1 M TBAP as electrolyte, SCE reference electrode. Scan rate of 0.05 Vs^{-1}.

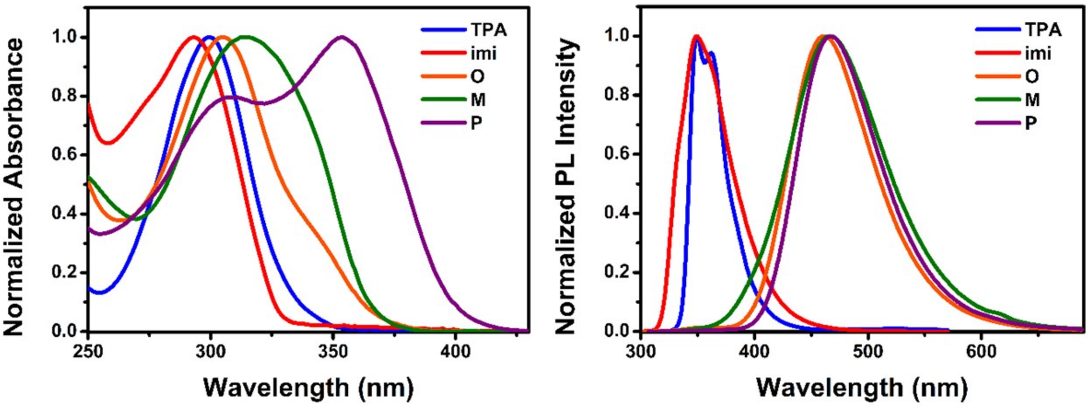

Figure S6. UV-vis absorption (left) and emission (right) spectra of triphenylamine (TPA), 1,2-diphenyl-1H-bezimidazole (IMI) and all dyads in dichloromethane solution.

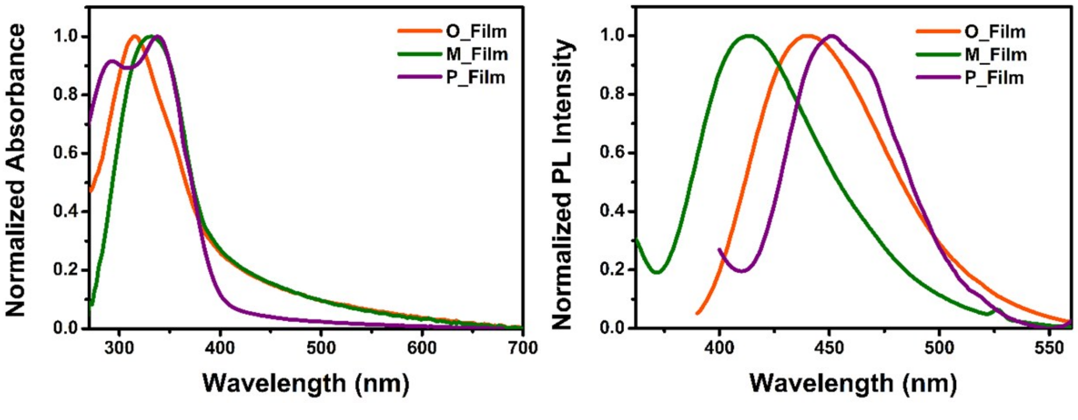

Figure S7. UV-vis absorption (left) and emission (right) spectra of **O**, **M**, and **P** in the solid state.

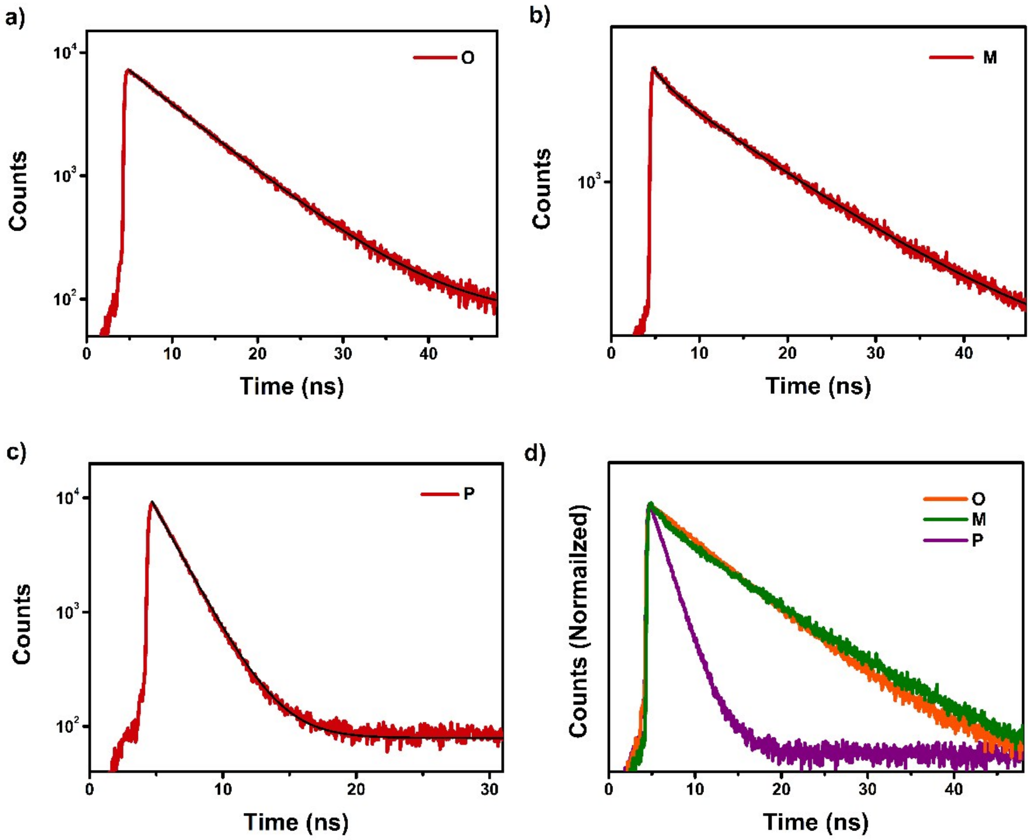

Figure S8. Fluorescence lifetimes (τ_F) of (a) **O**, (b) **M**, and (c) **P** at 500 nm (in CH_2Cl_2 at RT). (d) Fluorescence lifetimes (τ_F) comparison of all dyads at 500 nm (in CH_2Cl_2 at RT)

Table S3. Spectroscopic parameters of **O**, **M**, and **P** in various solvents

	O		**M**		**P**	
Solvents	λ_{abs} (nm)	λ_{em} (nm)	λ_{abs} (nm)	λ_{em} (nm)	λ_{abs} (nm)	λ_{em} (nm)
Hexane	305	415	315	371	350	404
Cyclohexane	306	418	314	372	351	406
Toluene	308	438	316	391	355	424
Ether	304	439	314	397	349	435
THF	306	461	316	449	353	460
DCM	305	472	314	478	354	479
ACN	303	501	312	538	349	513
MeOH	301	509	309	543	350	516

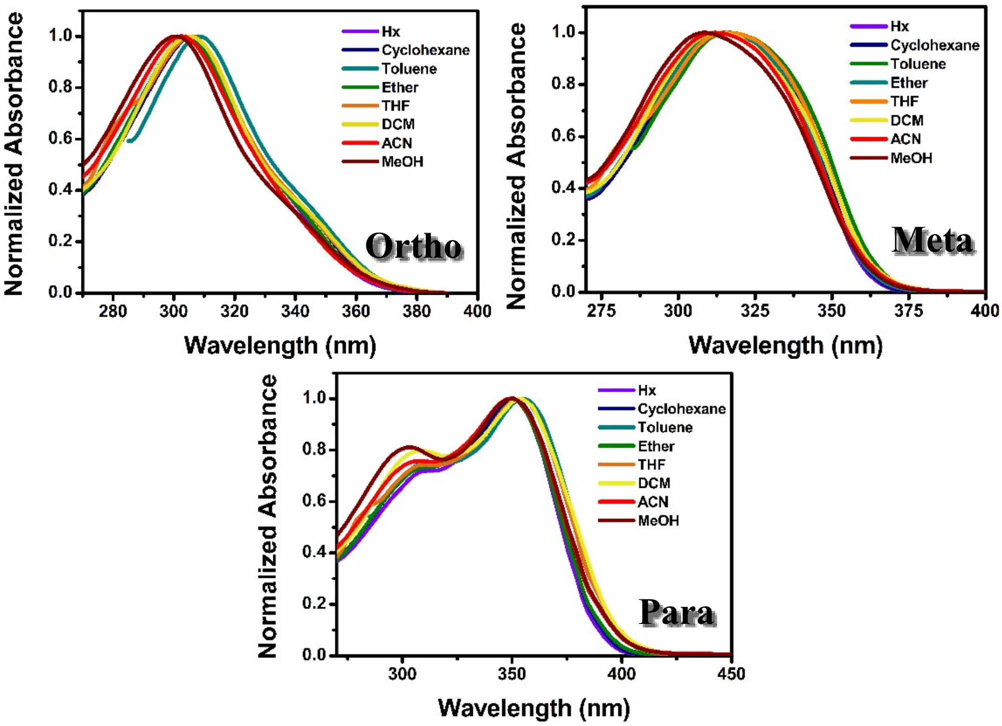

Figure S9. UV-vis absorption spectra of **O**, **M**, and **P** in various solvents at room temperature.

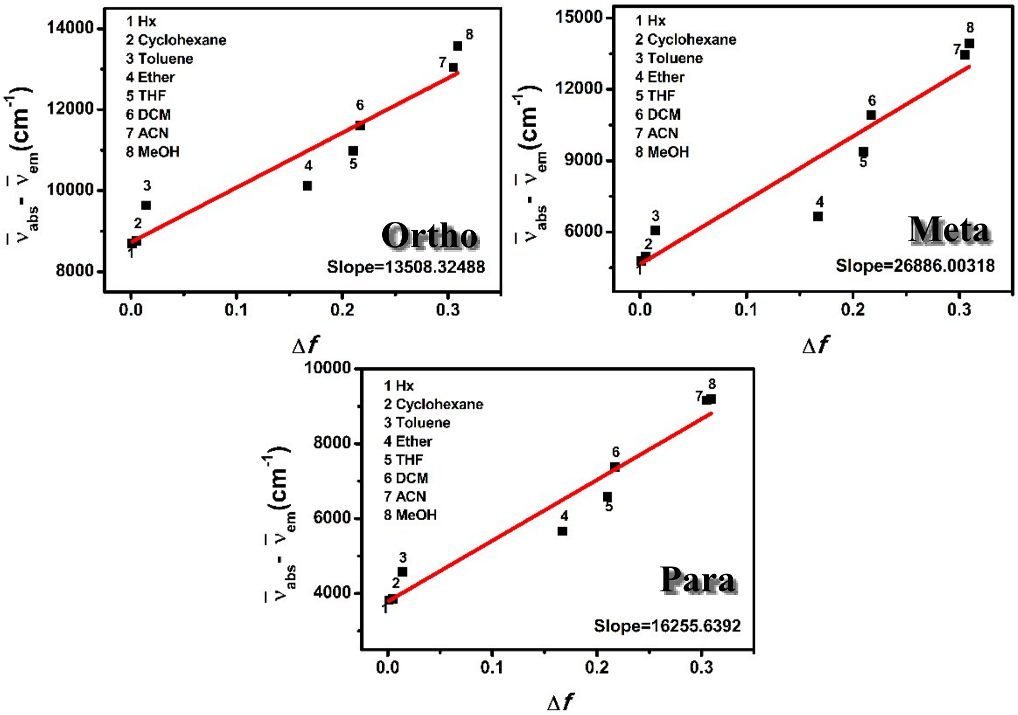

Figure S10. Lippert-Mataga plots for dyads **O**, **M**, and **P**.

Table S4. Dipole moment values of **O**, **M**, and **P** in the ground and excited states

Compounds	$\Delta\mu$	μ_g	μ_e
O	31.5 D	3.8 D	35.2 D
M	62.9 D	4.2 D	67.1 D
P	51.5 D	3.9 D	55.4 D

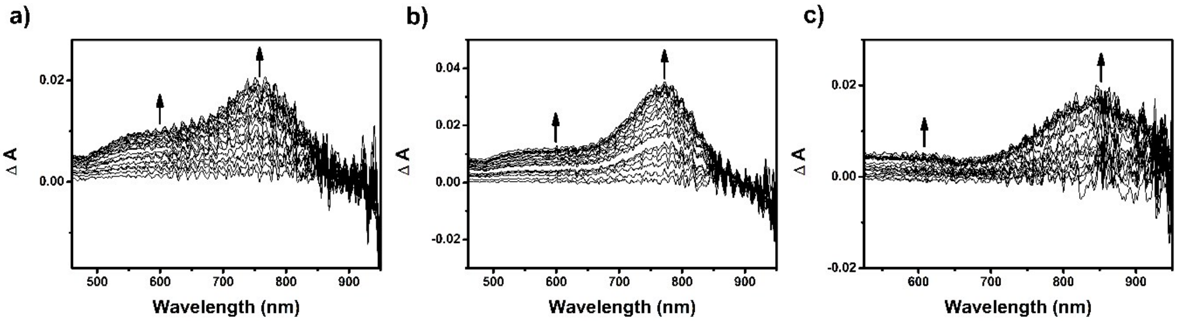

Figure S11. UV/vis/NIR optical absorption spectral change during the electrochemical oxidation from neutral to cation of (a) **O**, (b) **M**, and (c) **P** in CH_3CN with 0.1 M Bu_4NClO_4 at room temperature.

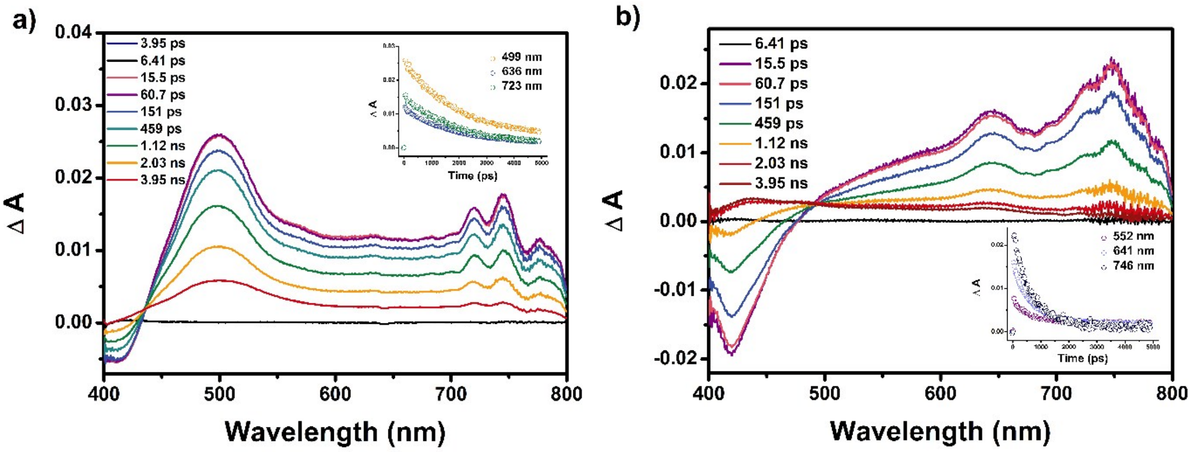

Figure S12. Transient absorption spectra of dyads (a) **O**, (b) **P** in CH_2Cl_2. Excitation wavelength is 320 nm. Inset: decay and rise profiles are monitored at selected wavelengths.

DFT/TD-DFT Calculation Details

All the calculations were performed on the platform of the Gaussian 16 package.[1] The ground-state geometry of all dyads has been optimized at the density function theory (DFT) level. Full geometry optimizations in their ground state were performed using the B3LYP functional[2] and the 6-31G[3] basis set for all atoms. No charge and no symmetry constraints were applied during the geometry optimizations. The nature of the stationary points located was further checked by computations of harmonic vibrational frequencies at the same level of theory. As well as, all of the Cartesian coordinates for optimized structure of all dyads are also summarized in Table S5. The Isodensity plots (isodensity contour = 0.05 a.u.) of the selected frontier orbitals (HOMO-3, HOMO-2, HOMO-1, HOMO, LUMO, LUMO+1, LUMO+2, LUMO+3) were visualized by Chem3D Ultra and GaussView 5.0 program. The excitation energies and oscillator strengths for the lowest 100 singlet–singlet transitions at the optimized geometry in the ground state were obtained in TD-DFT calculations using the same basis set and functional as for the ground state. The simulated absorption spectra were obtained by the GaussSum program based on TD-DFT results. To reduce the meaningless features, only 20 singlet–singlet transitions are summarized in Table S6.

Table S5-1. Cartesian coordinates for optimized structure for **O**

Atom	X	Y	Z
C	0.440296	-0.04884	-2.14854
C	-0.04344	-1.19061	-2.71347
C	0.672224	-1.76386	-3.70682
C	1.871413	-1.30557	-4.08996
C	2.39052	-0.24398	-3.46648
C	1.673229	0.368139	-2.51477
C	-1.14071	-1.85873	-2.27021
C	-0.27243	0.77075	-1.33044
C	-1.5166	-1.82782	-0.97733
C	-2.61634	-2.44639	-0.52161
C	-3.44334	-3.18347	-1.29525
C	-3.01173	-3.2654	-2.57393
C	-1.91482	-2.64545	-3.04181
C	0.284358	1.559527	-0.3909
C	-0.44424	2.345968	0.41911
C	-1.78534	2.459126	0.345447
C	-2.33621	1.663487	-0.59624
C	-1.61326	0.879727	-1.41174
N	-4.51598	-3.75518	-0.84359
C	-4.9674	-4.83187	-1.40905
C	-5.13608	-3.23318	0.1704
C	-6.2732	-5.19323	-1.38931
C	-6.75364	-6.3032	-1.97266
C	-5.93023	-7.13526	-2.62077
C	-4.62943	-6.82547	-2.66815
C	-4.17827	-5.70637	-2.07896
C	-5.89707	-3.95161	1.030908
C	-6.54062	-3.42219	2.083971
C	-6.45887	-2.11055	2.336449
C	-5.72208	-1.3539	1.514902
C	-5.08691	-1.91192	0.471768
C	-2.55584	3.210288	1.1785
N	-2.30275	4.135768	2.045076
C	-3.39882	4.304274	2.697233
C	-4.31941	3.494494	2.157917
N	-3.77851	2.867274	1.215346
C	-1.22237	4.814038	2.214995
C	-3.84109	5.127359	3.667377
C	-5.10738	5.048199	4.114988
C	-5.98054	4.177601	3.584679
C	-5.58837	3.392858	2.571164
C	-0.3819	5.056424	1.183474
C	0.746102	5.776275	1.292152
C	1.088243	6.312806	2.469495
C	0.272757	6.122014	3.513658
C	-0.85234	5.402233	3.37312
H	0.363824	-2.69948	-4.20117
H	2.446145	-1.81769	-4.88015
H	3.378831	0.143608	-3.76637
H	2.129827	1.293296	-2.12633
H	-0.8941	-1.32363	-0.21822
H	-2.762	-2.37682	0.571027
H	-3.61049	-3.7779	-3.3472
H	-1.73138	-2.73895	-4.12539
H	1.365767	1.514213	-0.17753
H	0.123876	2.817369	1.235532
H	-3.42395	1.651391	-0.78415
H	-2.18018	0.347413	-2.19448
H	-7.0509	-4.5452	-0.95002
H	-7.834	-6.52604	-1.9406
H	-6.31271	-8.05011	-3.10213
H	-3.92778	-7.50843	-3.17715
H	-3.08146	-5.59056	-2.11727
H	-5.97336	-5.05046	0.96202
H	-7.12411	-4.06888	2.761569
H	-6.9839	-1.66542	3.19733
H	-5.65788	-0.26574	1.6891
H	-4.57185	-1.18236	-0.17736
H	-3.23547	5.923758	4.118256
H	-5.44957	5.730189	4.912727
H	-7.01951	4.133979	3.951144
H	-6.28992	2.69419	2.087595
H	-0.62968	4.736876	0.157326
H	1.380594	5.954057	0.407159
H	2.011009	6.906677	2.573424
H	0.542644	6.54589	4.496217
H	-1.40884	5.247148	4.307244

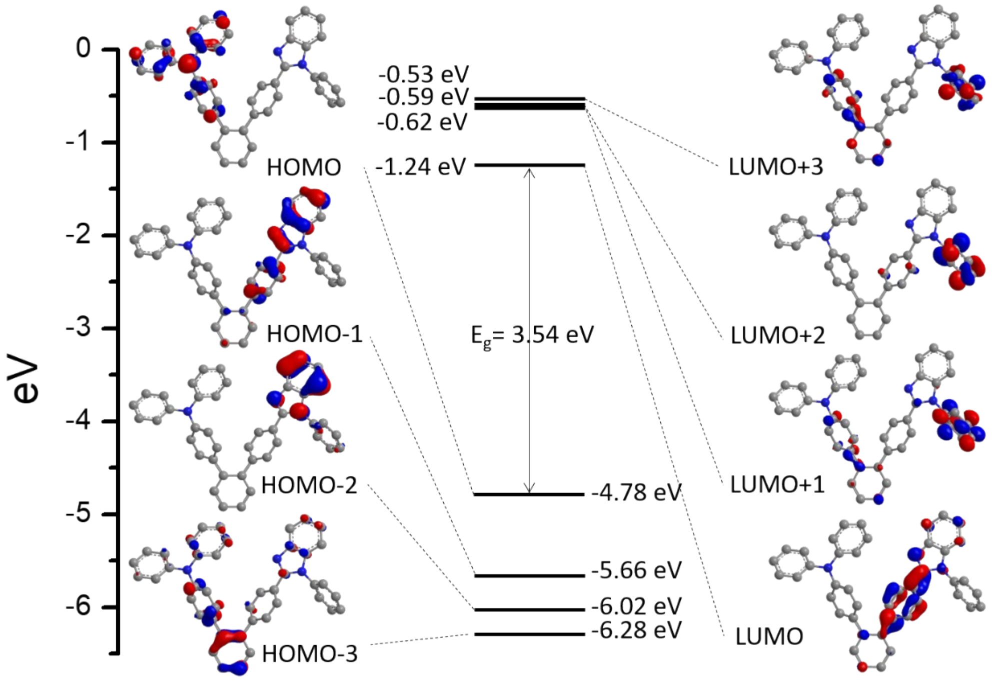

Figure S13-1. Energy levels and isodensity plots (isodensity contour = 0.05 a.u.) for selected occupied and unoccupied molecular orbitals of **O** obtained by DFT calculations.

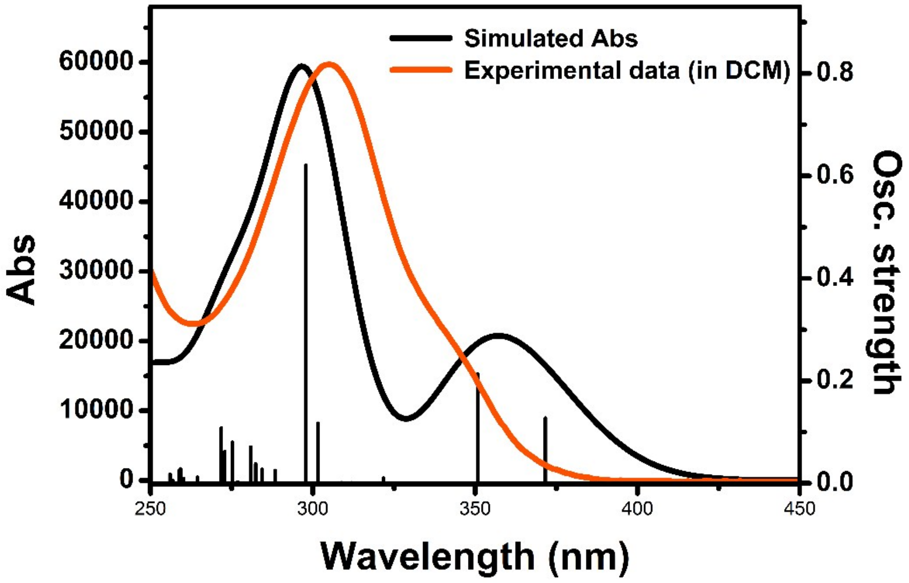

Figure S14-1. Electronic transition and simulated absorption spectra of **O** in the ground state geometry obtained by TD-DFT calculations.

Table S6-1. TD-DFT calculation: Transition assignment of **O**

No.	Excitation Energy (cm^{-1})	Wavelength (nm)	Oscillator strength	Assignment
1	26907.46	371.64	0.1277	HOMO->LUMO (95%)
2	28506.86	350.79	0.2137	HOMO->L+1 (94%)
3	31074.93	321.80	0.0104	HOMO->L+4 (87%)
4	32055.7	311.96	0.0011	HOMO->L+2 (98%)
5	32372.68	308.90	0.0014	HOMO->L+3 (90%)
6	33162.29	301.55	0.1176	HOMO->L+5 (90%)
7	33580.89	297.79	0.6209	H-1->LUMO (84%)
8	34678.61	288.36	0.0253	HOMO->L+6 (70%), HOMO->L+8 (17%)
9	35174.65	284.30	0.0272	H-1->L+1 (85%)
10	35416.61	282.35	0.0377	H-2->LUMO (68%)
11	35603.73	280.87	0.0713	HOMO->L+7 (53%), HOMO->L+8 (22%)
12	36118.31	276.87	0.0029	HOMO->L+6 (19%), HOMO->L+7 (22%), HOMO->L+8 (34%), HOMO->L+9 (15%)
13	36328.82	275.26	0.0803	H-1->L+2 (79%)
14	36652.25	272.83	0.0625	H-1->L+3 (75%)
15	36795.82	271.77	0.1082	HOMO->L+7 (12%), HOMO->L+9 (20%), HOMO->L+10 (44%)
16	37814.5	264.45	0.0123	H-3->LUMO (78%)
17	38425.87	260.24	0.0094	H-2->L+2 (88%)
18	38569.43	259.27	0.0285	H-2->L+1 (33%), H-2->L+3 (34%), HOMO->L+9 (11%)
19	38650.09	258.73	0.0244	H-2->L+3 (10%), HOMO->L+8 (10%), HOMO->L+9 (37%), HOMO->L+10 (21%)
20	38931.58	256.86	0.006	H-6->LUMO (22%), H-5->LUMO (10%), H-1->L+4 (20%), H-1->L+6 (16%)

Table S5-2. Cartesian coordinates for optimized structure for **M**

Atom	X	Y	Z
C	6.165422	-1.73715	-2.42346
C	5.848536	-2.18065	-3.6572
C	4.754567	-1.75788	-4.30147
C	3.928699	-0.87133	-3.73349
C	4.15658	-0.3707	-2.5019
C	5.283609	-0.8423	-1.91486
C	7.280078	-2.16313	-1.76221
C	3.318278	0.533341	-1.91733
C	7.661737	-1.72137	-0.54527
C	8.758636	-2.15326	0.100167
C	9.618764	-3.07226	-0.38866
C	9.236354	-3.50699	-1.60853
C	8.135635	-3.08412	-2.25326
C	3.490121	1.040091	-0.67761
C	2.66585	1.939969	-0.11498
C	1.584248	2.452817	-0.73039
C	1.368638	1.898113	-1.9411
C	2.198443	1.004649	-2.50659
N	10.67846	-3.48524	0.234865
C	11.69433	-3.93018	-0.43889
C	10.72065	-3.45319	1.531477
C	0.721488	3.351095	-0.18243
N	0.762567	4.108616	0.864639
C	-0.43158	4.565791	1.005432
C	-1.16408	4.103943	-0.01645
N	-0.42084	3.393786	-0.73632
C	11.87263	-3.34167	2.236481
C	11.93148	-3.30475	3.577479
C	10.81092	-3.38406	4.304396
C	9.645583	-3.49787	3.656832
C	9.617225	-3.52782	2.314698
C	12.57524	-4.83486	0.053086
C	13.62915	-5.30611	-0.6327
C	13.86681	-4.88245	-1.87944
C	13.02754	-3.98684	-2.41219
C	11.97925	-3.53673	-1.70401
C	-1.05477	5.431072	1.828354
C	-2.3598	5.716555	1.669116
C	-3.07144	5.182891	0.664021
C	-2.4608	4.372251	-0.21171
C	1.770051	4.420811	1.601981
C	3.022107	4.458516	1.091866
C	4.108511	4.800135	1.802761
C	3.986491	5.141878	3.090936
C	2.762407	5.14499	3.632538
C	1.693177	4.804374	2.894721
H	6.450168	-2.90259	-4.22692
H	4.532189	-2.14292	-5.31269
H	3.067065	-0.60141	-4.35985
H	5.505751	-0.4597	-0.91887
H	7.110431	-0.94478	0.005391
H	8.965138	-1.63422	1.053157
H	9.78393	-4.31945	-2.11858
H	7.974906	-3.58328	-3.22019
H	4.307568	0.724783	-0.01241
H	2.879968	2.173992	0.939394
H	0.501329	2.19012	-2.55899
H	1.880521	0.688822	-3.51103
H	12.84737	-3.19412	1.740243
H	12.90217	-3.18723	4.089127
H	10.84671	-3.35657	5.405718
H	8.710347	-3.58862	4.235563
H	8.612473	-3.69902	1.891364
H	12.43437	-5.30779	1.040328
H	14.29436	-6.06198	-0.18107
H	14.72969	-5.26058	-2.45158
H	13.2166	-3.60537	-3.43031
H	11.39953	-2.74779	-2.21351
H	-0.55185	5.980814	2.634077
H	-2.85286	6.426358	2.35587
H	-4.13641	5.438017	0.535766
H	-3.00633	3.948642	-1.07017
H	3.207073	4.286935	0.018132
H	5.101428	4.829911	1.322496
H	4.869478	5.425538	3.686627
H	2.641526	5.412158	4.696436
H	0.749414	4.770098	3.455629

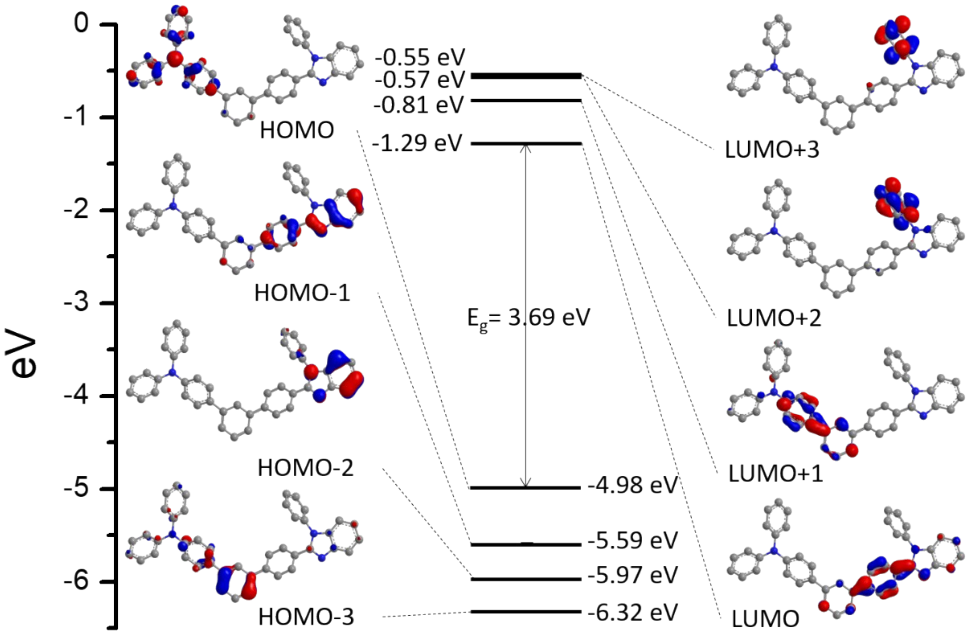

Figure S13-2. Energy levels and isodensity plots (isodensity contour = 0.05 a.u.) for selected occupied and unoccupied molecular orbitals of **M** obtained by DFT calculations.

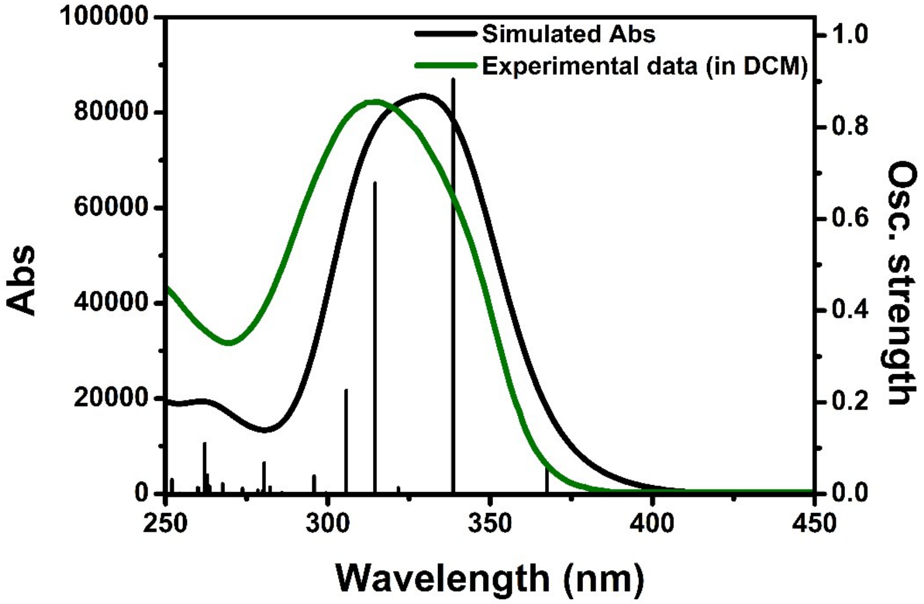

Figure S14-2. Electronic transition and simulated absorption spectra of **M** in the ground state geometry obtained by TD-DFT calculations.

Table S6-2. TD-DFT calculation: Transition assignment of **M**

No.	Excitation Energy (cm^{-1})	Wavelength (nm)	Oscillator strength	Assignment
1	27214.76	367.45	0.0684	HOMO->LUMO (98%)
2	29534.41	338.59	0.9051	HOMO->L+1 (87%)
3	31085.41	321.69	0.0132	HOMO->L+4 (96%)
4	31789.54	314.57	0.6782	H-1->LUMO (86%)
5	32715.46	305.67	0.2258	HOMO->L+5 (97%)
6	33397.81	299.42	0.0024	HOMO->L+2 (97%)
7	33566.38	297.92	0.0012	HOMO->L+3 (98%)
8	33809.15	295.78	0.0391	H-2->LUMO (92%)
9	34984.3	285.84	0.0025	H-1->L+1 (68%)
10	35439.2	282.17	0.015	HOMO->L+6 (12%), HOMO->L+8 (71%)
11	35657.77	280.44	0.0674	H-1->L+2 (69%), HOMO->L+9 (15%)
12	35723.1	279.93	0.0076	H-1->L+2 (13%), HOMO->L+9 (79%)
13	35907	278.50	0.0081	H-1->L+3 (92%)
14	36533.69	273.72	0.0121	HOMO->L+6 (69%), HOMO->L+8 (12%)
15	37370.09	267.59	0.0226	H-3->LUMO (78%), H-1->L+1 (10%)
16	37461.23	266.94	0	HOMO->L+7 (86%)
17	37943.55	263.55	0.0173	H-7->LUMO (34%), H-1->L+7 (31%)
18	38041.95	262.87	0.0411	H-2->L+2 (78%)
19	38147.6	262.14	0.1102	H-4->LUMO (50%), HOMO->L+10 (17%)
20	38436.35	260.17	0.0127	H-2->L+3 (80%)

Table S5-3. Cartesian coordinates for optimized structure for **P**

Atom	X	Y	Z	Atom	X	Y	Z
C	2.356202	-0.55598	0.264308	C	-6.48512	5.24776	2.58619
C	2.100803	-1.04561	-0.99272	C	-1.23004	4.951569	4.521141
C	0.890828	-0.72764	-1.50585	C	-0.22459	5.352454	5.275597
C	-0.08949	-0.1199	-0.80503	C	-0.46253	5.77569	6.517845
C	0.14407	0.453303	0.39451	C	-1.75423	5.642004	6.905306
C	1.394371	0.223674	0.893304	C	-2.77782	5.136314	6.103014
C	3.002887	-1.79138	-1.7168	H	3.313663	-0.81929	0.737477
C	-0.81897	1.146588	1.034609	H	0.623193	-1.18035	-2.47485
C	2.72411	-2.49386	-2.8141	H	-1.082	-0.09209	-1.30372
C	3.565305	-3.3311	-3.48997	H	1.680163	0.640132	1.872128
C	4.805063	-3.51407	-3.0308	H	1.691978	-2.54774	-3.09424
C	5.074998	-2.80193	-1.90342	H	3.190673	-3.86474	-4.37117
C	4.271045	-1.93552	-1.32274	H	6.091646	-2.9423	-1.51419
N	5.579182	-4.30227	-3.70205	H	4.773026	-1.41978	-0.49938
C	6.41787	-5.0317	-2.99648	H	6.010648	-6.64566	-4.99838
C	5.402323	-4.50308	-4.97414	H	5.659463	-6.9869	-7.26592
C	5.688705	-5.67828	-5.55517	H	5.060094	-5.1766	-8.87159
C	5.513244	-5.92958	-6.88093	H	4.564379	-2.93277	-7.83379
C	5.066114	-4.99663	-7.74367	H	4.651465	-2.59848	-5.58066
C	4.758791	-3.82749	-7.20826	H	7.880234	-5.18552	-4.58985
C	4.814055	-3.63609	-5.89791	H	9.475306	-6.32764	-3.33693
C	7.564193	-5.47256	-3.51569	H	9.017062	-7.06499	-1.12901
C	8.550977	-6.13237	-2.8792	H	6.919664	-6.29177	0.031363
C	8.320225	-6.41645	-1.61293	H	5.453515	-5.00585	-1.1365
C	7.217887	-6.05975	-0.993	H	0.186446	1.424688	2.939461
C	6.289738	-5.31978	-1.69913	H	-1.27936	2.666382	3.936881
C	-0.67765	1.659886	2.277025	H	-3.50018	2.806075	0.34394
C	-1.51193	2.501028	2.887964	H	-2.1782	1.55065	-0.60315
C	-2.53772	3.093745	2.261564	H	-4.96123	6.125753	5.84743
C	-2.68967	2.539011	1.039113	H	-7.15341	6.732348	5.39463
C	-1.89382	1.643117	0.411056	H	-8.14222	6.331804	3.27104
C	-3.3855	3.98659	2.752502	H	-6.88931	5.061408	1.574333
N	-3.44201	4.611261	3.895603	H	-0.95671	4.827974	3.515029
C	-4.63548	5.076584	3.927631	H	0.808173	5.431274	4.840572
C	-5.27877	4.811952	2.818789	H	0.328886	6.059229	7.229959
N	-4.48611	4.176459	2.100047	H	-1.89595	5.714859	8.013469
C	-2.54082	4.859255	4.818357	H	-3.66699	4.860856	6.653085
C	-5.30214	5.824883	4.839028				
C	-6.54606	6.224119	4.617831				
C	-7.16055	6.017447	3.432078				

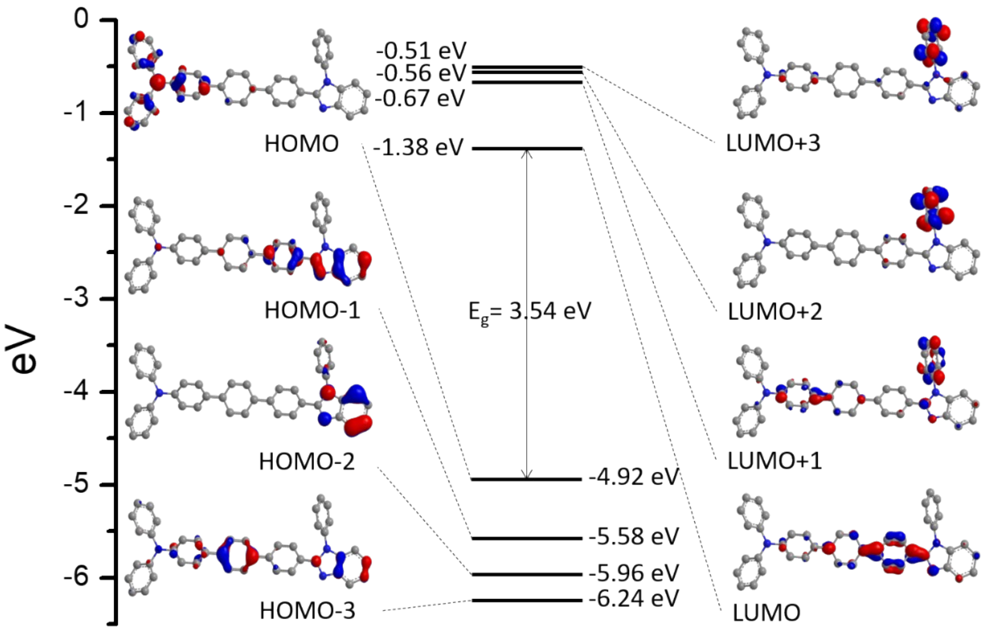

Figure S13-3. Energy levels and isodensity plots (isodensity contour = 0.05 a.u.) for selected occupied and unoccupied molecular orbitals of **P** obtained by DFT calculations.

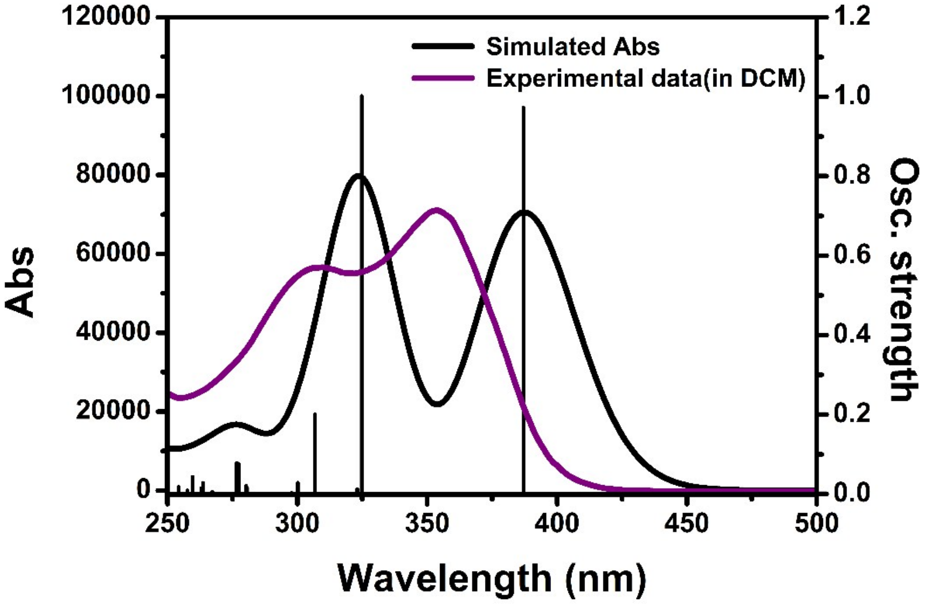

Figure S14-3. Electronic transition and simulated absorption spectra of **P** in the ground state geometry obtained by TD-DFT calculations.

Table S6-3. TD-DFT calculation: Transition assignment of **P**

No.	Excitation Energy (cm^{-1})	Wavelength (nm)	Oscillator strength	Assignment
1	25839.58	387.00	0.9732	HOMO->LUMO (96%)
2	30791.83	324.76	1.0022	H-1->LUMO (76%), HOMO->L+1 (16%)
3	30954.75	323.05	0.0124	HOMO->L+4 (96%)
4	31585.48	316.60	0.0013	H-1->LUMO (19%), HOMO->L+1 (71%)
5	32596.9	306.78	0.2006	HOMO->L+5 (96%)
6	33291.34	300.38	0.0006	HOMO->L+2 (83%)
7	33315.54	300.16	0.0289	H-2->LUMO (83%)
8	33585.73	297.75	0.003	HOMO->L+3 (80%)
9	34639.09	288.69	0.0013	HOMO->L+6 (70%), HOMO->L+7 (10%)
10	35627.93	280.68	0.0158	HOMO->L+8 (19%), HOMO->L+9 (12%), HOMO->L+10 (57%)
11	35640.83	280.58	0.005	H-1->L+1 (51%), H-1->L+2 (10%), H-1->L+3 (13%)
12	35681.97	280.25	0.021	HOMO->L+6 (10%), HOMO->L+9 (55%)
13	36052.98	277.37	0.0765	H-3->LUMO (36%), H-1->L+2 (46%)
14	36150.58	276.62	0.0785	H-3->LUMO (44%), H-1->L+2 (18%), H-1->L+3 (18%)
15	36879.7	271.15	0.0001	H-1->L+2 (12%), HOMO->L+7 (49%)
16	37424.13	267.21	0.006	H-2->L+1 (11%), H-1->L+1 (21%), H-1->L+3 (49%)
17	37935.48	263.61	0.0286	H-2->L+1 (27%), H-2->L+2 (14%), H-2->L+3 (15%), HOMO->L+8 (26%)
18	38027.43	262.97	0.0145	H-2->L+2 (33%), HOMO->L+8 (33%), HOMO->L+10 (10%)
19	38287.95	261.18	0.0007	H-6->LUMO (28%), H-1->L+6 (25%), HOMO->L+6 (12%)
20	38509.75	259.67	0.0435	H-2->L+2 (44%), H-2->L+3 (22%)

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