Electronic Supplementary Information (ESI)

Materials and Instrumentations

Tetrahydrofuran (THF) was distilled from sodium benzophenone ketyl under dry nitrogen immediately prior to use. Chemicals and reagents were purchased from commercial sources and used as received without further purification. 1,2-Di([1,1'-biphenyl]-4-yl)ethyne (**1a**)[1], 1,2-di([1,1'-biphenyl]-2-yl)ethyne (**1c**)[2] and 1,2-bis(2,6-dimethylphenyl)ethyne (**1d**)[2] were prepared according to the known procedures. ^{1}H and ^{13}C NMR spectra were measured on a Bruker AV 500 spectrometer in proper deuterated solvents using tetramethylsilane (TMS; $\delta = 0$) as internal reference at room temperature. High resolution mass spectra (HRMS) were recorded on a GCT premier CAB048 mass spectrometer operating in a MALDT-TOF mode. LC-MS measurements were carried out on a Waters ACQUITY UPLC H-Class_XEVO TQD. Single crystal X-ray diffraction intensity data were collected on a Bruker–Nonices Smart Apex CCD diffracto-meter with graphite monochromated MoKα radiation. Processing of the intensity data was carried out using the SAINT and SADABS routines, and the structure and refinement were conducted using the SHELTL suite of X-ray programs (version 6.10). UV-vis absorption spectra were measured on a SHIMADZU UV-2600 spectrophotometer. Photoluminescence spectra were recorded on a Horiba Fluoromax-4 fluorescence spectrophotometer. Fluorescence quantum yields were measured using a Hamamatsu absolute PL quantum yield spectrometer C11347 Quantaurus_QY. The fluorescence lifetimes were determined by the compact fluorescence lifetime spectrometer C11367 of Hamamatsu. Thermogravimetric analysis (TGA) analysis was carried out on a TA TGA Q5000 and differential scanning calorimetry (DSC) analysis was performed on a DSC Q1000 under dry nitrogen at a

heating rate of 10 °C min^{-1}. The frontier orbitals of the molecules based on the ground state geometries are calculated using the density function theory (DFT) method at B3LYP/6-31G (d, p) by Gaussian 09 program.

Synthesis

1,2-Di([1,1'-biphenyl]-3-yl)ethyne (1b): A mixture of 3-bromobiphenyl (5 g, 22 mmol), acetylenedicarboxylic acid (1.14 g, 10 mmol), 1,4-bis(diphenylphosphino)butane (426 mg, 1 mmol) and $Pd(PPh_3)_2Cl_2$ (352 mg, 0.5 mmol) in 80 ml of DMSO was combined with DBU (3.04 mg, 20 mmol), and then heated to 110 ^oC for 3 h under nitrogen. After cooled to room temperature, the reaction mixture was quenched with saturated aqueous ammonium chloride and extracted with dichloromethane three times. The combined extracts were washed with brine, dried over $MgSO_4$, and filtered. After solvent evaporation, the residue was purified by silica-gel column chromatography using hexane/dichloromethane as eluent. White solid of **1c** in 70 % yield (2.3 g) was obtained. ^1H NMR (500 MHz, $CDCl_3$), δ (TMS, ppm): 7.82–7.79 (m, 2H), 7.65–7.61 (m, 4H), 7.60–7.56 (m, 2H), 7.56–7.53 (m, 2H), 7.50–7.42 (m, 6H), 7.41–7.35 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$), δ (TMS, ppm): 141.45, 140.36, 130.40, 130.39, 128.84, 127.62, 127.19, 127.14, 123.67, 89.49. HRMS ($C_{26}H_{18}$): *m/z* 330.1427 (M^+, calcd 330.1409).

4,4'-(Ethyne-1,2-diyl)bis(N,N-diphenylaniline) (3a): The procedure was analogous to that described for **1c**. Yellow solid, yield 67 %. ^1H NMR (500 MHz, $CDCl_3$), δ (TMS, ppm): 7.34 (d, J = 8.5 Hz, 4H), 7.29–7.24 (m, 8H), 7.10 (d, J = 7.5 Hz, 8H), 7.07–7.02 (m, 4H), 6.99 (d, J = 8.5 Hz, 4H). ^{13}C NMR (125 MHz, $CDCl_3$), δ (TMS, ppm): 147.63, 147.28, 132.40, 129.38, 124.88, 123.43, 122.53, 116.60, 88.86. LC-MS ($C_{38}H_{28}N_2$): *m/z* 513.3 ($M + H^+$, calcd 512.2).

4',4'''-(Ethyne-1,2-diyl)bis(N,N-diphenyl-[1,1'-biphenyl]-4-amine) (3b): The procedure was analogous to that described for **1c**. Yellow solid, yield 78 %. ^1H NMR (500 MHz, $CDCl_3$), δ (TMS, ppm): 7.60–7.54 (m, 8H), 7.51–7.46 (m, 4H), 7.30–7.26 (m, 8H), 7.17–7.10 (m, 12H), 7.07–7.02 (m,

4H). ^{13}C NMR (125 MHz, $CDCl_3$), δ (TMS, ppm): 147.57, 140.33, 133.99, 132.01, 129.32, 127.63, 126.42, 124.56, 123.69, 123.10, 121.65, 90.06. LC-MS ($C_{50}H_{36}N_2$): *m/z* (M + H^+, calcd 664.2878).

2,3-Di([1,1'-biphenyl]-4-yl)-1-phenyl-1H-phosphindole-1-oxide ((*p*-BP)$_2$PIO): A mixture of **1a** (3.3 g, 10 mmol), diphenylphosphine oxide (4.04 g, 20 mmol), and Ag_2O (4.62 g, 20 mmol) in DMF (125 mL) was stirred at 100 ^{o}C for 10 h under nitrogen. After cooling to room temperature, the mixture was diluted with ethyl acetate (100 mL) and the insoluble solids were removed on a Celite plug. The filtrate was washed with saturated brine three times, and dried over anhydrous $MgSO_4$. After filtration, the solvent was evaporated under reduced pressure, and the residue was purified by column chromatography on silica gel by using petroleum ether/ethyl acetate (2/1 v/v) as eluent to afford the product as a yellow solid in 48% yield (2.5 g). ^{1}H NMR (500 MHz, $CDCl_3$), δ (TMS, ppm): 7.85–7.80 (m, 2 H), 7.76–7.68 (m, 3 H), 7.66 (d, *J* = 7.4, 2 H), 7.53–7.32 (m, 18 H), 7.32–7.26 (m, 2 H,). ^{13}C NMR (125 MHz, $CDCl_3$), δ (TMS, ppm): 149.55 (d, *J* = 21.6 Hz), 143.77 (d, *J* = 26.9Hz), 141.45, 140.38, 140.24 (d, *J* = 7.6 Hz), 133.91(d, *J* = 95.7 Hz), 133.27 (d, *J* = 15.1 Hz), 132.97, 132.23, 131.73 (d, *J* = 9.5 Hz), 131.64 (d, *J* = 105.2 Hz), 131.00 (d, *J* = 10.6 Hz), 130.04 (d, *J* = 99.7 Hz), 129.60, 129.48 (d, *J* = 5.7 Hz), 129.14 (d, *J* = 10.3 Hz), 129.11 (d, *J* = 9.4 Hz), 128.98, 128.92, 128.89, 128.69, 127.74, 127.66, 127.39, 127.94 (d, *J* = 25.7 Hz), 126.93, 124.07 (d, *J* = 10.8 Hz). HRMS ($C_{38}H_{27}OP$): *m/z* 531.1886 (M^+, calcd 531.1878).

2,3-Di([1,1'-biphenyl]-3-yl)-1-phenyl-1H-phosphindole-1-oxide ((*m*-BP)$_2$PIO): The procedure was analogous to that described for (*p*-BP)$_2$PIO. Pale yellow solid, yield 37 %. ^{1}H NMR (500 MHz, $(CD_3)_2CO$), δ (TMS, ppm): 7.91–7.80 (m, 4 H), 7.73–7.59 (m, 5 H), 7.56–7.40 (m, 10 H), 7.40–7.21 (m, 8 H). ^{13}C NMR (125 MHz, $CDCl_3$), δ (TMS, ppm): 150.28 (d, *J* = 21.6 Hz), 143.72 (d, *J* = 26.8 Hz), 142.25, 140.76, 140.49 (d, *J* = 5.3 Hz), 135.99 (d, *J* = 14.9 Hz), 134.92, 133.63 (d, *J* = 133.3 Hz), 133.04, 133.03, 133.02, 132.26 (d, *J* = 2.7 Hz), 131.10 (d, *J* = 105.1 Hz), 131.09, 131.00, 129.87 (d, *J* = 99.3 Hz), 129.47 (d, *J* = 58.3 Hz), 129.24 (d, *J* = 21.4 Hz), 129.00, 128.90, 128.57, 128.16 (d, *J* = 6.4 Hz), 127.91, 127.88, 127.87, 127.83, 127.59 (d, *J* = 25.3 Hz), 127.22, 127.03 (d, *J*

= 32.9 Hz), 126.60, 124.11 (d, *J* = 10.8 Hz). HRMS ($C_{38}H_{27}OP$): *m/z* 531.1858 (M^+, calcd 531.1878).

2,3-Di([1,1'-biphenyl]-2-yl)-1-phenyl-1H-phosphindole-1-oxide ((*o*-BP)$_2$PIO): The procedure was analogous to that described for (*p*-BP)$_2$PIO. White solid, yield 31%. ^{1}H NMR (500 MHz, $CDCl_3$), δ (TMS, ppm): 7.70–7.62 (m, 1H), 7.62–7.53 (m, 3H), 7.50–7.38 (m, 4H), 7.30–6.98 (m, 13H), 6.93–6.91 (m, 1H), 6.68 (s, 2H), 6.57 (s, 1H), 5.98 (s, 1H), 5.29 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$), δ (TMS, ppm): 149.88 (d, *J* = 22.5 Hz), 145.34 (d, *J* = 27.3 Hz), 142.10 (d, *J* = 5.5 Hz), 141.13 (d, *J* = 0.8 Hz), 140.99, 140.90, 135.69 (d, *J* = 96.2 Hz), 133.08, 132.68, 132.31 (d, *J* = 2.1 Hz), 131.84 (d, *J* = 10.9 Hz), 130.90 (d, *J* = 136.0 Hz), 130.80 (d, *J* = 130.3 Hz), 130.19 , 129.75, 129.37, 129.27, 129.14 (d, *J* = 9.3 Hz), 128.97, 128.90, 128.74, 128.59 (d, *J* = 12.4 Hz), 128.45, 127.91 (d, *J* = 12.9 Hz), 127.80, 127.52 (d, *J* = 1.2 Hz), 127.02, 126.46, 126.32, 126.28, 123.95 (d, *J* = 9.3 Hz). HRMS ($C_{38}H_{27}OP$): *m/z* 531.1865 (M^+, calcd 531.1878).

2,3-Bis(2,6-dimethylphenyl)-1-phenyl-1H-phosphindole-1-oxide ((*o*-DMP)$_2$PIO): The procedure was analogous to that described for (*p*-BP)$_2$PIO. White solid, yield 43%. ^{1}H NMR (500 MHz, $CDCl_3$), δ (TMS, ppm): 7.95–7.90 (m, 1 H), 7.53–7.44 (m, 5 H), 7.34–7.30 (m, 2 H), 7.10–7.05 (m, 2 H), 7.00–6.96 (m, 2 H), 6.93–6.87 (m, 2 H), 6.62 (d, *J* = 7.5 Hz, 1 H), 2.74 (s, 3 H), 2.07 (s, 3 H), 2.03 (s, 3 H), 1.13 (s, 3 H). ^{13}C NMR (125 MHz, $CDCl_3$), δ (TMS, ppm): 149.36 (d, *J* = 23.6 Hz), 144.77 (d, *J* = 28.6 Hz), 140.56 (d, *J* = 90.5 Hz), 139.13, 139.11, 137.27, 139.12 (d, *J* = 2.7 Hz), 135.67, 137.02 (d, *J* = 4.9 Hz), 132.88 (d, *J* = 15.2 Hz), 132.28 (d, *J* = 2.7 Hz), 131.33 (d, *J* = 100.2 Hz), 130.62 (d, *J* = 10.4 Hz), 130.49 (d, *J* = 7.0 Hz), 129.82 (d, *J* = 8.9 Hz), 129.28 (d, *J* = 104.0 Hz), 128.77 (d, *J* = 10.4 Hz), 128.66 (d, *J* = 12.1 Hz), 128.30 (d, *J* = 1.3 Hz), 128.03, 127.96, 127.60 (d, *J* = 1.5 Hz), 127.20, 123.99 (d, *J* = 11.0 Hz), 22.16, 21.64, 20.88, 19.59. HRMS ($C_{30}H_{27}OP$): *m/z* 435.1876 (M^+, calcd 435.1878).

2,3-Bis(4-(diphenylamino)phenyl)-1-phenyl-1H-phosphindole 1-oxide ((TPA)$_2$PIO): The procedure was analogous to that described for (*p*-BP)$_2$PIO. Yellow orange solid, yield 39 %. ^{1}H

NMR (500 MHz, $CDCl_3$), δ (TMS, ppm): 7.84–7.76 (m, 2H), 7.70–7.64 (m, 1H), 7.53–7.38 (m, 5H), 7.36–7.27 (m, 5H), 7.25–6.19 (m, 6H), 7.17–6.98 (m, 16H), 6.79 (d, J = 8.5 Hz, 2H).^{13}C NMR (125 MHz, $CDCl_3$), δ (TMS, ppm): 148.16, 148.00, 147.26, 147.22 (d, J = 15.3 Hz), 144.10 (d, J = 27.0 Hz), 133.07 (d, J = 96.6 Hz), 132.81,132.04, 132.02 (d, J = 105.3 Hz), 130.97 (d, J = 10.5 Hz), 130.03, 130.00, 129.96, 129.63, 129.71 (d, J = 131.3 Hz), 129.34 (d, J = 18.4 Hz), 129.03, 128.88 (d, J = 11.8 Hz), 128.70 (d, J = 10.4 Hz), 127.70 (d, J = 15.3 Hz), 126.12 (d, J = 10.0 Hz), 124.97 (d, J = 10.4 Hz), 123.69 (d, J = 10.7 Hz), 123.44 (d, J = 14.9 Hz), 122.74, 121.74. HRMS ($C_{50}H_{37}N_2OP$): *m/z* 712.2645 (M^+, calcd 712.2644).

2,3-Bis(4'-(diphenylamino)-[1,1'-biphenyl]-4-yl)-1-phenyl-1H-phosphindole 1-oxide ((TPAP)$_2$PIO): The procedure was analogous to that described for (p-BP)$_2$PIO. Yellow orange solid, yield 36 %. ^{1}H NMR (500 MHz, $CDCl_3$), δ (TMS, ppm): 7.85–7.78 (m, 2H), 7.76–7.70 (m, 1H), 7.67 (d, J = 8.0 Hz, 2H), 7.56–7.53 (m, 2H), 7.51–7.46 (m, 2H), 7.45–7.34 (m, 7H), 7.34–7.21 (m, 13H), 7.19–7.11 (m, 6H), 7.10 – 6.97 (m, 10H). ^{13}C NMR (125 MHz, $CDCl_3$), δ (TMS, ppm): 149.46 (d, J = 21.5 Hz), 147.66, 147.57, 147.56, 147.32, 143.85 (d, J = 26.8 Hz), 140.84, 139.74, 133.95(d, J = 23.0 Hz), 133.73 (d, J = 95.4 Hz), 132.97, 132.74 (d, J = 15.0 Hz), 132.22, 132.21, 132.06 (d, J = 105.1 Hz), 131.27, 131.01 (d, J = 10.5 Hz), 130.82 (d, J = 95.7 Hz), 129.61, 129.50 (d, J = 5.8 Hz), 129.30 (d, J = 9.7 Hz), 129.15, 129.07, 129.06, 128.93 (d, J = 12.3 Hz), 127.56 (d, J = 26.6 Hz), 127.04, 126.32, 124.50 (d, J = 14.4 Hz), 124.04 (d, J = 10.7 Hz), 123.76, 123.71, 123.13, 122.97. HRMS ($C_{62}H_{45}N_2OP$): *m/z* 864.3282 (M^+, calcd 864.3270).

X-Ray crystallography

Crystal data for (o-BP)$_2$PIO (CCDC 1504481): $C_{38}H_{27}OP$, M_W = 530.18, monoclinic, C2/c, a = 18.1818(9), b = 8.7095(4), c = 37.051(2) Å; β = 99.620(6)^o, V = 5784.68 Å^3, Z = 8, ρ_{calcd} = 1.22 g cm^{-3}, μ = 1.306 mm^{-1} (MoKa, λ = 1.5418), F(000) = 380, T = 173(2) K, $2\theta_{max}$ = 66.5 (97.85)^o, 5228 measured reflections, 3271 independent reflections (R_{int} = 0.0253), GOF on F^2 = 1.002, R_1 = 0.0348, wR_2 = 0.0872 (all data), Δe 0.319 and –0.163 eÅ^{-3}.

Crystal data for (*o*-DMP)$_2$PIO (CCDC 1504480): $C_{30}H_{27}OP$, M_W = 434.18, triclinic, P1, a = 8.8585(5), b = 11.2910(6), c = 12.4815(8) Å, α = 92.334 (5)^o, β = 92.130(5)^o, γ = 104.326(5)^o, V = 1207.15 Å^3, Z = 2, ρ_{calcd} = 1.19 g cm^{-3}, μ = 1.316 mm^{-1} (MoKa, λ = 1.5418), F(000) = 792, T = 173.15 K; $2\theta_{max}$ = 66.5(98.86)^o, 8330 measured reflections, 3413 independent reflections (R_{int} = 0.0376), GOF on F^2 = 1.002, R_1 = 0.0655, wR_2 = 0.1449 (all data), Δe 0.227 and –0.248 eÅ^{-3}.

Device fabrication

The multilayer OLEDs were fabricated by the vacuum-deposition method. Organic layers were deposited by high-vacuum (5 × 10^{-4} Pa) thermal evaporation onto a glass (3 cm × 4 cm) substrate pre-coated with an indium tin oxide (ITO) layer. Dipyrazinoquinoxaline-2,3,6,7,10,11-hexacarbonitrile (HATCN) was used as the hole-injecting layer, *N*,*N*-bis(naphthalene)-*N*,*N*-bis(phenyl)benzidine (NPB) was used as the hole-transporting layer (HTL), DPE-BFDB and TPE-BFDB were used as the emitting layers, 1,3,5-tri(1-phenyl-1*H*-benzo[d]imidazol-2-yl)phenyl (TPBi) was used as the electron-transporting layer (ETL) and LiF/Al was used as the cathode. All organic layers were deposited sequentially. Thermal deposition rates for the organic materials, LiF and Al were 0.5, 0.5 and 1 Å S^{-1}, respectively. The active area of each device was 12 mm^2. The electroluminescence spectra were measured on a Hitachi MPF-4 spectrofluorometer. The current density-voltage (J-V) characteristics of the OLEDs were recorded on a Keithley 2400 Source Meter. The current density-voltage-luminance curves (J-V-L) characterizations were carried out with a 3645 DC power supply combined with a 1980A spot photometer and they were recorded simultaneously. All measurements were done at room temperature under ambient conditions.

Additional data

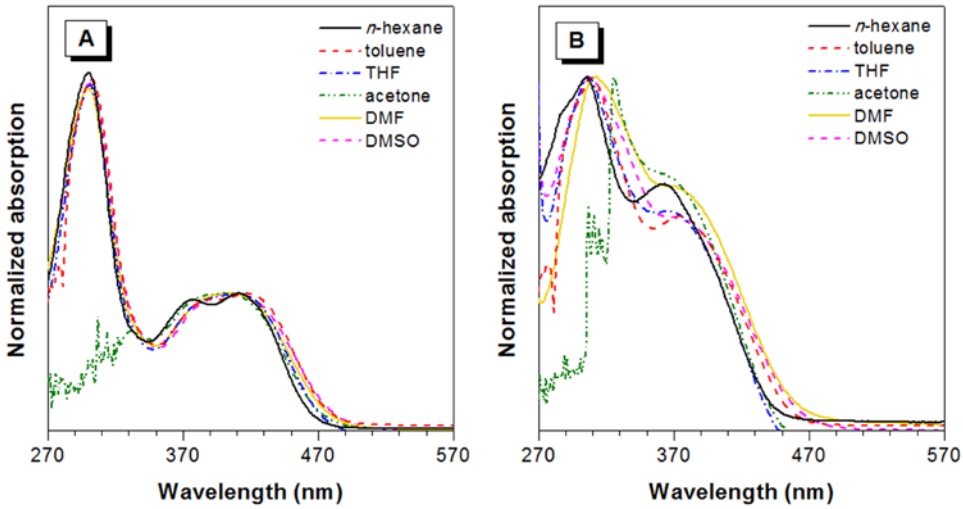


Fig. S1 Absorption spectra of $(TPA)_2PIO$ and $(TPAP)_2PIO$ in various solvents.

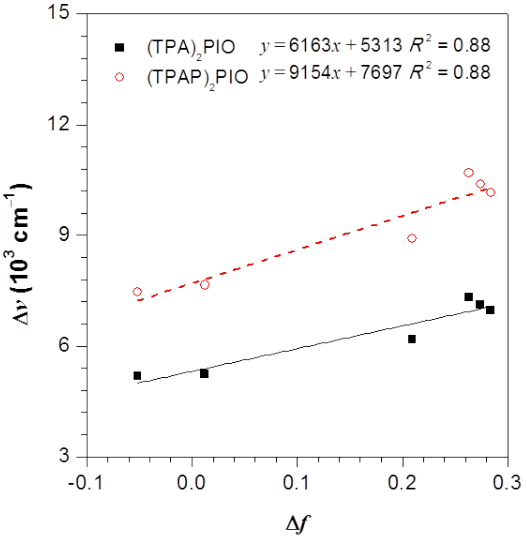


Fig. S2 Plots of Stokes shift ($\Delta\nu$) of $(TPA)_2PIO$ and $(TPAP)_2PIO$ *vs* solvent orientation polarizability (Δf). Δf = orientation polarizability = $(\varepsilon - 1)/(2\varepsilon + 1) - (n^2 - 1)/(2n^2 + 1)$, where ε = dielectric constant and n = refractive index.

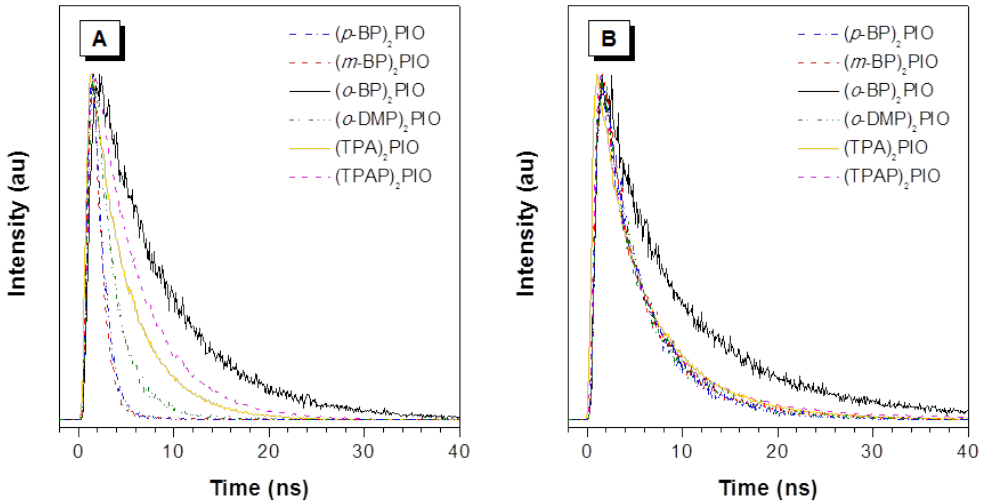
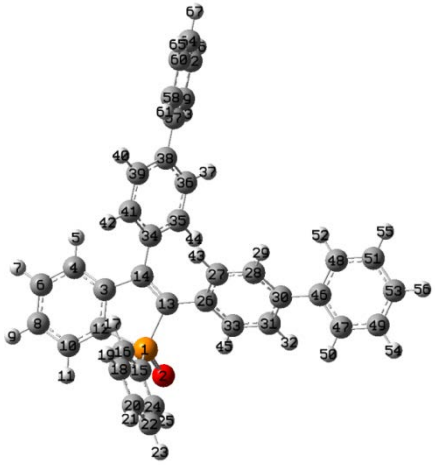


Fig. S3 Fluorescence decay curves of $(p\text{-BP})_2$PIO, $(m\text{-BP})_2$PIO, $(o\text{-BP})_2$PIO, $(o\text{-DMP})_2$PIO, $(\text{TPA})_2$PIO and $(\text{TPAP})_2$PIO in (A) THF solutions and (B) films.

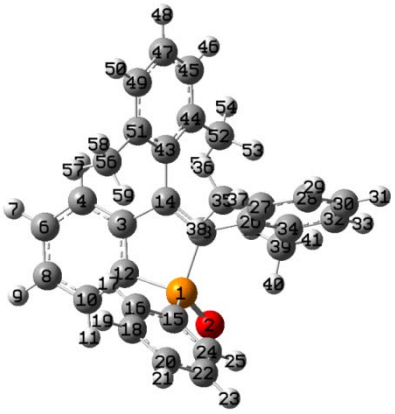
Table S1. Cartesian coordinates for the calculated structures



1 P1	2.8483	–1.5155	-0.8937 P
2 O2	3.5813	-1.1054	-2.1424 O
3 C3	0.7973	-3.1496	-0.5567 C
4 C4	0.0669	-4.3389	-0.4982 C
5 H5	-1.0043	-4.3193	-0.3295 H
6 C6	0.7277	-5.5608	-0.6697 C
7 H7	0.1578	-6.4843	-0.6243 H
8 C8	2.1015	-5.6073	-0.9070 C
9 H9	2.5980	-6.5628	-1.0449 H
10 C10	2.8389	-4.4181	-0.9772 C

11	H11	3.9062	-4.4439	-1.1768 H
12	C12	2.1851	-3.2066	-0.7988 C
13	C13	1.1898	-0.7780	-0.5849 C
14	C14	0.2584	-1.7629	-0.4350 C
15	C15	3.8440	-1.2242	0.6114 C
16	C16	3.3894	-1.5529	1.8966 C
17	H17	2.4082	-1.9998	2.0307 H
18	C18	4.1955	-1.3078	3.0063 C
19	H19	3.8405	-1.5636	4.0003 H
20	C20	5.4588	-0.7331	2.8397 C
21	H21	6.0853	-0.5426	3.7064 H
22	C22	5.9146	-0.4042	1.5630 C
23	H23	6.8959	0.0427	1.4329 H
24	C24	5.1097	-0.6484	0.4487 C
25	H25	5.4474	-0.4000	-0.5526 H
26	C26	1.0223	0.6825	-0.4926 C
27	C27	0.1879	1.2831	0.4684 C
28	C28	0.0665	2.6650	0.5458 C
29	H29	-0.5593	3.0992	1.3196 H
30	C30	0.7693	3.5107	-0.3307 C
31	C31	1.6109	2.9091	-1.2809 C
32	H32	2.1510	3.5323	-1.9871 H
33	C33	1.7441	1.5267	-1.3585 C
34	C34	-1.1986	-1.5435	-0.2394 C
35	C35	-1.9434	-0.8121	-1.1777 C
36	C36	-3.3094	-0.6136	-1.0064 C
37	H37	-3.8555	-0.0253	-1.7374 H
38	C38	-3.9877	-1.1325	0.1097 C
39	C39	-3.2391	-1.8629	1.0473 C
40	H40	-3.7379	-2.2963	1.9088 H
41	C41	-1.8729	-2.0699	0.8742 C
42	H42	-1.3209	-2.6423	1.6141 H
43	H43	-0.3517	0.6603	1.1733 H
44	H44	-1.4407	-0.3931	-2.0433 H

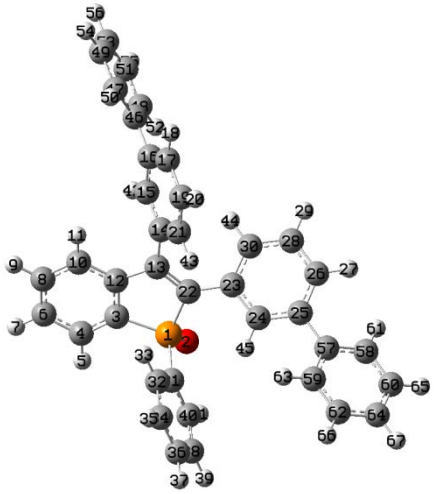
45	H45	2.3999	1.0853	-2.1026 H
46	C46	0.6309	4.9858	-0.2487 C
47	C47	1.7303	5.8298	-0.4827 C
48	C48	-0.6042	5.5795	0.0642 C
49	C49	1.5994	7.2152	-0.4072 C
50	H50	2.7005	5.3934	-0.7000 H
51	C51	-0.7350	6.9649	0.1409 C
52	H52	-1.4741	4.9490	0.2220 H
53	C53	0.3662	7.7896	-0.0947 C
54	H54	2.4652	7.8469	-0.5843 H
55	H55	-1.7017	7.4011	0.3760 H
56	H56	0.2643	8.8692	-0.0356 H
57	C57	-5.4456	-0.9182	0.2905 C
58	C58	-5.9906	-0.6964	1.5667 C
59	C59	-6.3190	-0.9317	-0.8103 C
60	C60	-7.3594	-0.4961	1.7361 C
61	H61	-5.3316	-0.6542	2.4287 H
62	C62	-7.6877	-0.7304	-0.6412 C
63	H63	-5.9241	-1.1278	-1.8026 H
64	C64	-8.2143	-0.5120	0.6328 C
65	H65	-7.7575	-0.3180	2.7309 H
66	H66	-8.3449	-0.7531	-1.5057 H
67	H67	-9.2807	-0.3554	0.7647 H



1	P1	1.5931	-0.2847	-1.1441 P
2	O2	2.1682	0.2536	-2.4250 O

3	C3	-0.3366	-2.0051	-0.6301 C
4	C4	-1.0403	-3.2108	-0.5856 C
5	H5	-2.0626	-3.2338	-0.2216 H
6	C6	-0.4189	-4.3850	-1.0256 C
7	H7	-0.9676	-5.3219	-0.9957 H
8	C8	0.8904	-4.3660	-1.5087 C
9	H9	1.3564	-5.2844	-1.8522 H
10	C10	1.5996	-3.1593	-1.5609 C
11	H11	2.6133	-3.1325	-1.9498 H
12	C12	0.9817	-1.9948	-1.1223 C
13	C13	-0.0288	0.3770	-0.5293 C
14	C14	-0.8676	-0.6590	-0.2475 C
15	C15	2.7835	-0.1029	0.2358 C
16	C16	2.7803	-0.9230	1.3739 C
17	H17	2.0567	-1.7278	1.4644 H
18	C18	3.7202	-0.7229	2.3848 C
19	H19	3.7168	-1.3654	3.2604 H
20	C20	4.6691	0.2954	2.2662 C
21	H21	5.4013	0.4485	3.0538 H
22	C22	4.6821	1.1087	1.1322 C
23	H23	5.4248	1.8950	1.0339 H
24	C24	3.7447	0.9104	0.1180 C
25	H25	3.7603	1.5212	-0.7789 H
26	C26	-0.2541	1.8460	-0.3745 C
27	C27	-0.2982	2.4571	0.9023 C
28	C28	-0.5036	3.8390	0.9939 C
29	H29	-0.5346	4.2993	1.9778 H
30	C30	-0.6628	4.6217	-0.1434 C
31	H31	-0.8259	5.6920	-0.0539 H
32	C32	-0.6014	4.0235	-1.3977 C
33	H33	-0.7168	4.6292	-2.2925 H
34	C34	-0.3843	2.6483	-1.5405 C
35	C35	-0.1233	1.6766	2.1830 C
36	H36	-1.0367	1.1337	2.4455 H

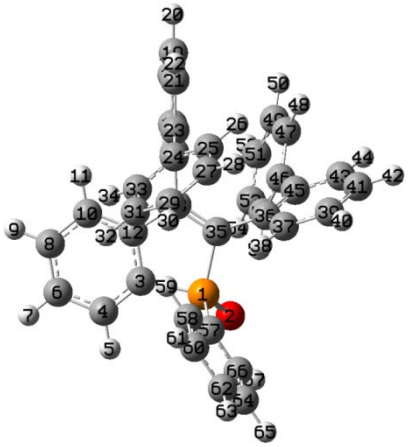
37	H37	0.1079	2.3519	3.0114 H
38	H38	0.6880	0.9480	2.1110 H
39	C39	-0.2879	2.0809	-2.9400 C
40	H40	0.7494	1.8568	-3.2019 H
41	H41	-0.6902	2.7924	-3.6666 H
42	H42	-0.8386	1.1434	-3.0448 H
43	C43	-2.2201	-0.5789	0.3961 C
44	C44	-3.3385	-0.0696	-0.3022 C
45	C45	-4.5812	-0.0234	0.3415 C
46	H46	-5.4374	0.3697	-0.2000 H
47	C47	-4.7344	-0.4726	1.6484 C
48	H48	-5.7044	-0.4225	2.1347 H
49	C49	-3.6381	-0.9992	2.3242 C
50	H50	-3.7526	-1.3638	3.3416 H
51	C51	-2.3804	-1.0758	1.7150 C
52	C52	-3.2445	0.4134	-1.7291 C
53	H53	-2.8098	1.4160	-1.7796 H
54	H54	-4.2375	0.4581	-2.1846 H
55	H55	-2.6221	-0.2445	-2.3420 H
56	C56	-1.2446	-1.7104	2.4894 C
57	H57	-1.1106	-2.7612	2.2081 H
58	H58	-1.4506	-1.6824	3.5630 H
59	H59	-0.2909	-1.2082	2.3167 H



1	P1	1.1063	1.8766	1.1604 P
2	O2	1.5900	1.8036	2.5797 O
3	C3	-0.3027	2.9594	0.7685 C
4	C4	-0.4487	4.3222	0.9892 C
5	H5	0.3345	4.8867	1.4867 H
6	C6	-1.6231	4.9586	0.5671 C
7	H7	-1.7582	6.0213	0.7436 H
8	C8	-2.6151	4.2266	-0.0858 C
9	H9	-3.5186	4.7259	-0.4234 H
10	C10	-2.4642	2.8544	-0.3156 C
11	H11	-3.2400	2.3020	-0.8344 H
12	C12	-1.3081	2.2077	0.1289 C
13	C13	-0.9782	0.7600	-0.0198 C
14	C14	-1.9416	-0.1591	-0.6850 C
15	C15	-3.2455	-0.3093	-0.1912 C
16	C16	-4.1737	-1.1623	-0.8096 C
17	C17	-3.7697	-1.8623	-1.9582 C
18	H18	-4.4631	-2.5438	-2.4411 H
19	C19	-2.4791	-1.7148	-2.4631 C
20	H20	-2.1801	-2.2680	-3.3486 H
21	C21	-1.5655	-0.8729	-1.8329 C
22	C22	0.2473	0.4024	0.4600 C
23	C23	0.8260	-0.9514	0.5686 C
24	C24	2.1941	-1.1611	0.3292 C

25	C25	2.7820	-2.4292	0.4464 C
26	C26	1.9689	-3.5075	0.8288 C
27	H27	2.3959	-4.5028	0.9036 H
28	C28	0.6137	-3.3125	1.0911 C
29	H29	-0.0031	-4.1534	1.3946 H
30	C30	0.0416	-2.0505	0.9647 C
31	C31	2.4465	2.3501	0.0040 C
32	C32	2.2504	2.4761	-1.3795 C
33	H33	1.2719	2.2854	-1.8115 H
34	C34	3.3107	2.8471	-2.2043 C
35	H35	3.1550	2.9438	-3.2749 H
36	C36	4.5715	3.0960	-1.6540 C
37	H37	5.3962	3.3854	-2.2989 H
38	C38	4.7705	2.9730	-0.2786 C
39	H39	5.7498	3.1651	0.1499 H
40	C40	3.7111	2.6007	0.5513 C
41	H41	3.8476	2.4964	1.6232 H
42	H42	-3.5465	0.2538	0.6867 H
43	H43	-0.5592	-0.7640	-2.2238 H
44	H44	-1.0096	-1.9079	1.1862 H
45	H45	2.8215	-0.3192	0.0584 H
46	C46	-5.5463	-1.3169	-0.2617 C
47	C47	-6.6541	-1.4378	-1.1175 C
48	C48	-5.7723	-1.3462	1.1247 C
49	C49	-7.9421	-1.5837	-0.6052 C
50	H50	-6.5058	-1.3917	-2.1922 H
51	C51	-7.0604	-1.4909	1.6372 C
52	H52	-4.9288	-1.2805	1.8053 H
53	C53	-8.1512	-1.6107	0.7746 C
54	H54	-8.7848	-1.6676	-1.2855 H
55	H55	-7.2105	-1.5188	2.7125 H
56	H56	-9.1546	-1.7240	1.1739 H
57	C57	4.2298	-2.6226	0.1724 C
58	C58	4.9954	-3.5165	0.9400 C

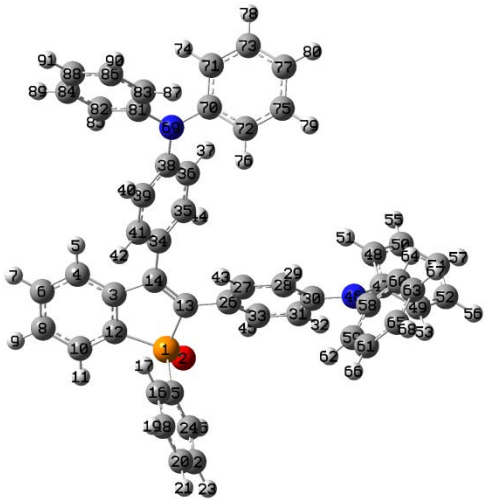
59	C59	4.8718	-1.9191	-0.8606 C
60	C60	6.3525	-3.7022	0.6829 C
61	H61	4.5277	-4.0490	1.7626 H
62	C62	6.2296	-2.1030	-1.1165 C
63	H63	4.2969	-1.2384	-1.4813 H
64	C64	6.9763	-2.9965	-0.3471 C
65	H65	6.9258	-4.3923	1.2955 H
66	H66	6.7029	-1.5525	-1.9246 H
67	H67	8.0340	-3.1403	-0.5471 H



1	P1	1.0207	-1.9868	0.1444 P
2	O2	0.5290	-3.3362	-0.3083 O
3	C3	1.0108	-1.6354	1.9324 C
4	C4	1.6308	-2.3133	2.9734 C
5	H5	2.2543	-3.1800	2.7742 H
6	C6	1.4348	-1.8694	4.2883 C
7	H7	1.9090	-2.3927	5.1130 H
8	C8	0.6280	-0.7590	4.5377 C
9	H9	0.4783	-0.4206	5.5589 H
10	C10	0.0031	-0.0747	3.4879 C
11	H11	-0.6288	0.7842	3.6907 H
12	C12	0.1923	-0.5154	2.1772 C
13	C13	-0.3953	0.0909	0.9470 C
14	C14	-1.3260	1.2553	1.0598 C
15	C15	-2.6419	0.9936	1.4720 C

16	H16	-2.9276	-0.0294	1.6951 H
17	C17	-3.5886	2.0118	1.5592 C
18	H18	-4.6025	1.7805	1.8712 H
19	C19	-3.2282	3.3173	1.2293 C
20	H20	-3.9561	4.1212	1.2893 H
21	C21	-1.9217	3.5923	0.8336 C
22	H22	-1.6302	4.6127	0.6034 H
23	C23	-0.9482	2.5826	0.7539 C
24	C24	0.4421	2.9768	0.3831 C
25	C25	0.6833	3.6939	-0.7994 C
26	H26	-0.1425	3.8913	-1.4761 H
27	C27	1.9676	4.1334	-1.1209 C
28	H28	2.1332	4.6812	-2.0442 H
29	C29	3.0354	3.8710	-0.2615 C
30	H30	4.0340	4.2204	-0.5073 H
31	C31	2.8087	3.1635	0.9207 C
32	H32	3.6295	2.9687	1.6055 H
33	C33	1.5249	2.7184	1.2390 C
34	H34	1.3556	2.1876	2.1705 H
35	C35	-0.0701	-0.5410	-0.2080 C
36	C36	-0.5036	-0.2042	-1.5907 C
37	C37	0.4339	0.4128	-2.4364 C
38	H38	1.4253	0.6256	-2.0515 H
39	C39	0.1100	0.7800	-3.7402 C
40	H40	0.8551	1.2605	-4.3673 H
41	C41	-1.1710	0.5268	-4.2268 C
42	H42	-1.4391	0.8005	-5.2432 H
43	C43	-2.1061	-0.0971	-3.4061 C
44	H44	-3.0950	-0.3228	-3.7933 H
45	C45	-1.8014	-0.4826	-2.0893 C
46	C46	-2.8639	-1.1718	-1.3018 C
47	C47	-4.1551	-0.6200	-1.2451 C
48	H48	-4.3466	0.3330	-1.7294 H
49	C49	-5.1805	-1.2634	-0.5532 C

50 H50	-6.1700	-0.8157	-0.5177 H
51 C51	-4.9341	-2.4749	0.0950 C
52 H52	-5.7311	-2.9789	0.6346 H
53 C53	-3.6575	-3.0371	0.0376 C
54 H54	-3.4574	-3.9868	0.5256 H
55 C55	-2.6294	-2.3978	-0.6571 C
56 H56	-1.6506	-2.8656	-0.7124 H
57 C57	2.6961	-1.6420	-0.4965 C
58 C58	3.3954	-0.4610	-0.2084 C
59 H59	2.9428	0.3084	0.4096 H
60 C60	4.6732	-0.2638	-0.7289 C
61 H61	5.2081	0.6554	-0.5091 H
62 C62	5.2614	-1.2443	-1.5328 C
63 H63	6.2581	-1.0883	-1.9359 H
64 C64	4.5692	-2.4215	-1.8189 C
65 H65	5.0247	-3.1835	-2.4445 H
66 C66	3.2873	-2.6218	-1.3039 C
67 H67	2.7316	-3.5293	-1.5178 H

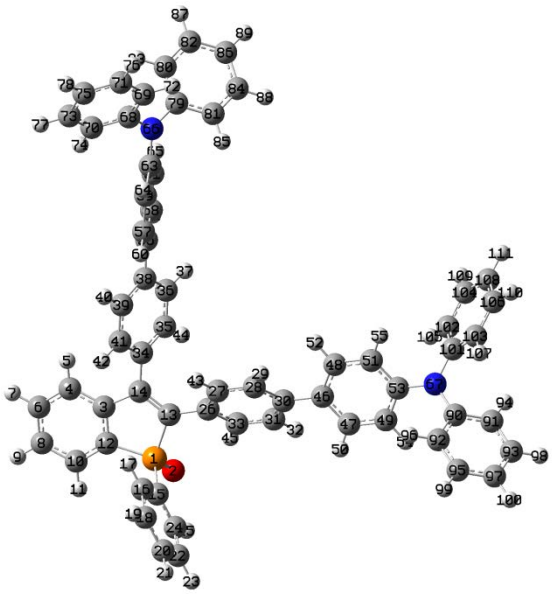


1 P1	-3.0037	7.3564	-1.8485 P
2 O2	-4.6895	7.5248	-4.1338 O
3 C3	1.9717	7.5162	-1.4588 C

4	C4	4.4253	8.4911	-1.5016 C
5	H5	6.0386	7.2563	-1.2322 H
6	C6	4.7913	11.0774	-1.9169 C
7	H7	6.7012	11.8291	-1.9488 H
8	C8	2.7456	12.6930	-2.3086 C
9	H9	3.0620	14.6925	-2.6421 H
10	C10	0.2808	11.7270	-2.2882 C
11	H11	-1.3226	12.9642	-2.6220 H
12	C12	-0.0831	9.1655	-1.8558 C
13	C13	-1.3072	4.3757	-1.2670 C
14	C14	1.2322	4.8158	-1.1226 C
15	C15	4.7067	8.1160	1.0611 C
16	C16	3.5577	8.0748	3.4485 C
17	H17	1.5757	7.5708	3.6290 H
18	C18	4.9547	8.6791	5.5970 C
19	H19	4.0581	8.6449	7.4431 H
20	C20	7.5060	9.3266	5.3758 C
21	H21	8.5918	9.7966	7.0534 H
22	C22	8.6569	9.3691	3.0045 C
23	H23	10.6395	9.8710	2.8305 H
24	C24	7.2626	8.7649	0.8477 C
25	H25	8.1262	8.7856	-1.0129 H
26	C26	2.7109	1.9997	-0.9295 C
27	C27	2.0064	0.1637	0.8642 C
28	C28	3.3938	-2.0406	1.1791 C
29	H29	2.8044	-3.4259	2.5702 H
30	C30	5.5701	-2.4942	-0.2771 C
31	C31	6.3064	-0.6608	-2.0496 C
32	H32	7.9915	-0.9636	-3.1761 H
33	C33	4.9052	1.5376	-2.3663 C
34	C34	3.2014	2.8432	-0.8065 C
35	C35	3.3854	0.8236	-2.5195 C
36	C36	5.2363	-1.0205	-2.2630 C
37	H37	5.3609	-2.5373	-3.6354 H

38	C38	6.9594	-0.9404	-0.2414 C
39	C39	6.7805	1.0660	1.4887 C
40	H40	8.0762	1.1546	3.0741 H
41	C41	4.9525	2.9321	1.1869 C
42	H42	4.8471	4.4531	2.5614 H
43	H43	-0.3479	0.4692	2.0281 H
44	H44	2.0757	0.7255	-4.0946 H
45	H45	-5.5166	2.9388	-3.7348 H
46	N46	-6.9900	-4.7421	0.0449 N
47	C47	-8.0828	-5.9649	-2.0873 C
48	C48	-6.6909	-6.2661	-4.3254 C
49	C49	-10.5654	-6.8932	-1.9792 C
50	C50	-7.7731	-7.4543	-6.4108 C
51	H51	-4.7682	-5.5608	-4.4165 H
52	C52	-11.6190	-8.1096	-4.0633 C
53	H53	-11.6547	-6.6557	-0.2590 H
54	C54	-10.2370	-8.3915	-6.2929 C
55	H55	-6.6710	-7.6695	-8.1292 H
56	H56	-13.5431	-8.8156	-3.9485 H
57	H57	-11.0693	-9.3271	-7.9178 H
58	C58	-7.3639	-5.7702	2.4999 C
59	H59	-7.9225	-4.1890	4.5565 H
60	C60	-7.1922	-8.3877	2.8998 C
61	C61	8.2797	-5.2103	6.9569 C
62	H62	-8.0744	-2.1664	4.2592 H
63	C63	-7.5876	-9.3936	5.3006 C
64	H64	-6.7535	-9.6192	1.3207 H
65	C65	-8.1239	-7.8154	7.3459 C
66	H66	-8.7116	-3.9593	8.5261 H
67	H67	-7.4494	-11.4233	5.5750 H
68	H68	-8.4181	-8.6046	9.2166 H
69	N69	8.8273	-2.8337	0.0422 N
70	C70	8.2657	-5.3970	-0.5543C
71	C71	10.0173	-6.8749	-1.8896 C

72	C72	5.9663	-6.4868	0.1956 C
73	C73	9.4795	-9.3920	-2.4446 C
74	H74	11.7936	-6.0402	-2.4819 H
75	C75	5.4311	-8.9955	-0.3991 C
76	H76	4.6080	-5.3598	1.2383 H
77	C77	7.1837	-10.4666	-1.7127 C
78	H78	10.8560	-10.5096	-3.4789 H
79	H79	3.6422	-9.8089	0.1938 H
80	H80	6.7656	-12.4244	-2.1606 H
81	C81	11.2797	-2.1951	0.9459 C
82	C82	12.5464	-0.0588	0.0138 C
83	C83	12.4705	-3.7047	2.7729 C
84	C84	14.9432	0.5591	0.9120 C
85	H85	11.6427	1.1042	-1.4125 H
86	C86	14.8820	-3.0910	3.6340 C
87	H87	11.4967	-5.3542	3.5031 H
88	C88	16.1298	-0.9539	2.7190 C
89	H89	15.8985	2.2179	0.1707 H
90	H90	15.7774	-4.2790	5.0483 H
91	H91	18.0034	-0.4749	3.4036 H



1	P1	-3.8394	10.8485	-1.9113 P
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3	C3	1.1244	11.1483	-1.4348 C
4	C4	3.5477	12.1954	-1.4089 C
5	H5	5.1939	11.0003	-1.1606 H
6	C6	3.8399	14.8047	-1.7288 C
7	H7	5.7260	15.6142	-1.7090 H
8	C8	1.7503	16.3700	-2.0912 C
9	H9	2.0094	18.3887	-2.3504 H
10	C10	-0.6843	15.3307	-2.1395 C
11	H11	-2.3196	16.5310	-2.4522 H
12	C12	-0.9757	12.7456	-1.8041 C
13	C13	-2.0577	7.9047	-1.3969 C
14	C14	0.4621	8.4166	-1.2005 C
15	C15	-5.6244	11.4606	0.9823 C
16	C16	-4.5283	11.3590	3.3928 C
17	H17	-2.5401	10.8918	3.6020 H
18	C18	-5.9867	11.8550	5.5280 C
19	H19	-5.1319	11.7731	7.3922 H
20	C20	-8.5464	12.4541	5.2702 C
21	H21	-9.6802	12.8388	6.9376 H
22	C22	-9.6446	12.5560	2.8758 C
23	H23	-11.6338	13.0193	2.6739 H
24	C24	-8.1891	12.0597	0.7321 C
25	H25	-9.0116	12.1266	-1.1459 H
26	C26	-3.3816	5.4675	-1.1752 C
27	C27	-2.6533	3.6097	0.5842 C
28	C28	-3.9741	1.3508	0.7896 C
29	H29	-3.4046	-0.0125	2.2134 H
30	C30	-6.0790	0.8319	-0.7496 C
31	C31	-6.8104	2.6965	-2.4937 C
32	H32	-8.3977	2.3431	-3.7448 H
33	C33	-5.5082	4.9700	-2.6968 C
34	C34	2.4901	6.4945	-0.9234 C

35	C35	2.7731	4.5630	-2.7198 C
36	C36	4.6802	2.7706	-2.4864 C
37	H37	4.8199	1.2738	-3.8825 H
38	C38	6.3874	2.8243	-0.4501 C
39	C39	6.0976	4.7616	1.3437 C
40	H40	7.4098	4.8886	2.9160 H
41	C41	4.1954	6.5644	1.1091 C
42	H42	4.0253	8.0408	2.5251 H
43	H43	-1.0646	3.9622	1.8296 H
44	H44	1.4722	4.4683	-4.3023 H
45	H45	-6.1113	6.3773	-4.0624 H
46	C46	-7.4811	-1.5807	-0.5227 C
47	C47	-10.1132	-1.6884	-0.8668 C
48	C48	-6.2362	-3.8565	0.0503 C
49	C49	-11.4372	-3.9482	-0.6650 C
50	H50	-11.1498	0.0339	-1.2767 H
51	C51	-7.5458	-6.1214	0.2889 C
52	H52	-4.1987	-3.8603	0.2929 H
53	C53	-10.1738	-6.2059	-0.0717 C
54	H54	-13.4673	-3.9718	-0.9463 H
55	H55	-6.5335	-7.8455	0.7405 H
56	C56	8.4165	0.9113	-0.2095 C
57	C57	9.1968	0.0095	2.1644 C
58	C58	9.6402	-0.0801	-2.3489 C
59	C59	11.0849	-1.8012	2.3975 C
60	H60	8.2517	0.6768	3.8593 H
61	C61	11.5521	-1.8677	-2.1369 C
62	H62	9.1413	0.6183	-4.2127 H
63	C63	12.3033	-2.7685	0.2454 C
64	H64	11.6118	-2.4953	4.2526 H
65	H65	12.4908	-2.5640	-3.8205 H
66	N66	14.2361	-4.6067	0.4702 N
67	N67	-11.5198	-8.5136	0.1593 N
68	C68	16.0127	-4.4663	2.4836 C

69	C69	16.7312	-6.6578	3.7950 C
70	C70	17.0826	-2.1403	3.1800 C
71	C71	18.4929	-6.5190	5.7469 C
72	H72	15.9048	-8.4594	3.2718 H
73	C73	18.8164	-2.0162	5.1578 C
74	H74	16.5492	-0.4421	2.1632 H
75	C75	19.5396	-4.2009	6.4485 C
76	H76	19.0282	-8.2333	6.7411 H
77	H77	19.6269	-0.2015	5.6712 H
78	H78	20.9016	-4.0985	7.9791 H
79	C79	14.4156	-6.6035	-1.3232 C
80	C80	16.7743	-7.3218	-2.3016 C
81	C81	12.2397	-7.8871	-2.1333 C
82	C82	16.9452	-9.2914	-4.0408 C
83	H83	18.4612	-6.3303	-1.6903 H
84	C84	12.4263	-9.8305	-3.8999 C
85	H85	10.4130	-7.3513	-1.3724 H
86	C86	14.7764	-10.5520	-4.8583 C
87	H87	18.7851	-9.8233	-4.7795 H
88	H88	10.7241	-10.8039	-4.5070 H
89	H89	14.9156	-12.0767	-6.2237 H
90	C90	-13.9288	-8.5563	1.3506 C
91	C91	-15.9071	-10.0023	0.3325 C
92	C92	-14.3652	-7.1584	3.5636 C
93	C93	-18.2582	-10.0560	1.5162 C
94	H94	-15.5871	11.0785	-1.3825 H
95	C95	-16.7336	-7.1966	4.7130 C
96	H96	12.8427	-6.0464	4.3684 H
97	C97	-18.6923	-8.6496	3.7060 C
98	H98	-19.7671	-11.1850	0.7021 H
99	H99	-17.0375	-6.1027	6.4233 H
100	H100	-20.5312	-8.6850	4.6147 H
101	C101	-10.4608	-10.7930	-0.7929 C
102	C102	-9.2508	-10.8347	-3.1541 C

103	C103	-10.6150	-13.0383	0.6126 C
104	C104	-8.2068	-13.0709	-4.0718 C
105	H105	-9.1371	-9.1105	-4.2572 H
106	C106	-9.5965	-15.2726	-0.3377 C
107	H107	-11.5362	-13.0178	2.4439 H
108	C108	-8.3792	-15.3049	-2.6783 C
109	H109	-7.2782	-13.0685	-5.9025 H
110	H110	-9.7340	-16.9922	0.7750 H
111	H111	-7.5764	-17.0467	-3.4065 H

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