Supporting Information

for

A novel π-conjugated poly(phenyl diimide) with full utilization of carbonyls as highly stable organic electrode for Li-ion batteries

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Experimental Section

1. Materials and instrumentation

THF and toluene were distilled from sodium/ benzophenone prior to use. Ac_2O was distilled from phosphorus pentoxide under reduced pressure. Other solvents were purchased and were used without further purification. Sodium periodate (99%), tris(dibenzylideneacetone)dipalladium ($Pd_2(dba)_3$) (98%) and triotolylphosphine (P(o-tolyl)$_3$, 97%) were purchased from Energy Chemical Inc. and used as received. Sodium acetate (98.5%) purchased from TCI Chemicals. If no other special indicated, other reagents and solvents were used as commercially available without further purification. Column chromatographic purification of products was accomplished using 200-300 mesh silica gel.

BET test:

Analysis Report

Operator: operator Date:7/23/2020 Operator: operator Date:2020/07/23

Sample ID: 2 Filename: QW2_200723_01_jun2.QPS

Sample Desc: Comment:

Sample weight: 0. 3600 g

Analysis Time: 269.7 min End of run: 7/23/2020 4:08:11

Instrument: QuadraSorb Station 2

Void Vol.: He Mode.Cell: 9mm large bulbRun mode Standard

Instrument version:5.13

Thermal delay: 180 sec He evac time: 3 min

Outgas Time: 5.0 hrs OutgasTemp: 200.0 C

Analysis gas: Nitrogen Bath Temp: 77.3 K

Press. Tolerance:0.050/0.050 (ads/des)Equil time: 30/30 sec (ads/des) Equil timeout: 300/300 sec (ads/des)

Data Reduction Parameters

Adsorbate Nitrogen Temperature 77.350K

BET summary

Slope = 64.276

Intercept = 5.716e+01

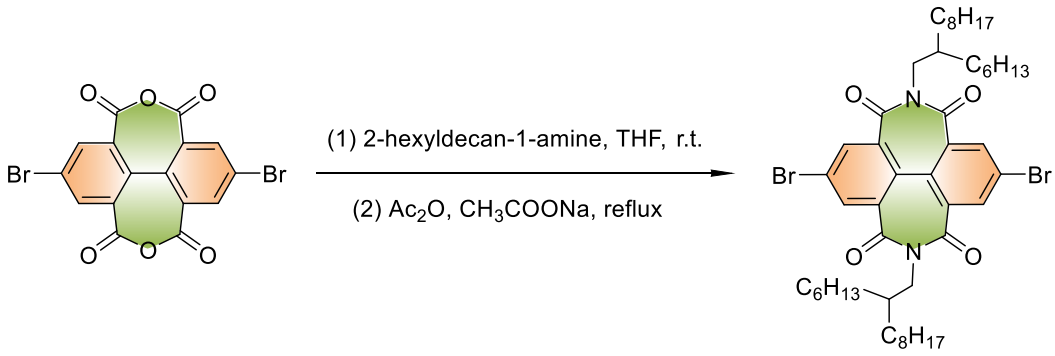
Correlation coefficient, r = 0.997828

C constant= 2.124

Surface Area = 28.677 m^2/g

2. Synthetic procedures

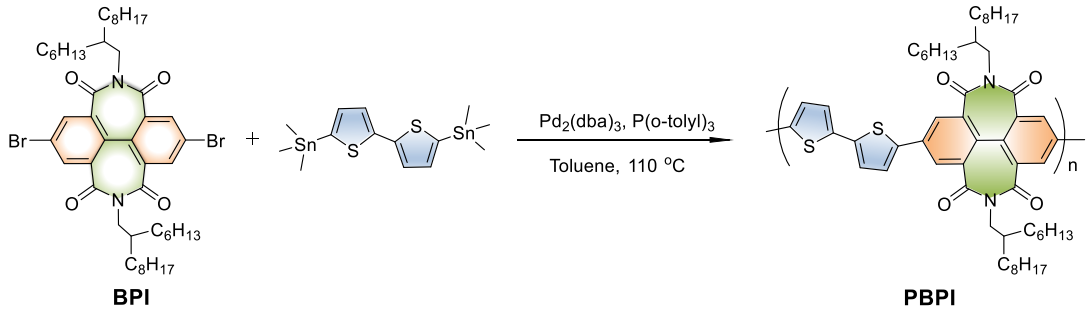
Synthesis of **BPI**



4 **BPI**

To a solution of compound **4** [1] (0.452 g, 1 mmol) in dry THF (20mL) was added 2-hexyldecan-1-amine (0.388 g, 1.5 mmol) at room temperature under nitrogen and stirred overnight. After the solvent was removed under reduced pressure, anhydrous sodium acetate (0.33 g, 10 mmol) and acetic anhydride (5 mL) were added, then the resulting mixture was heated to reflux for another 4 hours. After cooling to room temperature, the mixture continued to stir at this temperature for several hours. The reaction mixture was diluted with water and thoroughly extracted with dichloromethane. The combined organic phases were washed with water and dried over Na_2SO_4. After concentrated under reduced pressure, the residue was purified by column chromatography on silica gel with dichloromethane/ hexane (1:2) to give **BPI** as colorless oil (403 mg, 45% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.97 (s, 4H), 4.11 (m, J = 11.2 Hz, 2H), 3.76 (m, J = 9.3 Hz, 2H), 1.90 (m, 4H), 1.24 (m, 48H), 0.87 (t, J = 3.8 Hz, 12H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.32, 153.25, 149.37, 142.46, 138.23, 130.34, 124.05, 118.62, 116.07, 49.75, 36.96, 31.43, 29. 68, 29.47, 29.28. FT-IR (KBr, cm^{-1}) ν 3253, 3026, 2928, 2906, 2863, 1712, 1661, 1567, 1479,1386, 1329, 1172, 943, 916, 854, 772, 746, 724. Anal. Calcd for $C_{48}H_{70}Br_2O_4N_2$: C, 64.14; H, 7.85; N, 3.12 Found: C, 64.22; H, 7.80 N, 3.08. HRMS (MALDI-FT) (m/z): $(M^+H)^+$ Calcd for $C_{48}H_{71}Br_2O_4N_2$ 898.3682; Found, 899.3745.

Synthesis of **PBPI**



BPI **PBPI**

2,5-Bis(trimethylstannyl)thiophene [2] (123mg, 0.250 mmol) and **BPI** (0.225 g, 0.250 mmol) were placed in a 50 mL two-necked flask purged by argon gas. After dissolving in deoxidized toluene (10 mL), argon bubbling was conducted for 30 min. $Pd_2(dba)_3$ (13.7 mg, 0.0150 mmol) and P(o-Tolyl)$_3$ (38.0 mg, 0.125 mmol) were then added to start the polymerization and the solution was stirred at 110 °C for 72 h. The reaction was then quenched with a 5M HCl solution (2 mL). The solution was extracted with chloroform and washed with water and KF(aq), and then precipitated in 200 mL of methanol. The precipitate was purified by Soxhlet extraction using acetone to remove the residual monomer and then extracted with chloroform. After evaporating the chloroform, the resulting solid was collected and dried overnight under vacuum to afford **PBPI** as an orange solid (150 mg, 64%), ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.05 (s, 4H), 7.43 (s, 2H), 7.26 (s, 2H), 4.19 (s, 2H), 3.85 (s, 2H), 2.01 (s, 2H), 1.24 (d, 48H), 0.85 (s,12H). Mn = 2.03 × 104, Mw = 5.09 × 104, PDI = 2.50 by GPC. FT-IR (KBr, cm^{-1}) ν 2968, 2901, 2360, 1705, 1653, 1594, 1449, 1394, 1316, 1264, 1123, 1066, 902, 788, 771, 712.

3. TGA and DSC curves for PBPI.

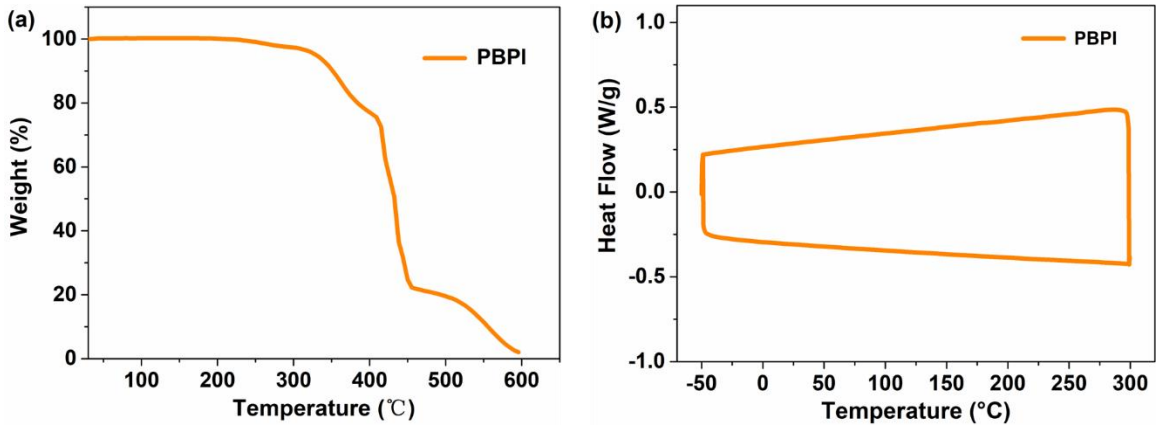


Fig. S1. (a) TGA measurements and (b) DSC measurements for **PBPI**.

4. UV-vis absorption and fluorescence emission spectra for PBPI.

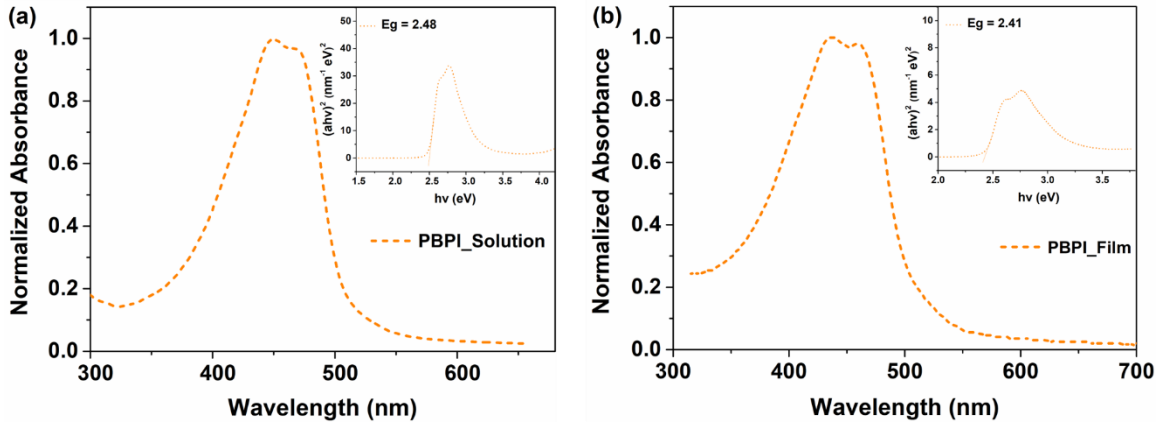


Fig. S2. UV-vis absorption of **PBPI** dissolved in DCM (5×10^{-5} M) and in film state.

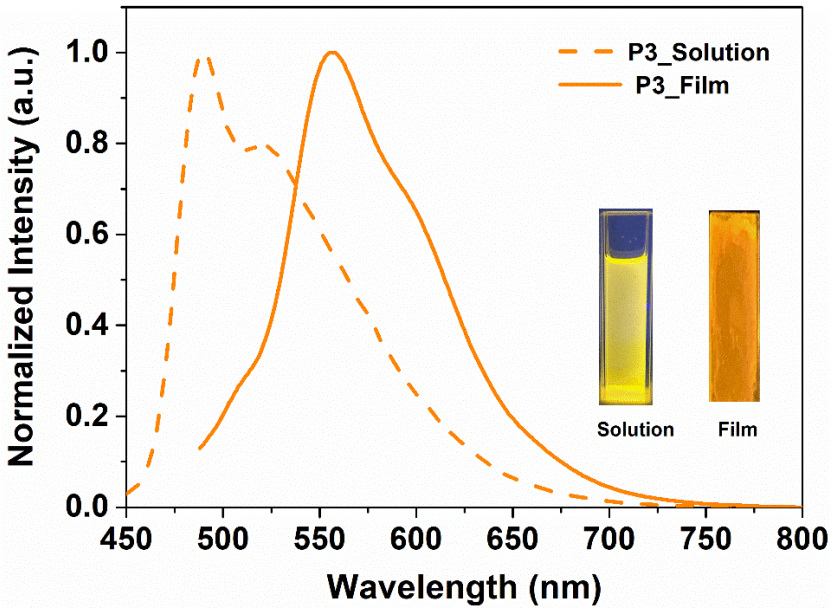


Fig. S3. Fluorescence Emission spectrum of **PBPI** dissolved in DCM (5×10^{-5} M) and in film state.

5. Cyclic voltammograms in THF for PBPI

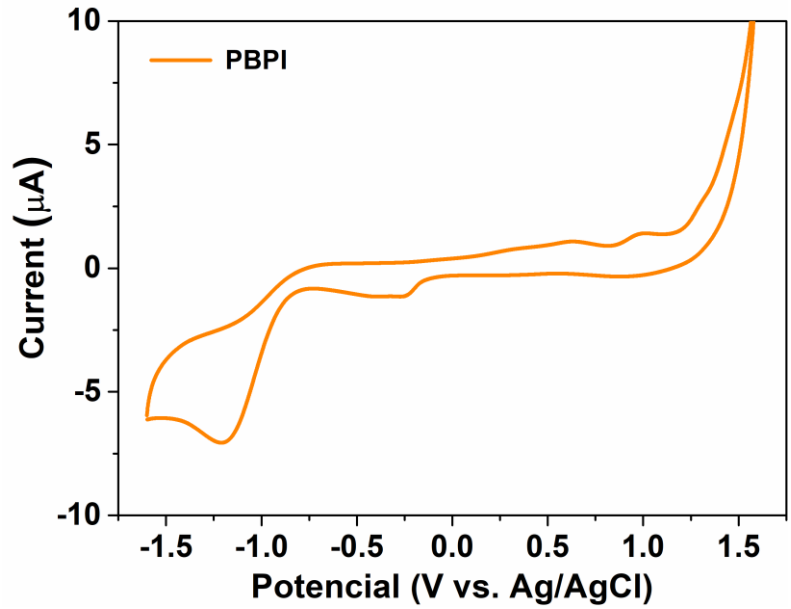


Fig. S4. Cyclic voltammograms of **PBPI** dissolved in THF (0.1 M $Bu_4^+NPF_6^-$ as supporting electrolyte; Ag/AgCl as a reference electrode; scan rate of 50 mV s^{-1}).

Table S1. Optical electrochemical and DFT calculation data of **PBPI**.

polymers	Mn[a] (kD)	λ_{abs} (nm)		λ_{em} (nm)		LUMO[d] (eV)	HOMO[e] (eV)	Eg[f] (eV)	LUMO[g] (eV)	HOMO[g] (eV)
		Sol[b]	Film[c]	Sol[b]	Film[c]					
PBPI	20.3	450, 469	440, 463	489	558	-2.81	-5.29	2.48	-2.17	-5.56

[a]GPC versus polystyrene standards in TCB stabilised with 0.0125% BHT as eluent. [b]Solution absorption spectra in dichloroform. [c]Thin film absorption spectra from spin-cast from dichloroform solution. [d]Cyclic voltammetry determined with Fc/Fc^+ as an internal reference (LUMO = −4.7 − ($E_{1/2}^{red}$ − $E_{1/2}^{red}$ Fc/Fc^+). [e]Estimated from HOMO = LUMO − *E*opt. [f]Optical energy gap estimated from the absorption onset of Solutions. [g]Estimated from DFT calculation.

5. Electrochemical results.

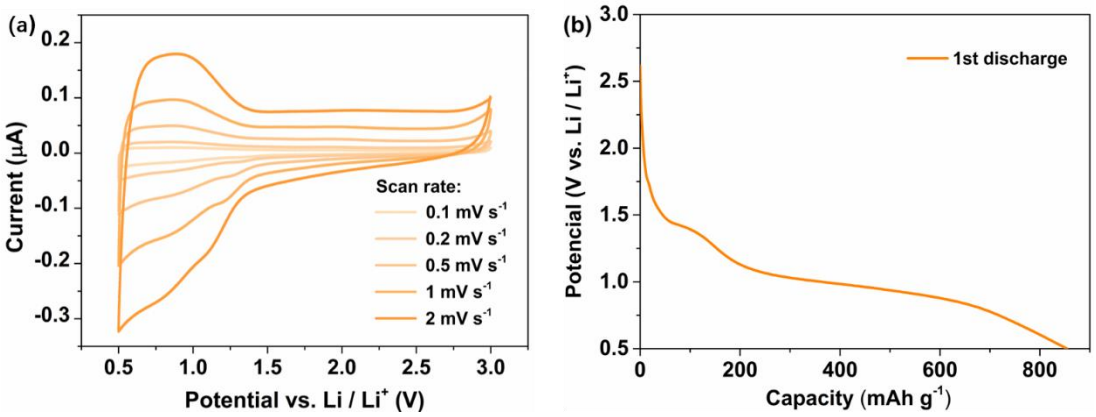


Fig. S5. (a) Cyclic voltammetry at different scan rates of the **PBPI** electrode. (b) The first cycle galvanostatic discharge curve of the **PBPI** electrode.

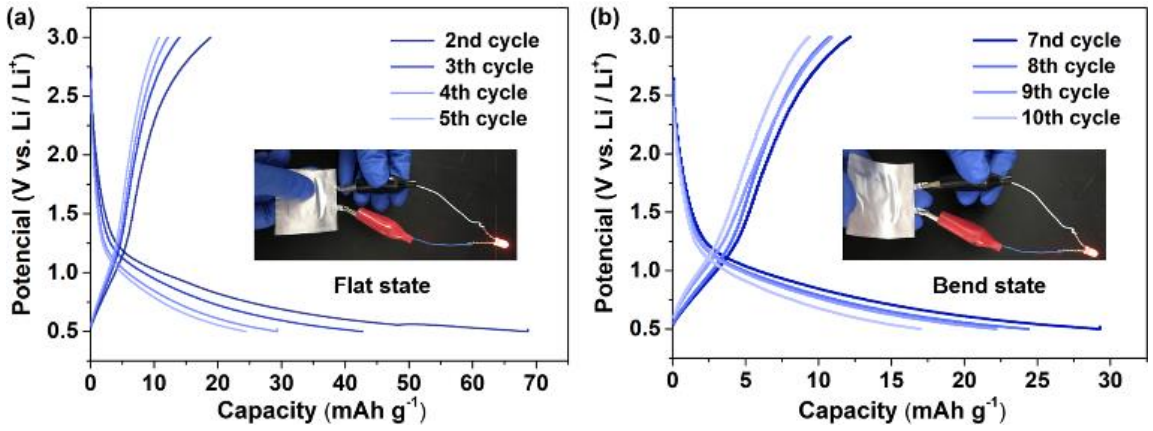


Fig. S6. Charge/discharge curves and digital photos of the flexible LIB lightening a LED under various states (insertion) of the battery in the flat and bend state .

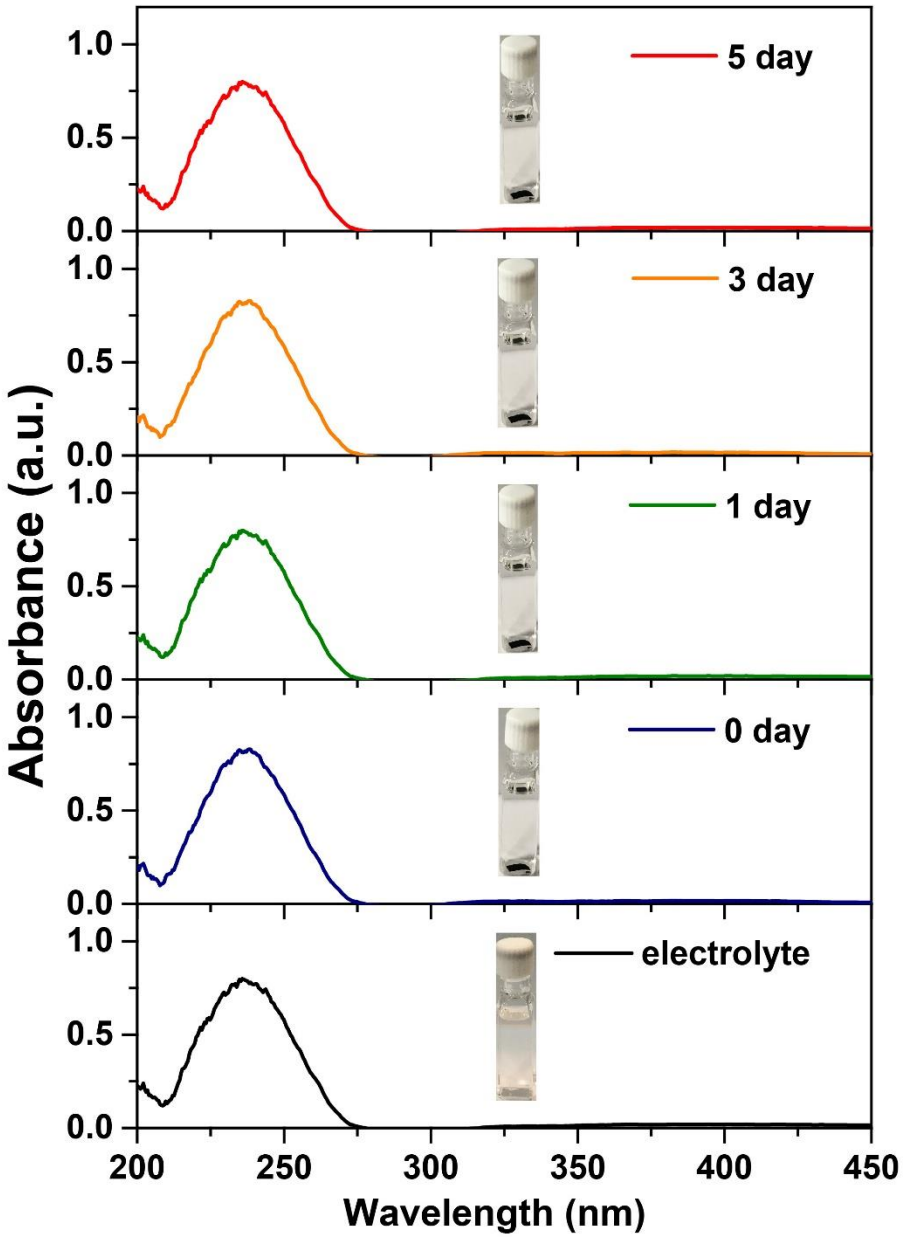


Fig. S7. Solubility test of **PBPI** electrode in electrolyte.

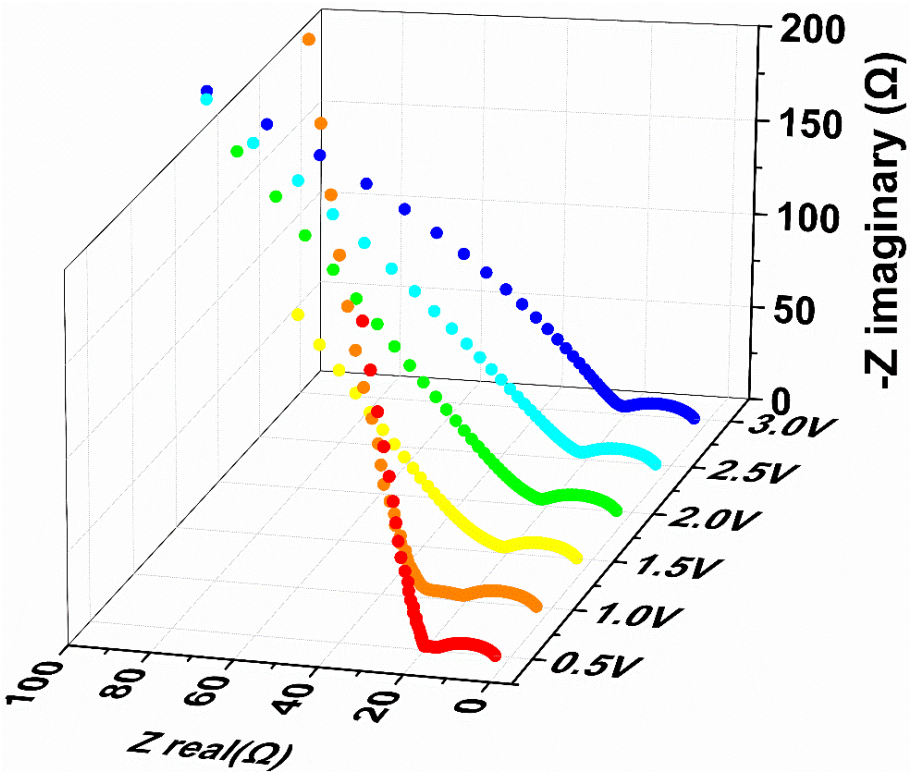


Fig. S8. Electrochemical impedance spectroscopy at various potential of **PBPI** electrode.

7. ^{1}H NMR and ^{13}C NMR of BPI and PBPI.

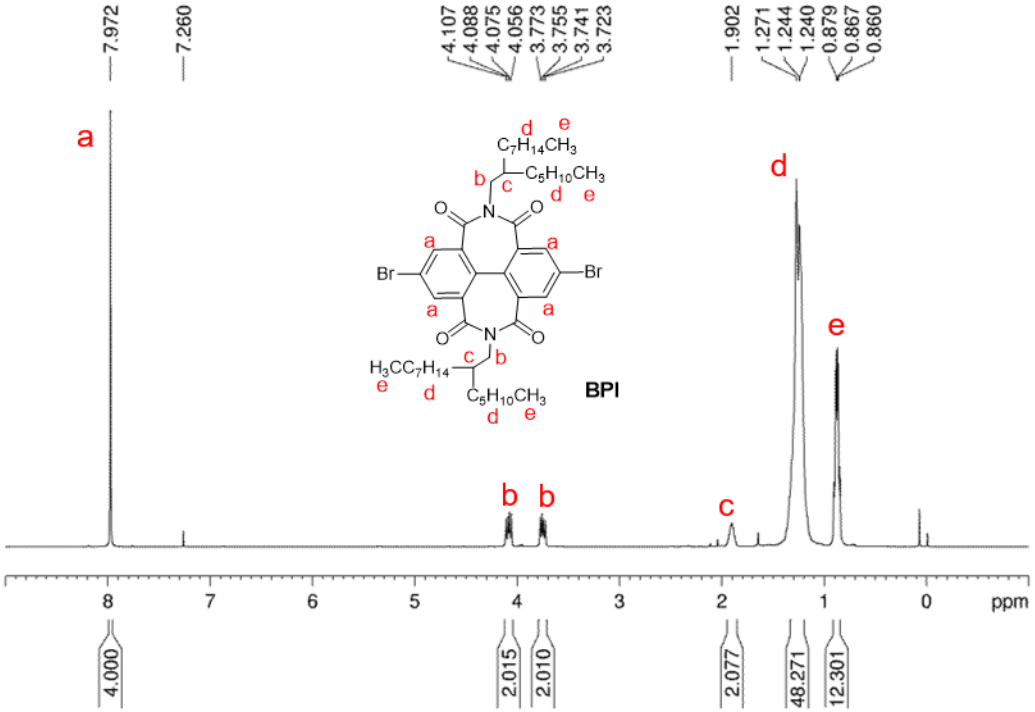


Fig. S9. ^{1}H NMR spectrum of **BPI** (400M Hz, $CDCl_3$)

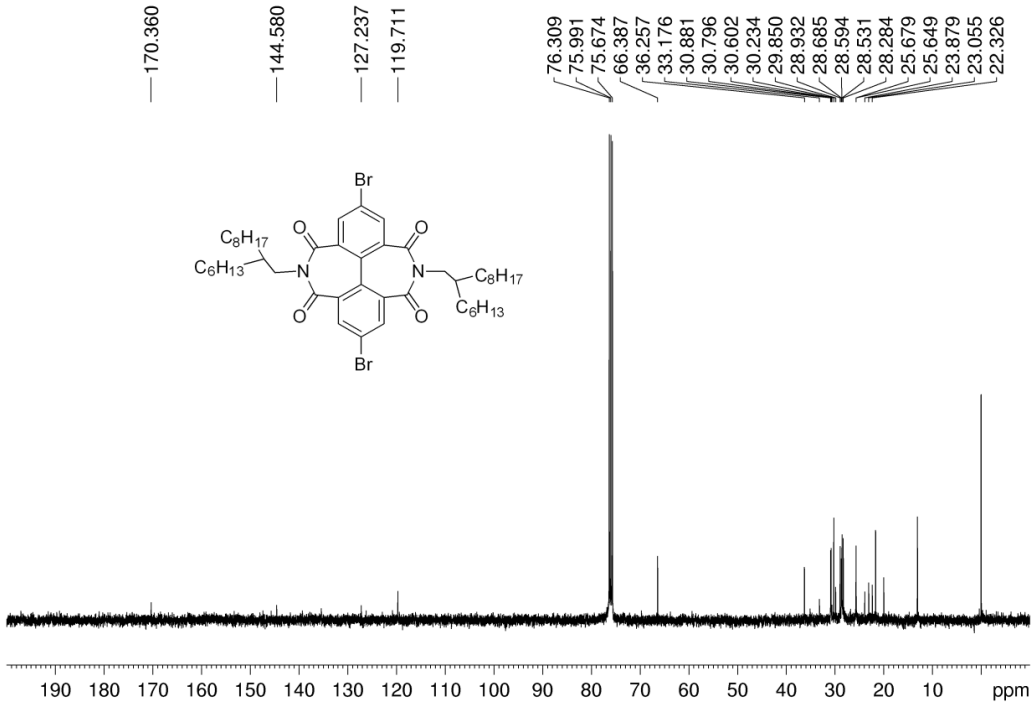


Fig. S10. ^{13}C NMR spectrum of **BPI** (100M Hz, $CDCl_3$)

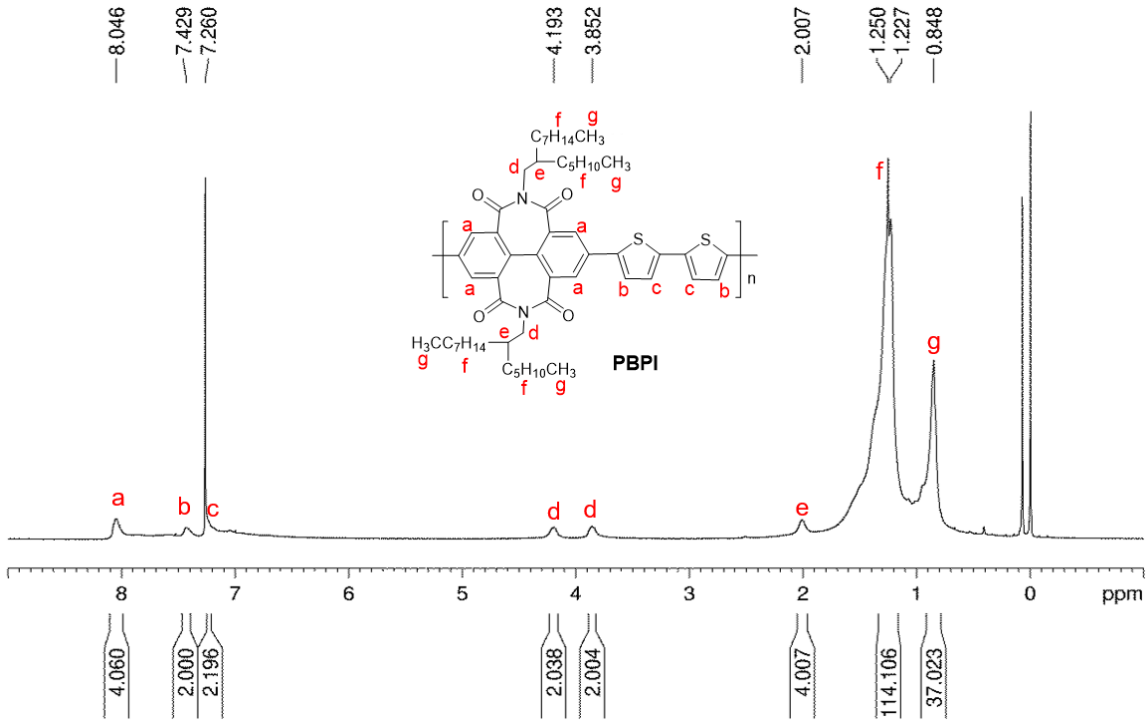


Fig. S11. ^{1}H NMR spectrum of **PBPI** (400M Hz, $CDCl_3$)

8. DFT computations

The HOMO and LUMO energy levels of the compounds studied in this work were calculated using density functional theory (DFT) at the B3LYP/6-31G(d) level of theory with the Gaussian09 package. All of the geometries were optimized followed by harmonic frequencies at the same level of theory to verify that these stationary points were local minima. And the moleculars, **PBPI-unit** and **PBPI-unit-1** orbitals were extracted from the output using Gauss View 5 and assuming an isovalue of 0.05. Meanwhile, the structures of were studied and fully optimized in the dichloromethane without symmetry constraints.

Table S2. Comparison of HOMO/LUMO energy levels of **PBPI-unit** in CH_2Cl_2 solution. (DFT, B3LYP/6-31g*)

compound	**HOMO**		**LUMO**		**gap**
	hartree	eV	hartree	eV	eV
PBPI-unit	-0.20428	-5.56	-0.07981	-2.17	3.39
PBPI-unit-1	-0.20505	-5.58	-0.07937	-2.16	4.42

Table S1X. Cartesian coordinates of optimized geometry of **PBPI-unit** in CH_2Cl_2 solution (DFT, B3LYP/6-31g*)

Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.331144	-0.407895	-2.267516
2	6	0	0.872075	-1.691756	-2.640153
3	6	0	1.713451	-2.582202	-3.322654
4	6	0	2.986879	-2.198194	-3.720819
5	6	0	3.442868	-0.929016	-3.389291
6	6	0	2.650063	-0.052558	-2.635169

7	6	0	0.462140	0.537246	-1.539563
8	6	0	-0.910550	0.664858	-1.851896
9	6	0	-1.710438	1.612592	-1.207730
10	6	0	-1.223336	2.407093	-0.162749
11	6	0	0.123170	2.238660	0.186025
12	6	0	0.963724	1.367459	-0.510507
13	1	0	1.340707	-3.574185	-3.550037
14	1	0	4.430535	-0.601575	-3.692454
15	1	0	-2.736861	1.716015	-1.541201
16	1	0	0.543774	2.791930	1.016621
17	6	0	2.382964	1.426125	-0.010991
18	6	0	3.374306	1.216920	-2.284949
19	8	0	2.605217	1.524506	1.187675
20	8	0	4.107794	1.755837	-3.100987
21	6	0	-1.687438	-0.148553	-2.851714
22	6	0	-0.488537	-2.275578	-2.377303
23	8	0	-0.595567	-3.445284	-2.037190
24	8	0	-2.533329	0.381576	-3.557309
25	7	0	3.409107	1.613528	-0.940295
26	7	0	-1.615780	-1.544229	-2.765826
27	6	0	-4.019164	-2.210691	-2.230166
28	1	0	-4.298187	-1.150136	-2.154788
29	6	0	5.886588	1.471917	-0.352449
30	1	0	6.105901	1.051607	-1.344339
31	6	0	-3.646742	-2.716132	-0.822204
32	1	0	-3.354888	-3.773740	-0.891179
33	1	0	-2.752659	-2.178281	-0.479876
34	6	0	-4.737809	-2.558854	0.245797
35	1	0	-5.621962	-3.150812	-0.026784
36	1	0	-5.067857	-1.509863	0.280428
37	6	0	5.653500	0.305459	0.627662
38	1	0	4.763612	-0.251324	0.305131
39	1	0	5.407974	0.717432	1.616557
40	6	0	-5.211367	-2.977126	-2.865572
41	1	0	-5.018516	-3.135810	-3.936530
42	1	0	-5.272050	-3.982168	-2.424582
43	6	0	-6.570443	-2.272322	-2.734374
44	1	0	-6.791685	-2.075949	-1.677133
45	1	0	-6.509140	-1.287417	-3.220145

46	6	0	7.069201	2.393922	0.050574
47	1	0	6.807436	3.441084	-0.159924
48	1	0	7.216702	2.339318	1.138529
49	6	0	8.393489	2.090368	-0.667126
50	1	0	8.685221	1.046360	-0.493492
51	1	0	8.240092	2.187230	-1.751990
52	6	0	6.813683	-0.690552	0.765720
53	1	0	7.696182	-0.188846	1.185025
54	1	0	7.108808	-1.052721	-0.230429
55	6	0	-4.265371	-2.986531	1.642292
56	1	0	-3.377651	-2.399226	1.920325
57	1	0	-3.936570	-4.035897	1.607736
58	6	0	-5.336998	-2.827124	2.728502
59	1	0	-6.226170	-3.412956	2.451326
60	1	0	-5.663458	-1.776990	2.763728
61	6	0	-4.862260	-3.256204	4.122929
62	1	0	-3.968119	-2.675890	4.395576
63	1	0	-4.542775	-4.308573	4.089316
64	6	0	-5.926792	-3.085642	5.214264
65	1	0	-6.821964	-3.665691	4.943701
66	1	0	-6.245830	-2.033056	5.248928
67	6	0	-5.450204	-3.513859	6.608232
68	1	0	-4.554847	-2.935397	6.877285
69	1	0	-5.133747	-4.566248	6.574944
70	6	0	-6.517232	-3.336502	7.693496
71	1	0	-6.145923	-3.650553	8.675953
72	1	0	-6.828804	-2.287603	7.774397
73	1	0	-7.412087	-3.930618	7.469596
74	6	0	-7.724948	-3.071500	-3.352455
75	1	0	-7.505630	-3.266374	-4.412973
76	1	0	-7.783210	-4.057698	-2.867971
77	6	0	-9.084919	-2.371089	-3.237051
78	1	0	-9.303789	-2.175237	-2.176578
79	1	0	-9.029142	-1.385420	-3.722974
80	6	0	-10.241009	-3.171356	-3.850822
81	1	0	-10.295151	-4.156980	-3.366755
82	1	0	-10.024353	-3.364655	-4.911186
83	6	0	-11.596240	-2.467211	-3.727215
84	1	0	-12.400304	-3.064119	-4.173130

85	1	0	-11.855698	-2.290253	-2.675940
86	1	0	-11.583926	-1.493587	-4.232884
87	6	0	6.453768	-1.891003	1.652101
88	1	0	5.573159	-2.398380	1.230974
89	1	0	6.149094	-1.529212	2.645378
90	6	0	7.593479	-2.905864	1.810268
91	1	0	8.470873	-2.404118	2.244839
92	1	0	7.906085	-3.258949	0.816126
93	6	0	7.216880	-4.112873	2.679355
94	1	0	6.337161	-4.610362	2.244479
95	1	0	6.905412	-3.760100	3.673886
96	6	0	8.348841	-5.136260	2.837034
97	1	0	9.227760	-4.642595	3.278165
98	1	0	8.664091	-5.486267	1.842510
99	6	0	7.964461	-6.346464	3.698072
100	1	0	7.085704	-6.838421	3.257155
101	1	0	7.650825	-5.997640	4.692380
102	6	0	9.097789	-7.366562	3.849244
103	1	0	8.791292	-8.217210	4.469048
104	1	0	9.409040	-7.760049	2.873478
105	1	0	9.979303	-6.912360	4.318709
106	6	0	9.538416	3.014539	-0.232873
107	1	0	9.245171	4.061183	-0.404040
108	1	0	9.692873	2.915653	0.852048
109	6	0	10.860478	2.734609	-0.959014
110	1	0	11.154967	1.688340	-0.787523
111	1	0	10.707281	2.833342	-2.044175
112	6	0	12.005826	3.658557	-0.525357
113	1	0	12.158472	3.560700	0.559007
114	1	0	11.712270	4.703823	-0.698285
115	6	0	13.323093	3.371666	-1.253591
116	1	0	14.119798	4.047645	-0.921979
117	1	0	13.660275	2.343677	-1.071085
118	1	0	13.210855	3.494982	-2.338034
119	1	0	3.618555	-2.881628	-4.278997
120	6	0	-2.066006	3.369206	0.545412
121	6	0	-1.677396	4.436743	1.327292
122	16	0	-3.819047	3.273145	0.485615
123	6	0	-2.758100	5.181233	1.859842

124	1	0	-0.639626	4.703480	1.492829
125	6	0	-3.998445	4.695783	1.496359
126	1	0	-2.627212	6.065505	2.474274
127	6	0	-5.312742	5.194990	1.844071
128	6	0	-6.530867	4.914840	1.260078
129	16	0	-5.526442	6.317543	3.180685
130	6	0	-7.623619	5.594611	1.869193
131	1	0	-6.637617	4.254113	0.406141
132	6	0	-7.239784	6.391600	2.913221
133	1	0	-8.651582	5.498918	1.537492
134	1	0	-7.854746	7.018863	3.544513
135	6	0	4.622852	2.346626	-0.497566
136	6	0	-2.820127	-2.299046	-3.197928
137	1	0	-2.505280	-3.335853	-3.318879
138	1	0	-3.104164	-1.897715	-4.172715
139	1	0	4.370881	2.811315	0.456028
140	1	0	4.799159	3.128379	-1.238664

Table S2X. Cartesian coordinates of optimized geometry of **PBPI-unit-1** in CH_2Cl_2 solution (DFT, B3LYP/6-31g*)

Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.495814	-1.575502	-1.106907
2	6	0	1.189403	-2.740477	-0.368869
3	6	0	2.157236	-3.736011	-0.171452
4	6	0	3.407730	-3.643468	-0.767704
5	6	0	3.715261	-2.517727	-1.521997
6	6	0	2.794553	-1.469347	-1.654221
7	6	0	0.493428	-0.519430	-1.343652
8	6	0	-0.854449	-0.839775	-1.626829
9	6	0	-1.776591	0.156889	-1.956471
10	6	0	-1.440020	1.515535	-1.931362
11	6	0	-0.121072	1.835471	-1.584801
12	6	0	0.840995	0.851543	-1.342701
13	1	0	1.900356	-4.593464	0.439718

14	1	0	4.682008	-2.424492	-2.003098
15	1	0	-2.776251	-0.154403	-2.237613
16	1	0	0.181142	2.871492	-1.496178
17	6	0	2.197520	1.444906	-1.056330
18	6	0	3.358724	-0.288320	-2.392200
19	8	0	2.272546	2.467214	-0.386727
20	8	0	4.032656	-0.447991	-3.396599
21	6	0	-1.477789	-2.209619	-1.618641
22	6	0	-0.123489	-3.074144	0.282800
23	8	0	-0.141670	-3.583922	1.394296
24	8	0	-2.315324	-2.511406	-2.456496
25	7	0	3.310225	0.964637	-1.747062
26	7	0	-1.285513	-3.021935	-0.493253
27	6	0	-3.643936	-3.307579	0.434317
28	1	0	-4.024890	-2.594880	-0.311002
29	6	0	5.679465	1.804641	-1.137225
30	1	0	6.362391	2.541791	-1.589480
31	6	0	-3.313243	-2.529731	1.723769
32	1	0	-2.890853	-3.228361	2.459797
33	1	0	-2.516571	-1.806648	1.503486
34	6	0	-4.487700	-1.772783	2.359286
35	1	0	-5.268073	-2.480805	2.669818
36	1	0	-4.950221	-1.113771	1.609513
37	6	0	6.352148	0.422576	-1.269149
38	1	0	6.433773	0.167538	-2.333911
39	1	0	5.696588	-0.336844	-0.818391
40	6	0	-4.718416	-4.410720	0.635427
41	1	0	-4.447050	-5.300867	0.049553
42	1	0	-4.713679	-4.735691	1.685533
43	6	0	-6.140560	-3.996282	0.227074
44	1	0	-6.441718	-3.095574	0.777726
45	1	0	-6.136013	-3.715094	-0.836233
46	6	0	5.438198	2.234181	0.335905
47	1	0	4.457670	2.712786	0.418812
48	1	0	5.391360	1.341756	0.976763
49	6	0	6.496989	3.202465	0.888555
50	1	0	7.497286	2.754623	0.817048
51	1	0	6.521847	4.101241	0.254122
52	6	0	7.742233	0.304031	-0.627760

53	1	0	7.674056	0.483572	0.453436
54	1	0	8.400176	1.088263	-1.030376
55	6	0	-4.063810	-0.936241	3.574496
56	1	0	-3.294199	-0.213223	3.266035
57	1	0	-3.584145	-1.592328	4.316085
58	6	0	-5.225418	-0.186362	4.239465
59	1	0	-5.992627	-0.910107	4.552792
60	1	0	-5.708437	0.466806	3.497419
61	6	0	-4.797122	0.653306	5.450000
62	1	0	-4.032068	1.378675	5.135280
63	1	0	-4.310425	0.000387	6.189932
64	6	0	-5.956400	1.401080	6.121137
65	1	0	-6.721054	0.676479	6.439125
66	1	0	-6.444960	2.053539	5.381860
67	6	0	-5.525461	2.242694	7.329286
68	1	0	-4.761878	2.966866	7.011090
69	1	0	-5.037534	1.591167	8.068284
70	6	0	-6.688149	2.986835	7.994353
71	1	0	-6.347174	3.578899	8.851632
72	1	0	-7.175046	3.671553	7.288684
73	1	0	-7.451829	2.286629	8.355294
74	6	0	-7.181473	-5.099964	0.454820
75	1	0	-6.881114	-6.003160	-0.097187
76	1	0	-7.186022	-5.381008	1.518623
77	6	0	-8.599998	-4.696288	0.032273
78	1	0	-8.899734	-3.792577	0.583820
79	1	0	-8.596101	-4.415582	-1.031632
80	6	0	-9.645603	-5.795674	0.259764
81	1	0	-9.648973	-6.077313	1.322477
82	1	0	-9.348137	-6.698016	-0.293358
83	6	0	-11.059094	-5.380943	-0.162170
84	1	0	-11.782293	-6.185847	0.013264
85	1	0	-11.396701	-4.500683	0.398999
86	1	0	-11.095202	-5.126591	-1.228844
87	6	0	8.387791	-1.068418	-0.864196
88	1	0	8.478737	-1.245227	-1.946146
89	1	0	7.718475	-1.853961	-0.482428
90	6	0	9.766380	-1.218029	-0.207565
91	1	0	9.672418	-1.045127	0.874874

92	1	0	10.435925	-0.430582	-0.584527
93	6	0	10.412241	-2.588993	-0.446674
94	1	0	10.514581	-2.757958	-1.529025
95	1	0	9.737588	-3.376399	-0.078469
96	6	0	11.783971	-2.746328	0.222075
97	1	0	11.681344	-2.579348	1.304855
98	1	0	12.459963	-1.959011	-0.144047
99	6	0	12.429801	-4.117150	-0.017670
100	1	0	12.536593	-4.282418	-1.099309
101	1	0	11.752936	-4.903954	0.345014
102	6	0	13.796308	-4.268056	0.658923
103	1	0	14.230805	-5.256423	0.469204
104	1	0	14.505193	-3.515765	0.291036
105	1	0	13.715536	-4.142131	1.745843
106	6	0	6.232703	3.620398	2.340881
107	1	0	5.232068	4.072406	2.410993
108	1	0	6.206138	2.724034	2.978513
109	6	0	7.272615	4.603750	2.893289
110	1	0	8.272305	4.147691	2.833544
111	1	0	7.306996	5.495855	2.249927
112	6	0	7.001581	5.036916	4.339926
113	1	0	6.964698	4.146390	4.983601
114	1	0	6.004359	5.495984	4.398593
115	6	0	8.046719	6.016860	4.883290
116	1	0	7.823697	6.309084	5.916038
117	1	0	9.049856	5.572561	4.871620
118	1	0	8.083440	6.931488	4.278358
119	1	0	4.136613	-4.437825	-0.643508
120	6	0	-2.407523	2.565668	-2.245752
121	6	0	-2.164403	3.874229	-2.608641
122	16	0	-4.137004	2.267128	-2.198437
123	6	0	-3.336341	4.625977	-2.867884
124	1	0	-1.165531	4.280118	-2.723989
125	6	0	-4.502980	3.906726	-2.699625
126	1	0	-3.325655	5.658150	-3.199307
127	6	0	-5.865832	4.373519	-2.867576
128	6	0	-6.324549	5.672894	-2.796335
129	16	0	-7.192525	3.282329	-3.237360
130	6	0	-7.723295	5.794096	-3.032034

131	1	0	-5.678551	6.511070	-2.559566
132	6	0	-8.330364	4.591616	-3.275527
133	1	0	-8.257324	6.737736	-3.010150
134	1	0	-9.374349	4.390604	-3.474971
135	6	0	-2.383935	-3.966726	-0.164974
136	6	0	4.419694	1.922114	-2.028273
137	1	0	-1.966972	-4.692878	0.533254
138	1	0	-2.642539	-4.475803	-1.095255
139	1	0	3.992601	2.920631	-1.929586
140	1	0	4.691303	1.757895	-3.072195

Table S3X. Cartesian coordinates of optimized geometry of **PBPI-unit-2Li** in CH_2Cl_2 solution (DFT, B3LYP/6-31g*)
Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.204840	-1.445572	-2.587602
2	6	0	-0.013316	-0.455513	-3.666990
3	6	0	-0.357918	-0.934141	-4.942069
4	6	0	-0.719692	-2.260332	-5.169886
5	6	0	-0.908757	-3.091621	-4.055610
6	6	0	-0.569242	-2.693611	-2.762713
7	6	0	1.162679	-1.299053	-1.622136
8	6	0	2.187580	-0.233577	-1.649143
9	6	0	3.476169	-0.531921	-1.227966
10	6	0	3.814542	-1.742601	-0.577361
11	6	0	2.716382	-2.532918	-0.150323
12	6	0	1.412781	-2.293060	-0.557293
13	1	0	-0.354070	-0.231857	-5.774252
14	1	0	-1.383187	-4.061713	-4.173259
15	1	0	4.227535	0.242916	-1.360587
16	1	0	2.890185	-3.335940	0.562672
17	6	0	0.352760	-2.910494	0.232736
18	6	0	-1.012864	-3.565339	-1.698641
19	8	0	0.550235	-3.251826	1.437644
20	8	0	-1.568334	-4.657406	-1.859078
21	6	0	1.943425	1.138657	-2.046163

22	6	0	-0.020505	0.969267	-3.472321
23	8	0	-0.581830	1.763925	-4.294807
24	8	0	2.803462	2.024548	-2.088015
25	7	0	-0.899430	-3.094109	-0.315489
26	7	0	0.565862	1.522393	-2.327887
27	6	0	0.349124	3.272384	-0.527325
28	1	0	1.376729	3.056954	-0.206415
29	6	0	-3.376722	-3.062430	0.152602
30	1	0	-3.555238	-3.422609	-0.868588
31	6	0	-0.611212	2.393842	0.299218
32	1	0	-1.645596	2.627430	0.001099
33	1	0	-0.445487	1.344151	0.023924
34	6	0	-0.488709	2.527810	1.823381
35	1	0	-0.722012	3.555611	2.133292
36	1	0	0.555364	2.348182	2.121736
37	6	0	-3.470114	-1.515638	0.156594
38	1	0	-2.457797	-1.092993	0.108240
39	1	0	-3.896856	-1.177800	1.112977
40	6	0	0.098641	4.793060	-0.336359
41	1	0	0.189065	5.304408	-1.305793
42	1	0	-0.939345	4.956150	-0.011057
43	6	0	1.057624	5.480927	0.647887
44	1	0	1.015775	4.979531	1.624162
45	1	0	2.088492	5.354129	0.286100
46	6	0	-4.414840	-3.742064	1.072512
47	1	0	-4.242400	-4.827983	1.047752
48	1	0	-4.228812	-3.428441	2.111681
49	6	0	-5.887544	-3.479736	0.729574
50	1	0	-6.110995	-2.408750	0.826437
51	1	0	-6.068144	-3.738548	-0.324090
52	6	0	-4.280722	-0.921713	-1.006766
53	1	0	-5.279893	-1.375204	-1.043618
54	1	0	-3.787736	-1.194715	-1.951569
55	6	0	-1.406014	1.560675	2.584772
56	1	0	-1.179172	0.528328	2.277325
57	1	0	-2.449486	1.740276	2.286214
58	6	0	-1.291335	1.673224	4.110591
59	1	0	-1.523497	2.704113	4.416461
60	1	0	-0.247343	1.496565	4.411356

61	6	0	-2.207794	0.703235	4.867968
62	1	0	-1.976895	-0.328786	4.562219
63	1	0	-3.250874	0.881383	4.567017
64	6	0	-2.096241	0.814694	6.393934
65	1	0	-2.329677	1.845238	6.700616
66	1	0	-1.053234	0.637027	6.697004
67	6	0	-3.013217	-0.156127	7.149265
68	1	0	-2.780567	-1.186206	6.842960
69	1	0	-4.055151	0.022550	6.847632
70	6	0	-2.895922	-0.038278	8.672453
71	1	0	-3.562881	-0.743758	9.181403
72	1	0	-1.872142	-0.245729	9.008147
73	1	0	-3.156667	0.971728	9.012388
74	6	0	0.767026	6.975473	0.835722
75	1	0	0.808582	7.479560	-0.141557
76	1	0	-0.263956	7.102065	1.199264
77	6	0	1.733038	7.669698	1.804592
78	1	0	1.693401	7.164432	2.781405
79	1	0	2.763999	7.546199	1.440565
80	6	0	1.442231	9.163536	1.998202
81	1	0	0.411892	9.287292	2.361451
82	1	0	1.483864	9.669390	1.022979
83	6	0	2.410757	9.847187	2.969046
84	1	0	2.176822	10.911779	3.085820
85	1	0	2.366601	9.384967	3.963170
86	1	0	3.446268	9.770117	2.614766
87	6	0	-4.423677	0.603460	-0.928955
88	1	0	-3.423914	1.059902	-0.885113
89	1	0	-4.922072	0.872682	0.014454
90	6	0	-5.206549	1.210208	-2.100758
91	1	0	-6.205163	0.751148	-2.148246
92	1	0	-4.707662	0.944428	-3.045991
93	6	0	-5.354464	2.735024	-2.015744
94	1	0	-4.355934	3.194502	-1.958609
95	1	0	-5.861613	2.996142	-1.075182
96	6	0	-6.126972	3.347392	-3.191153
97	1	0	-7.124374	2.886801	-3.250190
98	1	0	-5.619623	3.091617	-4.134612
99	6	0	-6.279397	4.871270	-3.099648

100	1	0	-5.282941	5.331777	-3.037091
101	1	0	-6.791431	5.126351	-2.161024
102	6	0	-7.047576	5.475049	-4.279878
103	1	0	-7.139380	6.563016	-4.183402
104	1	0	-6.541258	5.266522	-5.230842
105	1	0	-8.060649	5.059391	-4.346946
106	6	0	-6.858726	-4.271242	1.616514
107	1	0	-6.646199	-5.346150	1.517799
108	1	0	-6.674110	-4.020253	2.671867
109	6	0	-8.334751	-4.014783	1.286220
110	1	0	-8.548906	-2.940156	1.387896
111	1	0	-8.518695	-4.262547	0.229995
112	6	0	-9.308851	-4.808217	2.166673
113	1	0	-9.126292	-4.560656	3.222198
114	1	0	-9.095744	-5.881889	2.064671
115	6	0	-10.780145	-4.546019	1.828306
116	1	0	-11.449628	-5.126776	2.473425
117	1	0	-11.032455	-3.485664	1.954304
118	1	0	-11.001258	-4.816876	0.788333
119	1	0	-0.964538	-2.607830	-6.168911
120	6	0	5.168950	-2.092745	-0.206768
121	6	0	5.654776	-3.287254	0.307221
122	16	0	6.504062	-0.942117	-0.362771
123	6	0	7.044667	-3.284451	0.575341
124	1	0	5.028873	-4.160745	0.453948
125	6	0	7.681417	-2.098916	0.269736
126	1	0	7.571580	-4.148534	0.969260
127	6	0	9.074662	-1.743054	0.393534
128	6	0	9.716401	-0.574815	0.030001
129	16	0	10.238328	-2.867122	1.097667
130	6	0	11.114887	-0.577528	0.305408
131	1	0	9.199410	0.262249	-0.427467
132	6	0	11.548540	-1.739955	0.878914
133	1	0	11.770955	0.257052	0.081436
134	1	0	12.548723	-2.012517	1.187410
135	6	0	-1.979129	-3.552676	0.581212
136	6	0	0.254709	2.932698	-2.030089
137	1	0	-0.763216	3.110775	-2.383655
138	1	0	0.919400	3.594957	-2.595068

139	1	0	-1.740047	-3.167873	1.574019
140	1	0	-1.969096	-4.645977	0.639001
141	3	0	-2.089853	1.591245	-5.310815
142	3	0	1.691894	-2.374132	2.617284

Table S4X. Cartesian coordinates of optimized geometry of **PBPI-unit-4Li** in CH_2Cl_2 solution (DFT, B3LYP/6-31g*)

Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.031861	-1.190205	-2.517251
2	6	0	-0.269502	-0.171971	-3.519759
3	6	0	-0.610638	-0.608300	-4.888749
4	6	0	-0.647747	-1.985801	-5.162292
5	6	0	-0.688547	-2.947031	-4.158529
6	6	0	-0.565856	-2.536396	-2.739098
7	6	0	1.021295	-1.003795	-1.560632
8	6	0	1.988387	0.117702	-1.599028
9	6	0	3.339876	-0.172135	-1.334358
10	6	0	3.753956	-1.369828	-0.736322
11	6	0	2.712705	-2.246824	-0.263908
12	6	0	1.390681	-2.050363	-0.609764
13	1	0	-0.322112	0.058416	-5.707634
14	1	0	-0.423165	-3.976350	-4.428399
15	1	0	4.069528	0.603378	-1.560162
16	1	0	2.974926	-3.068348	0.401889
17	6	0	0.333725	-2.701297	0.220681
18	6	0	-0.918906	-3.444190	-1.774332
19	8	0	0.494900	-2.725148	1.482334
20	8	0	-1.445275	-4.628734	-2.010089
21	6	0	1.589178	1.429036	-1.951539
22	6	0	-0.267814	1.205944	-3.242302
23	8	0	-0.646299	2.103297	-4.114512
24	8	0	2.390250	2.390295	-2.250117
25	7	0	-0.797963	-3.148998	-0.346823
26	7	0	0.160175	1.657207	-1.941583

27	6	0	-0.018381	3.318430	-0.072715
28	1	0	1.050450	3.144431	0.123070
29	6	0	-3.289385	-3.094654	0.094305
30	1	0	-3.479436	-3.473825	-0.917926
31	6	0	-0.843330	2.385588	0.845639
32	1	0	-1.811013	2.859281	1.072352
33	1	0	-1.068976	1.469617	0.285244
34	6	0	-0.154803	1.976794	2.157394
35	1	0	0.122713	2.863850	2.741188
36	1	0	0.792231	1.471477	1.912301
37	6	0	-3.351514	-1.548329	0.059913
38	1	0	-2.334195	-1.151071	-0.051405
39	1	0	-3.726462	-1.172398	1.024150
40	6	0	-0.299781	4.820219	0.151915
41	1	0	0.300767	5.393635	-0.570516
42	1	0	-1.351771	5.022791	-0.104289
43	6	0	-0.018501	5.375135	1.554870
44	1	0	-0.679108	4.894912	2.288908
45	1	0	1.009720	5.120028	1.851647
46	6	0	-4.325400	-3.736094	1.043863
47	1	0	-4.164380	-4.824553	1.047871
48	1	0	-4.121858	-3.396884	2.071540
49	6	0	-5.801500	-3.470203	0.718556
50	1	0	-6.014989	-2.395632	0.793700
51	1	0	-6.003117	-3.752196	-0.325683
52	6	0	-4.200024	-0.972406	-1.085804
53	1	0	-5.220270	-1.376377	-1.047274
54	1	0	-3.769374	-1.314245	-2.038317
55	6	0	-1.015740	1.052744	3.029258
56	1	0	-1.302349	0.164667	2.446392
57	1	0	-1.955678	1.566564	3.280166
58	6	0	-0.326599	0.607801	4.325911
59	1	0	-0.033521	1.495640	4.905814
60	1	0	0.612900	0.086854	4.079721
61	6	0	-1.193798	-0.306032	5.201509
62	1	0	-1.491775	-1.190521	4.618817
63	1	0	-2.126546	0.218858	5.455908
64	6	0	-0.501491	-0.760342	6.492809
65	1	0	-0.197830	0.123691	7.073401

66	1	0	0.428837	-1.291893	6.239643
67	6	0	-1.374240	-1.665690	7.371689
68	1	0	-1.677769	-2.548803	6.791558
69	1	0	-2.302652	-1.134832	7.626242
70	6	0	-0.675025	-2.116025	8.658541
71	1	0	-1.324397	-2.759847	9.262993
72	1	0	0.239417	-2.679984	8.435798
73	1	0	-0.390256	-1.255235	9.276404
74	6	0	-0.205873	6.896467	1.641931
75	1	0	0.462252	7.386334	0.917693
76	1	0	-1.230003	7.153733	1.332241
77	6	0	0.057640	7.468996	3.040468
78	1	0	-0.611954	6.981630	3.765039
79	1	0	1.081174	7.211483	3.351974
80	6	0	-0.127861	8.989530	3.126693
81	1	0	-1.150524	9.247093	2.815937
82	1	0	0.541621	9.477022	2.403549
83	6	0	0.136819	9.552988	4.526791
84	1	0	-0.003885	10.639781	4.554887
85	1	0	-0.541485	9.109643	5.266487
86	1	0	1.163319	9.341079	4.851148
87	6	0	-4.265184	0.560039	-1.089041
88	1	0	-3.243067	0.964062	-1.120883
89	1	0	-4.703011	0.909967	-0.142037
90	6	0	-5.072877	1.133104	-2.261303
91	1	0	-6.098996	0.737364	-2.226200
92	1	0	-4.642356	0.768998	-3.207484
93	6	0	-5.122163	2.666347	-2.286713
94	1	0	-4.095177	3.061648	-2.309940
95	1	0	-5.565897	3.030418	-1.348200
96	6	0	-5.909712	3.236712	-3.473259
97	1	0	-6.937313	2.843959	-3.450726
98	1	0	-5.466795	2.871650	-4.413153
99	6	0	-5.955550	4.769890	-3.502131
100	1	0	-4.928474	5.161829	-3.523297
101	1	0	-6.401383	5.135282	-2.566082
102	6	0	-6.739997	5.329603	-4.693401
103	1	0	-6.754066	6.425646	-4.684762
104	1	0	-6.297005	5.009475	-5.644908

105	1	0	-7.780711	4.982534	-4.680278
106	6	0	-6.763013	-4.232083	1.641431
107	1	0	-6.561977	-5.311056	1.564211
108	1	0	-6.555282	-3.958457	2.686775
109	6	0	-8.243124	-3.969701	1.335049
110	1	0	-8.445108	-2.890833	1.413741
111	1	0	-8.451767	-4.242199	0.289466
112	6	0	-9.205728	-4.730880	2.255773
113	1	0	-8.998199	-4.458296	3.300434
114	1	0	-9.004891	-5.808908	2.177071
115	6	0	-10.681473	-4.462833	1.942313
116	1	0	-11.342263	-5.020046	2.616527
117	1	0	-10.920909	-3.397124	2.046176
118	1	0	-10.927785	-4.758083	0.914688
119	1	0	-0.618130	-2.315266	-6.203063
120	6	0	5.141991	-1.680255	-0.468442
121	6	0	5.704198	-2.873866	-0.036030
122	16	0	6.424578	-0.473094	-0.658670
123	6	0	7.108470	-2.831422	0.135870
124	1	0	5.119685	-3.774012	0.118769
125	6	0	7.682607	-1.612007	-0.160998
126	1	0	7.690270	-3.691078	0.455353
127	6	0	9.067620	-1.210560	-0.115585
128	6	0	9.645807	-0.011779	-0.487771
129	16	0	10.311050	-2.308574	0.486786
130	6	0	11.058038	0.028554	-0.299596
131	1	0	9.072975	0.816511	-0.891554
132	6	0	11.566305	-1.131044	0.215567
133	1	0	11.670234	0.890816	-0.542417
134	1	0	12.592637	-1.375377	0.453799
135	6	0	-1.899402	-3.616654	0.513025
136	6	0	-0.269575	3.002454	-1.562623
137	1	0	-1.344170	3.062521	-1.770361
138	1	0	0.209235	3.779205	-2.176510
139	1	0	-1.664959	-3.292437	1.527866
140	1	0	-1.909234	-4.710593	0.499890
141	3	0	2.555451	3.425803	-3.713261
142	3	0	-1.983072	1.122511	-4.963785
143	3	0	-2.245384	-4.533435	-3.647497

144	3	0	1.861043	-1.594200	2.071248

Table S5X. Cartesian coordinates of optimized geometry of **PBPI-unit-1-2Li** in CH_2Cl_2 solution (DFT, B3LYP/6-31g*)

Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.257175	-0.840545	-2.555450
2	6	0	-0.620139	0.284214	-3.434764
3	6	0	-1.128225	0.037953	-4.690316
4	6	0	-1.384023	-1.283625	-5.147012
5	6	0	-1.363700	-2.303411	-4.225704
6	6	0	-0.972270	-2.098377	-2.868165
7	6	0	0.791001	-0.783303	-1.661825
8	6	0	1.784344	0.312859	-1.654314
9	6	0	3.138392	-0.034386	-1.431962
10	6	0	3.537391	-1.267643	-0.933027
11	6	0	2.482759	-2.138581	-0.484296
12	6	0	1.169750	-1.910088	-0.793640
13	1	0	-1.398031	0.886223	-5.313370
14	1	0	-1.720905	-3.292154	-4.499117
15	1	0	3.877324	0.742690	-1.607863
16	1	0	2.714662	-2.949592	0.198972
17	6	0	0.168086	-2.670753	0.008721
18	6	0	-1.263207	-3.118833	-1.950261
19	8	0	0.427830	-3.049645	1.156230
20	8	0	-1.762185	-4.255200	-2.267254
21	6	0	1.496978	1.672653	-1.891237
22	6	0	-0.717343	1.688179	-2.959915
23	8	0	-1.565955	2.462594	-3.416741
24	8	0	2.382847	2.586001	-1.999127
25	7	0	-1.089134	-2.893849	-0.540496
26	7	0	0.133758	2.113986	-1.936846
27	6	0	0.221557	3.507564	0.160957
28	1	0	1.305336	3.348099	0.244102
29	6	0	-3.537625	-2.930997	0.048077

30	1	0	-3.790386	-3.221708	-0.980840
31	6	0	-0.496282	2.412300	0.989611
32	1	0	-1.409171	2.829538	1.440402
33	1	0	-0.827055	1.615472	0.311621
34	6	0	0.369065	1.761351	2.081189
35	1	0	0.691516	2.514438	2.813409
36	1	0	1.285904	1.372368	1.615025
37	6	0	-3.610438	-1.384779	0.147766
38	1	0	-2.592093	-0.976573	0.126784
39	1	0	-4.036911	-1.096161	1.119842
40	6	0	-0.081768	4.943208	0.640326
41	1	0	0.417767	5.652288	-0.037605
42	1	0	-1.160951	5.130765	0.529971
43	6	0	0.334468	5.277297	2.079478
44	1	0	-0.205384	4.631337	2.784527
45	1	0	1.403270	5.053891	2.214725
46	6	0	-4.521897	-3.653544	0.991995
47	1	0	-4.359395	-4.739080	0.906921
48	1	0	-4.272658	-3.392450	2.031984
49	6	0	-6.009727	-3.367689	0.748382
50	1	0	-6.214799	-2.298699	0.895514
51	1	0	-6.257204	-3.585640	-0.301375
52	6	0	-4.405687	-0.717082	-0.985555
53	1	0	-5.442188	-1.083039	-0.987571
54	1	0	-3.967686	-1.025927	-1.945133
55	6	0	-0.342784	0.612990	2.806350
56	1	0	-0.624487	-0.151987	2.068857
57	1	0	-1.283960	0.980913	3.242809
58	6	0	0.502958	-0.041804	3.907140
59	1	0	0.741666	0.706148	4.678506
60	1	0	1.465133	-0.361857	3.481248
61	6	0	-0.181782	-1.250119	4.558086
62	1	0	-0.370157	-2.007210	3.783706
63	1	0	-1.167515	-0.947039	4.943071
64	6	0	0.630588	-1.882259	5.695930
65	1	0	0.820516	-1.126513	6.473313
66	1	0	1.618292	-2.181490	5.314462
67	6	0	-0.053036	-3.099089	6.332349
68	1	0	-0.239491	-3.854777	5.556056

69	1	0	-1.041498	-2.801557	6.711210
70	6	0	0.760937	-3.725887	7.469423
71	1	0	0.246550	-4.592247	7.901684
72	1	0	1.742137	-4.064032	7.113445
73	1	0	0.933778	-3.003606	8.277191
74	6	0	0.072269	6.744086	2.447638
75	1	0	0.619516	7.397150	1.751189
76	1	0	-0.994546	6.968780	2.299162
77	6	0	0.466545	7.097180	3.887684
78	1	0	-0.081491	6.445543	4.584613
79	1	0	1.533498	6.873972	4.038491
80	6	0	0.201167	8.563162	4.253427
81	1	0	-0.864959	8.785837	4.103345
82	1	0	0.748712	9.214592	3.557236
83	6	0	0.596404	8.908648	5.693048
84	1	0	0.392390	9.960828	5.923269
85	1	0	0.040694	8.295649	6.413576
86	1	0	1.665594	8.731117	5.863557
87	6	0	-4.406345	0.815078	-0.914686
88	1	0	-3.366984	1.173806	-0.928488
89	1	0	-4.831235	1.140214	0.047203
90	6	0	-5.181306	1.475640	-2.062846
91	1	0	-6.230699	1.144985	-2.031165
92	1	0	-4.774921	1.119443	-3.020632
93	6	0	-5.127436	3.008622	-2.040048
94	1	0	-4.079598	3.326605	-2.135878
95	1	0	-5.476640	3.373325	-1.061994
96	6	0	-5.956852	3.667287	-3.149921
97	1	0	-7.007433	3.352473	-3.056711
98	1	0	-5.613515	3.296391	-4.127276
99	6	0	-5.887237	5.199880	-3.141129
100	1	0	-4.837846	5.513258	-3.235707
101	1	0	-6.229356	5.572384	-2.164731
102	6	0	-6.716304	5.850462	-4.253519
103	1	0	-6.644044	6.943952	-4.221127
104	1	0	-6.375494	5.522932	-5.243670
105	1	0	-7.776958	5.583776	-4.164519
106	6	0	-6.930660	-4.184152	1.665704
107	1	0	-6.736942	-5.256544	1.512151

108	1	0	-6.672434	-3.976903	2.714984
109	6	0	-8.423090	-3.904128	1.448648
110	1	0	-8.620030	-2.833979	1.611827
111	1	0	-8.682440	-4.103821	0.397930
112	6	0	-9.339460	-4.730709	2.360185
113	1	0	-9.078949	-4.532627	3.409757
114	1	0	-9.143953	-5.800026	2.195147
115	6	0	-10.828778	-4.444546	2.142114
116	1	0	-11.454942	-5.050578	2.807198
117	1	0	-11.061259	-3.389757	2.334713
118	1	0	-11.127702	-4.665382	1.109741
119	1	0	-1.722364	-1.456695	-6.164524
120	6	0	4.926787	-1.630368	-0.725665
121	6	0	5.454576	-2.838891	-0.303332
122	16	0	6.246106	-0.490232	-1.019711
123	6	0	6.867513	-2.856429	-0.202343
124	1	0	4.837634	-3.701437	-0.078728
125	6	0	7.475260	-1.668939	-0.551650
126	1	0	7.426458	-3.728255	0.123892
127	6	0	8.877970	-1.325117	-0.576994
128	6	0	9.474819	-0.097920	-0.789912
129	16	0	10.116133	-2.553762	-0.319822
130	6	0	10.898777	-0.135988	-0.743520
131	1	0	8.906883	0.810066	-0.963884
132	6	0	11.394568	-1.385513	-0.495108
133	1	0	11.526955	0.737176	-0.884739
134	1	0	12.425468	-1.699067	-0.401308
135	6	0	-2.119662	-3.461388	0.343913
136	6	0	-0.148250	3.427416	-1.335182
137	1	0	-1.219561	3.591428	-1.463980
138	1	0	0.365715	4.222091	-1.889782
139	1	0	-1.823705	-3.195587	1.360129
140	1	0	-2.111026	-4.556614	0.283480
141	3	0	3.576477	3.831554	-2.452963
142	3	0	-2.307660	-5.916638	-2.563795

Table S6X. Cartesian coordinates of optimized geometry of **PBPI-unit-1-4Li** in CH_2Cl_2 solution (DFT, B3LYP/6-31g*)

Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.028571	-1.302606	-2.490135
2	6	0	-0.278786	-0.332830	-3.535553
3	6	0	-0.630707	-0.829296	-4.881120
4	6	0	-0.660223	-2.218296	-5.092337
5	6	0	-0.690061	-3.134250	-4.046344
6	6	0	-0.567480	-2.658515	-2.646615
7	6	0	1.020818	-1.071295	-1.546110
8	6	0	1.991002	0.044148	-1.640975
9	6	0	3.342371	-0.238803	-1.364729
10	6	0	3.751801	-1.405851	-0.706479
11	6	0	2.707078	-2.255164	-0.189480
12	6	0	1.386445	-2.071331	-0.547281
13	1	0	-0.341214	-0.200993	-5.730277
14	1	0	-0.414150	-4.172233	-4.269551
15	1	0	4.075891	0.519869	-1.631607
16	1	0	2.962980	-3.040175	0.520976
17	6	0	0.324004	-2.669963	0.316511
18	6	0	-0.919283	-3.521781	-1.641027
19	8	0	0.480384	-2.603999	1.577366
20	8	0	-1.447730	-4.714815	-1.823566
21	6	0	1.592622	1.336885	-2.054236
22	6	0	-0.279629	1.056848	-3.319701
23	8	0	-0.676711	1.910247	-4.224510
24	8	0	2.393035	2.282147	-2.401512
25	7	0	-0.800002	-3.161198	-0.227992
26	7	0	0.163128	1.567780	-2.047377
27	6	0	0.001424	3.312797	-0.252639
28	1	0	1.073272	3.153941	-0.060774
29	6	0	-3.285877	-3.092718	0.217496
30	1	0	-3.446807	-3.442629	-0.810123
31	6	0	-0.807769	2.418785	0.716658
32	1	0	-1.776045	2.896814	0.931324
33	1	0	-1.033617	1.476898	0.201353
34	6	0	-0.104553	2.074243	2.039233

35	1	0	0.173601	2.988252	2.579371
36	1	0	0.843264	1.563752	1.808037
37	6	0	-3.373500	-1.546426	0.232495
38	1	0	-2.359764	-1.125626	0.206271
39	1	0	-3.819132	-1.212958	1.181966
40	6	0	-0.287545	4.821540	-0.092017
41	1	0	0.305730	5.367319	-0.841377
42	1	0	-1.342140	5.006438	-0.350938
43	6	0	-0.003505	5.436251	1.285195
44	1	0	-0.654993	4.979415	2.041862
45	1	0	1.028881	5.203405	1.585798
46	6	0	-4.339275	-3.776049	1.116681
47	1	0	-4.164181	-4.861925	1.092820
48	1	0	-4.173069	-3.465223	2.159947
49	6	0	-5.806640	-3.517890	0.748425
50	1	0	-6.035314	-2.447604	0.840858
51	1	0	-5.968107	-3.776866	-0.308768
52	6	0	-4.158380	-0.946359	-0.945790
53	1	0	-5.151156	-1.411129	-1.015150
54	1	0	-3.631880	-1.203156	-1.876264
55	6	0	-0.953880	1.187132	2.959607
56	1	0	-1.244100	0.273897	2.419044
57	1	0	-1.892629	1.709584	3.196607
58	6	0	-0.252752	0.798991	4.268093
59	1	0	0.044290	1.710759	4.807398
60	1	0	0.684885	0.268039	4.037053
61	6	0	-1.111691	-0.078258	5.188291
62	1	0	-1.417254	-0.983982	4.643455
63	1	0	-2.040785	0.457818	5.432512
64	6	0	-0.405621	-0.484431	6.488147
65	1	0	-0.095334	0.420249	7.032289
66	1	0	0.521599	-1.025862	6.244782
67	6	0	-1.269190	-1.356177	7.409118
68	1	0	-1.580178	-2.259161	6.864622
69	1	0	-2.194122	-0.815253	7.655012
70	6	0	-0.555680	-1.761096	8.703191
71	1	0	-1.198873	-2.381579	9.337914
72	1	0	0.355287	-2.334404	8.490303
73	1	0	-0.262503	-0.879166	9.286330

74	6	0	-0.206314	6.957786	1.313897
75	1	0	0.454277	7.426759	0.569221
76	1	0	-1.234160	7.192414	0.998623
77	6	0	0.055453	7.584868	2.689286
78	1	0	-0.605679	7.116428	3.433847
79	1	0	1.083060	7.350973	3.005965
80	6	0	-0.148134	9.105151	2.721181
81	1	0	-1.174710	9.339079	2.404695
82	1	0	0.513429	9.574423	1.978966
83	6	0	0.113387	9.721447	4.099485
84	1	0	-0.040107	10.806817	4.089183
85	1	0	-0.557805	9.296913	4.856514
86	1	0	1.143107	9.533288	4.428254
87	6	0	-4.321889	0.576178	-0.864116
88	1	0	-3.330552	1.042698	-0.776392
89	1	0	-4.864690	0.835660	0.057424
90	6	0	-5.057741	1.176342	-2.069445
91	1	0	-6.050795	0.710962	-2.160015
92	1	0	-4.515032	0.911833	-2.990436
93	6	0	-5.217714	2.700460	-1.998448
94	1	0	-4.225233	3.164495	-1.894855
95	1	0	-5.773102	2.964020	-1.086016
96	6	0	-5.931324	3.301757	-3.216010
97	1	0	-6.921783	2.834888	-3.325043
98	1	0	-5.372137	3.044030	-4.129001
99	6	0	-6.097014	4.825157	-3.142159
100	1	0	-5.107571	5.291309	-3.030670
101	1	0	-6.659257	5.083274	-2.233430
102	6	0	-6.805010	5.417054	-4.365326
103	1	0	-6.908371	6.505098	-4.281148
104	1	0	-6.247406	5.205531	-5.286407
105	1	0	-7.810682	4.994657	-4.483529
106	6	0	-6.790675	-4.313596	1.617292
107	1	0	-6.568368	-5.387317	1.526175
108	1	0	-6.629033	-4.058640	2.675380
109	6	0	-8.261739	-4.069618	1.256978
110	1	0	-8.486805	-2.996685	1.352319
111	1	0	-8.422599	-4.320653	0.197647
112	6	0	-9.246560	-4.869931	2.119137

113	1	0	-9.088165	-4.618035	3.177492
114	1	0	-9.021211	-5.941830	2.024587
115	6	0	-10.712968	-4.622749	1.749771
116	1	0	-11.390058	-5.208198	2.382605
117	1	0	-10.977920	-3.564553	1.867518
118	1	0	-10.910040	-4.898466	0.706209
119	1	0	-0.630768	-2.594226	-6.117254
120	6	0	5.139006	-1.705508	-0.421699
121	6	0	5.698424	-2.877937	0.067870
122	16	0	6.423388	-0.509885	-0.664906
123	6	0	7.102372	-2.828739	0.241873
124	1	0	5.112109	-3.768919	0.263539
125	6	0	7.678524	-1.625065	-0.110011
126	1	0	7.682138	-3.672636	0.604153
127	6	0	9.063685	-1.222404	-0.078345
128	6	0	9.641177	-0.035591	-0.487968
129	16	0	10.307893	-2.301006	0.556358
130	6	0	11.053468	0.011173	-0.301827
131	1	0	9.067728	0.780084	-0.915849
132	6	0	11.562338	-1.131651	0.248984
133	1	0	11.665121	0.865937	-0.571062
134	1	0	12.588768	-1.367746	0.494979
135	6	0	-1.897564	-3.605180	0.650229
136	6	0	-0.264242	2.928302	-1.724059
137	1	0	-1.340934	2.977778	-1.923845
138	1	0	0.206553	3.678208	-2.376780
139	1	0	-1.660253	-3.255442	1.655746
140	1	0	-1.904612	-4.698747	0.661263
141	3	0	2.565773	3.310244	-3.865983
142	3	0	-2.008122	0.895428	-5.046973
143	3	0	-2.258476	-4.663264	-3.461052
144	3	0	1.877050	-1.438428	2.023884

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