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Exploring Polymers of Intrinsic Microporosity – Microporous, soluble Poly(amide) and Poly(imide)

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Synthetic Procedures and Analytical Data for Monomers 1-3

Synthesis of 2,2'-diacetyl-9,9'-spirobifluorene.

3.975 g (30.34 mmol) anhydrous aluminium chloride was suspended in 40 mL of dichloromethane. 1.85 mL (26.55 mmol) acetyl chloride was added at 0°C. A solution of 2.0 g (6.321 mmol) 9,9'-spirobifluorene in 10 mL dichloromethane was added dropwise while keeping the temperature below 20°C. After stirring for 1h the temperature was allowed to rise to room temperature. After 16 h the reaction mixture was poured into 60 mL of iced water. The aqueous layer was extracted twice with dichloromethane. The combined organic phases were washed with water, 2% NaOH (aq), water and dried over potassium carbonate. Volatiles were removed by solvent evaporation. The crude product showed sufficient purity to be used directly in the synthesis of **(1)**.

¹H-NMR: (400.1 MHz, CDCl₃) δ=6.72 (d, J=7.6 Hz, 1H), 7.18 (t, J=7.5 Hz, 1H), 7.3 (s, 1H), 7.42 (t, J=7.5 Hz, 1H), 7.93 (2d, J= 7.88 Hz, J= 7.6 Hz , 2H), 8.02 (d, J=8.16 Hz, 1H); ¹³C-NMR: δ=197.7, 149.3, 148.5, 146.8, 140.6, 136.9, 129.4, 129.3, 128.4, 124.3, 124.0, 121.3, 120.2, 65.9, 26.8

*Synthesis of 2,2'-dicarboxyl-9,9'-spirobifluorene (**1**)^[19]*

0.77 mL of bromine was added to a solution of 2.0 g sodium hydroxide in 10 mL water at 0°C. 1.0 g of 2,2'-diacetyl-9,9'-spirobifluorene dissolved in a small amount of dioxane was added to this mixture. 7 mL water and 0.4 g NaS₂O₅ was added after stirring the mixture for 2 h at room temperature. The solution was acidified with conc. hydrochloric acid, the precipitate collected by filtration and washed with water. The crude product was purified by dissolving it in 1M aqueous NaOH followed by centrifugation and precipitation with 1M aqueous HCl. After washing with water the product was vacuum dried to yield a white solid.

$^1\text{H-NMR}$: (400.1 MHz, $\text{DMSO-}d_6$) δ =6.7 (d, J =7.6 Hz, 1H), 7.08 (s, 1H), 7.24 (t, J =7.5 Hz, 1H), 7.94 (t, J =7.5 Hz, 1H), 8.0 (d, J =7.88 Hz, 1H), 8.17 (2d, J =7.88 Hz, J = 7.64, 2H), 12.94 (s, 1H); $^{13}\text{C-NMR}$: (400.1 MHz, $\text{DMSO-}d_6$) δ = 65.0, 120.9, 121.7, 123.7, 123.9, 128.5, 129.4, 129.8, 130.2, 140.2, 145.7, 147.8, 148.2, 166.8

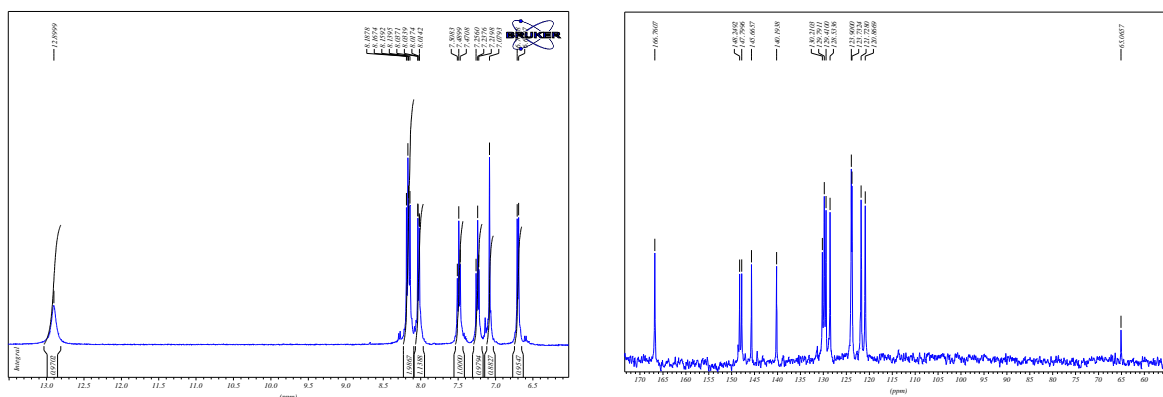


Figure S1. ^1H and ^{13}C NMR spectra of 2,2'-dicarboxyl-9,9'-spirobifluorene

Synthesis of 2,2'-dicarbonyl chloride-9,9'-spirobifluorene (2)

To a stirred suspension of **(1)** (2.5g, 6.18 mmol) in 25 mL of dry DCM (containing one drop of dry DMF) oxaloyl chloride (1.4 mL, 15.45 mmol) was slowly added under nitrogen atmosphere. The mixture was heated to reflux for 3h under nitrogen yielding a clear solution. The solvent was evaporated and the solid was dried under high vacuum at 80°C.

$^1\text{H-NMR}$: (CDCl_3): δ = 6.74 (d, 1H, J = 7.6 Hz), 7.24 (t, 1H, J = 7.5 Hz), 7.45 (s, 1H), 7.46 (t, 1H, J = 7.5 Hz), 7.97, (m, 2H, J = 8.16 Hz, J = 8.4 Hz), 8.23 (d, 1H, J = 7.8 Hz); $^{13}\text{C-NMR}$ (CDCl_3): δ = 65.5, 120.7, 122.0, 124.4, 126.8, 128.9, 129.5, 130.4, 132.7, 132.9, 139.9, 148.3, 149.1, 168.0

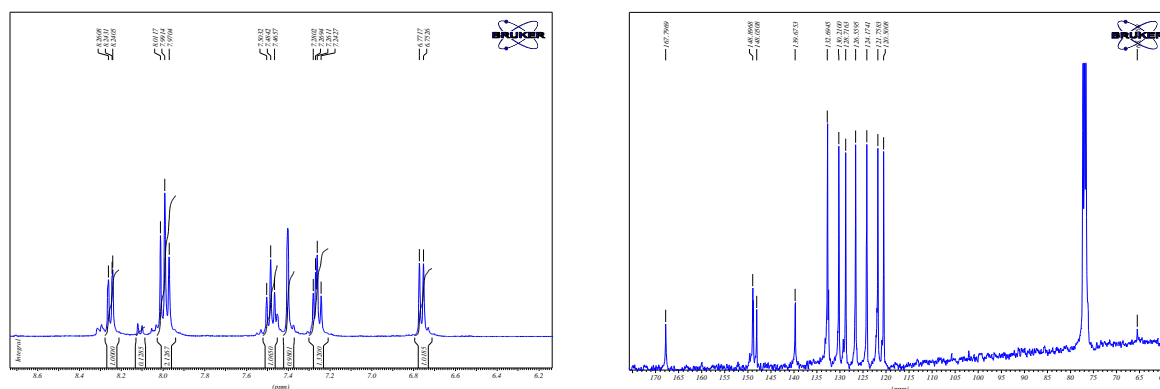


Figure S2. ^1H and ^{13}C NMR spectra of 2,2'-dicarbonyl chloride-9,9'-spirobifluorene

Synthesis of 2,2'-dinitro-9,9'-spirobifluorene

A mixture of 30 mL of concentrated nitric acid and 30 mL of acetic acid was added to a boiling solution of 3.00 g (9.5 mmol) of 9,9'-spirobifluorene in 100 mL of acetic acid over a period of 90 min and refluxed for an additional 75 min. After standing for one hour an equal volume of water was added, precipitating a yellow crystalline powder. The crude product was purified by column chromatography (silica gel, petroleum ether/ethylacetat: 4/1, 1 vol.-% acetic acid added). Yield: 1.5 g (3.7 mmol, 39%)

$^1\text{H-NMR}$: (CDCl_3): δ = 6.77 (d, 1H, J = 7.64 Hz), 7.26 (t, 1H, J = 7.5 Hz), 7.49 (t, 1H, J = 7.5 Hz), 7.54 (s, 1H), 7.97 (d, 1H, J = 7.88 Hz), 7.99 (d, 1H, J = 8.64 Hz), 8.33 (d, 1H, J = 8.4 Hz);
 $^{13}\text{C-NMR}$ (CDCl_3): δ = 65.8, 119.7, 120.8, 122.0, 124.5, 124.8, 129.2, 130.5, 139.6, 147.8, 148.1, 148.2, 148.3

Synthesis of 2,2'-diamino-9,9'-spirobifluorene (3)ⁱ

1.3 g (3.2 mmol) of 2,2'-dinitro-9,9'-spirobifluorene was repeatedly evacuated and flushed with argon. Abs. methanol (160 mL) and Pd/C (10% Pd, 0.4 g) were added. The resulting suspension was cooled to 0°C. Sodium borohydride (3.8 g, 105 mmol) was added in several portions. After complete addition the ice bath was removed and the mixture stirred for 12 h at room temperature. After that period the mixture was filtered through celite and the filtrate evaporated to dryness. The resulting residue was dissolved in dichloromethane (100 mL) and

washed twice with water. The combined aqueous phases were then extracted with dichloromethane, and the combined organic layers were washed with water and brine and dried over Na₂SO₄. The solid product was obtained after rotary evaporation of the solvent.

Yield: 1.04 g (3.01 mmol, 94%)

¹H-NMR: (DMSO-d₆): δ= 5.86 (d, 1H, J= 2.1 Hz), 6.51 (d, 1H, J= 7.4 Hz), 6.55 (d, 1H, J= 8.12), 6.93 (t, 1H, J= 7.4 Hz), 7.25, (t, 1H, J= 7.5 Hz), 7.58 (d, 1H, J= 8.12 Hz), 7.68 (d, 1H, J= 7.4 Hz); ¹³C-NMR (DMSO-d₆): δ= 109, 113.6, 118.6, 121.2, 123.6, 125.5, 127.8, 129.5, 142.9, 148.4, 149.4, 151.3, 65. 8

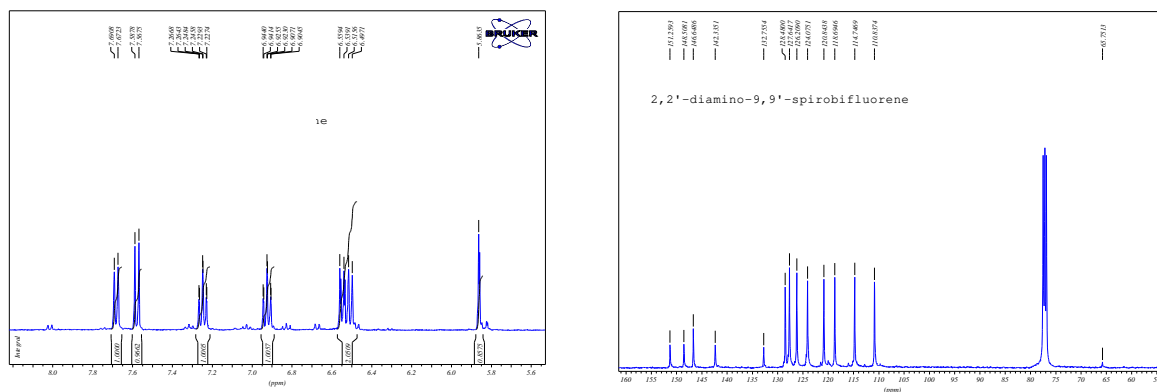


Figure S3. ¹H and ¹³C NMR spectra of 2,2'-diamino-9,9'-spirobifluorene

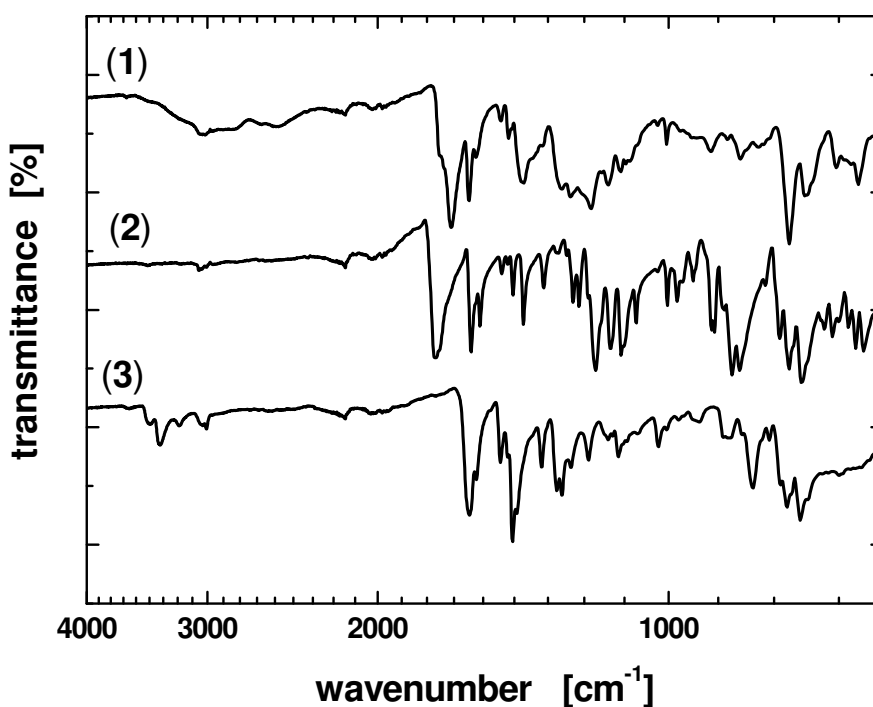


Figure S4. ATR-FTIR spectra of monomers 1-3

Spectral Data for Polymers P1-P4

$^1\text{H-NMR}$:

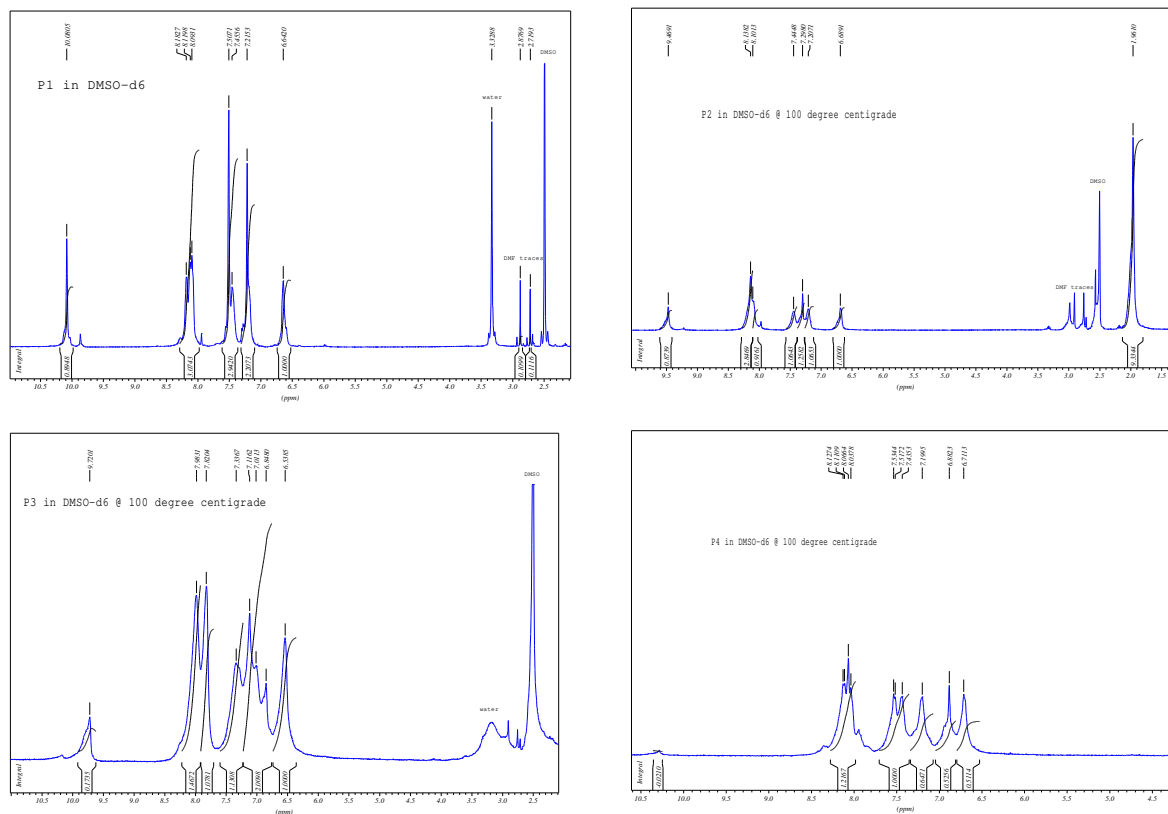


Figure S5. $^1\text{H-NMR}$ spectra of polymers **P1-P4** (P1 measured at 25 °C, P2-P4 measured at 100°C for better resolution)

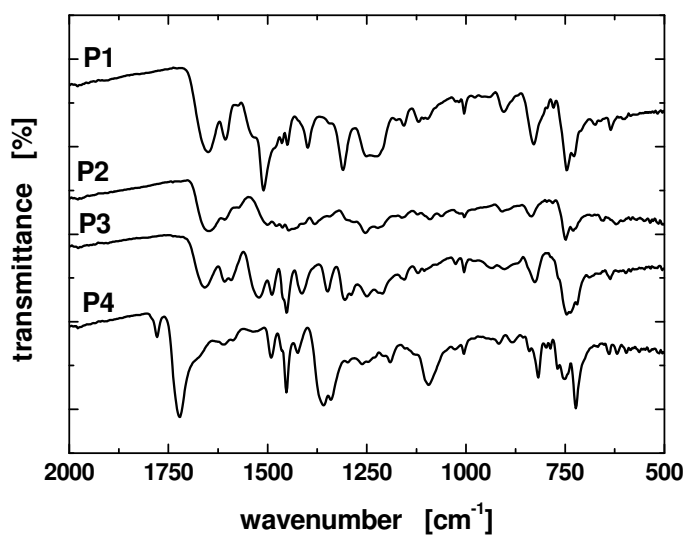


Figure S6. ATR-FTIR spectra of polymers **P1-P4**

Nitrogen Sorption

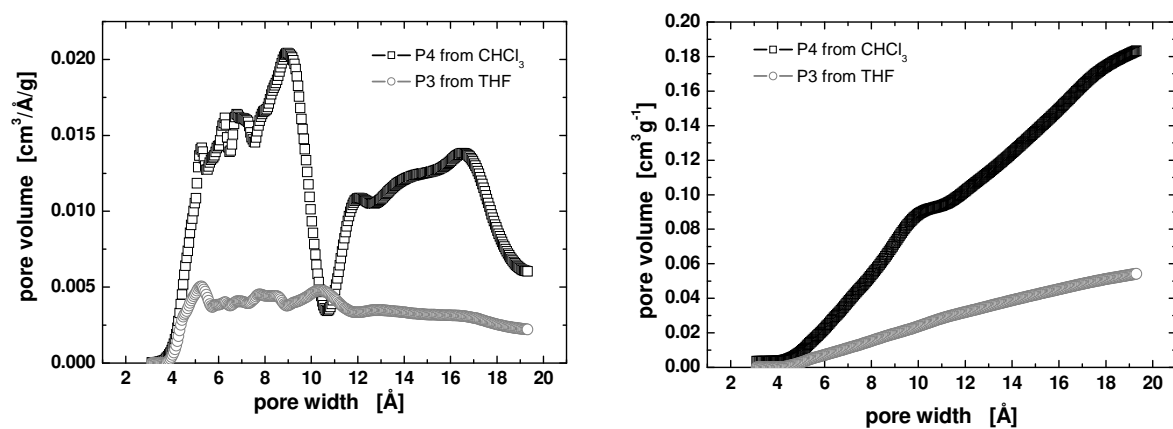


Figure S7. Results of Horvath-Kawazoe (HK) micropore analysis, left-hand side: pore size distribution, right-hand side: cumulative pore volume

Scanning Electron Microscopy

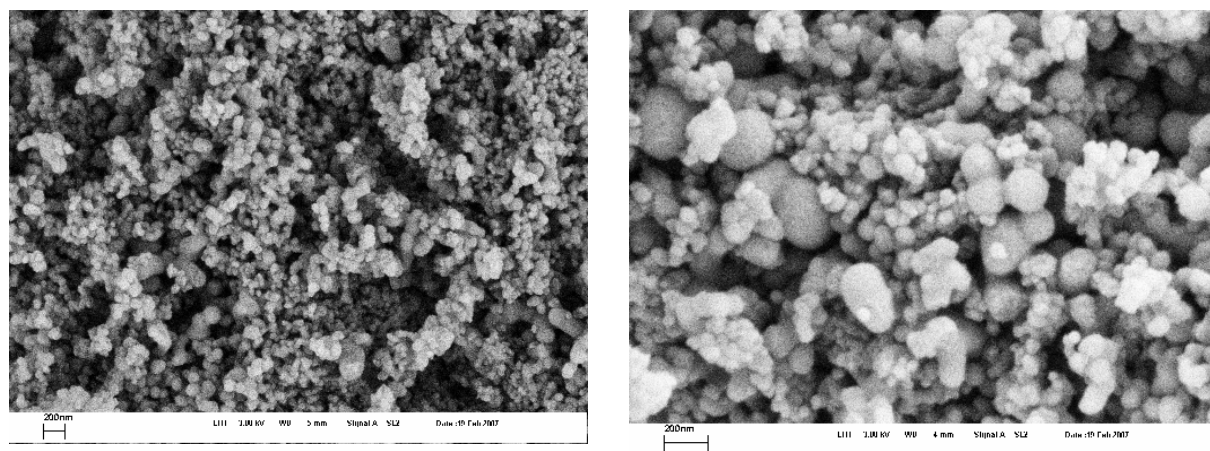


Figure S8. SEM micrographs of **P3** precipitated from DMAc into Methanol, scale bar: 200 nm

Molecular Modeling

Computational details: All computations were performed using the Gaussian 03 suite of programsⁱⁱ. Optimizations were carried out using the semiempirical AM1 method.

Optimized structures

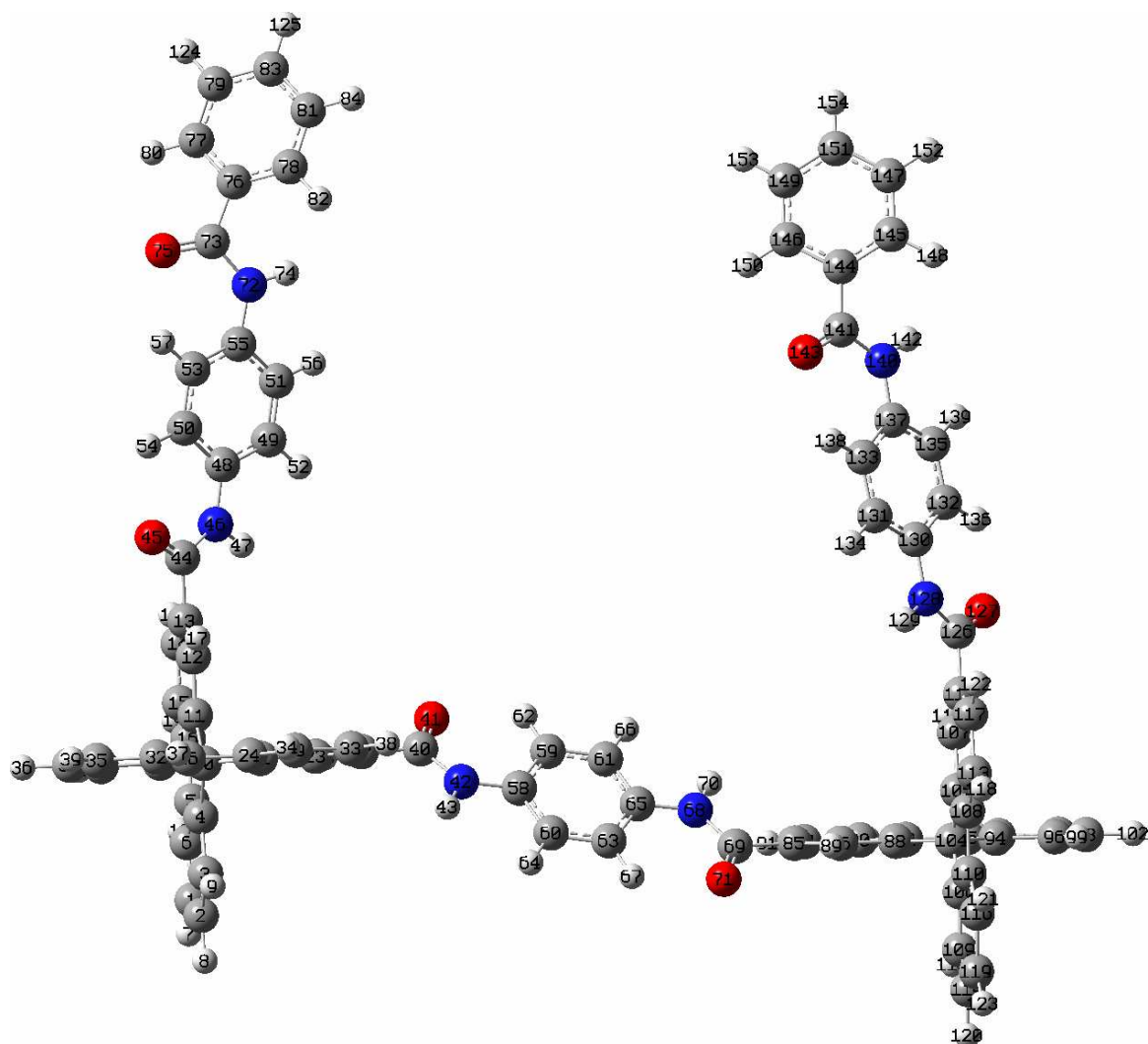


Figure S9. optimized structure of P1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-7.393458	-8.428153	-1.685461
2	6	0	-6.875497	-8.643337	-0.412191
3	6	0	-6.849406	-7.612816	0.540251
4	6	0	-7.349947	-6.372951	0.189368
5	6	0	-7.882812	-6.152360	-1.116642
6	6	0	-7.904457	-7.174805	-2.050522
7	1	0	-7.404382	-9.248667	-2.418395
8	1	0	-6.479121	-9.633683	-0.142302
9	1	0	-6.438691	-7.795414	1.543737
10	1	0	-8.312968	-7.010255	-3.057620
11	6	0	-8.092179	-4.126533	0.046837
12	6	0	-8.440522	-2.803596	0.239177
13	6	0	-9.025863	-2.102461	-0.831981
14	6	0	-9.266932	-2.726817	-2.055400
15	6	0	-8.926300	-4.072115	-2.248618
16	6	0	-8.338600	-4.767673	-1.204910
17	1	0	-8.280402	-2.296232	1.203527
18	1	0	-9.744227	-2.172379	-2.878316
19	1	0	-9.124615	-4.562300	-3.212381
20	6	0	-7.441587	-5.100742	1.010989
21	6	0	-6.089635	-4.621397	1.506540
22	6	0	-8.225308	-5.277482	2.297540
23	6	0	-4.959280	-4.289015	0.785839
24	6	0	-6.094980	-4.530317	2.931509
25	6	0	-9.530265	-5.694473	2.482205
26	6	0	-7.410576	-4.935459	3.418980
27	6	0	-3.813005	-3.870562	1.488739
28	1	0	-4.939152	-4.333359	-0.314501
29	6	0	-4.967235	-4.103209	3.613022

30	6	0	-10.032376	-5.773664	3.790480	93	1	0	7.233428	-3.209444	-4.703398
31	1	0	-10.168709	-5.957084	1.626252	94	6	0	10.605441	-2.278250	-2.303427
32	6	0	-7.914178	-5.016242	4.706545	95	6	0	9.747776	-2.503581	-3.422223
33	6	0	-3.819493	-3.773460	2.880028	96	6	0	11.922272	-1.904132	-2.495659
34	1	0	-4.969099	-4.018670	4.709172	97	6	0	10.221044	-2.351385	-4.714845
35	6	0	-9.238495	-5.440624	4.883515	98	6	0	12.393481	-1.751940	-3.808934
36	1	0	-11.071037	-6.101511	3.947430	99	1	0	12.591927	-1.725590	-1.641909
37	1	0	-7.292395	-4.751050	5.573273	100	6	0	11.557821	-1.971768	-4.899471
38	1	0	-2.928204	-3.416898	3.419446	101	1	0	9.564719	-2.522496	-5.579768
39	1	0	-9.651621	-5.506643	5.901142	102	1	0	13.439605	-1.452121	-3.972087
40	6	0	-2.607822	-3.502259	0.684739	103	1	0	11.945850	-1.845661	-5.921276
41	8	0	-2.708940	-2.823208	-0.353709	104	6	0	9.846605	-2.509571	-1.010222
42	7	0	-1.395373	-3.973417	1.169166	105	6	0	9.837801	-1.292273	-0.104369
43	1	0	-1.427410	-4.579927	1.958823	106	6	0	10.477904	-3.574246	-0.132881
44	6	0	-9.412219	-0.676400	-0.602067	107	6	0	9.384933	-0.012481	-0.359104
45	8	0	-10.043464	-0.333454	0.413425	108	6	0	10.404785	-1.622303	1.163973
46	7	0	-9.019348	0.213863	-1.592901	109	6	0	10.749314	-4.899850	-0.415842
47	1	0	-8.427430	-0.141910	-2.310959	110	6	0	10.799062	-3.028239	1.146483
48	6	0	-9.207546	1.606596	-1.595446	111	6	0	9.482269	0.950849	0.663499
49	6	0	-8.445998	2.392981	-2.491779	112	1	0	8.965793	0.270558	-1.337588
50	6	0	-10.141208	2.260488	-0.766724	113	6	0	10.509315	-0.664129	2.158705
51	6	0	-8.617767	3.766116	-2.556361	114	6	0	11.344577	-5.691685	0.578418
52	1	0	-7.703276	1.922790	-3.155250	115	1	0	10.504558	-5.332395	-1.396757
53	6	0	-10.308702	3.638391	-0.826723	116	6	0	11.386552	-3.816667	2.121807
54	1	0	-10.750382	1.685268	-0.048242	117	6	0	10.040559	0.630832	1.900844
55	6	0	-9.553933	4.422034	-1.722334	118	1	0	10.952901	-0.910003	3.134116
56	1	0	-8.006121	4.340361	-3.269696	119	6	0	11.657864	-5.159669	1.825306
57	1	0	-11.052109	4.109089	-0.160433	120	1	0	11.562303	-6.748695	0.363444
58	6	0	-0.128289	-3.807393	0.584616	121	1	0	11.634760	-3.401699	3.108892
59	6	0	0.135745	-2.865358	-0.430875	122	1	0	10.137728	1.397373	2.685329
60	6	0	0.944038	-4.603542	1.048721	123	1	0	12.122753	-5.797359	2.591985
61	6	0	1.413008	-2.731430	-0.955044	124	1	0	-12.592622	10.687385	-2.438188
62	1	0	-0.671596	-2.224989	-0.825003	125	1	0	-10.419064	11.901368	-2.247680
63	6	0	2.221767	-4.469236	0.525025	126	6	0	8.999997	2.332726	0.357991
64	1	0	0.781864	-5.350678	1.841891	127	8	0	9.259997	2.878107	-0.730422
65	6	0	2.485601	-3.528833	-0.491817	128	7	0	8.250036	2.940878	1.354638
66	1	0	1.575331	-1.983095	-1.747100	129	1	0	8.031723	2.390604	2.156170
67	1	0	3.027531	-5.110946	0.920116	130	6	0	7.661786	4.216460	1.319745
68	7	0	3.751519	-3.358264	-1.077126	131	6	0	6.769024	4.578979	2.355034
69	6	0	4.953435	-3.912528	-0.660280	132	6	0	7.929537	5.166426	0.312849
70	1	0	3.790339	-2.708232	-1.831335	133	6	0	6.172998	5.831198	2.389016
71	8	0	5.052870	-4.665503	0.326048	134	1	0	6.529545	3.866441	3.160495
72	7	0	-9.668869	5.819878	-1.810259	135	6	0	7.329520	6.416796	0.344001
73	6	0	-10.687361	6.609207	-1.294274	136	1	0	8.616344	4.927549	-0.516847
74	1	0	-8.988569	6.272180	-2.379889	137	6	0	6.439609	6.780828	1.381377
75	8	0	-11.648696	6.147171	-0.652742	138	1	0	5.483359	6.068227	3.216979
76	6	0	-10.574599	8.074340	-1.567168	139	1	0	7.564366	7.127048	-0.464739
77	6	0	-11.738161	8.770616	-1.914829	140	7	0	5.879047	8.068955	1.364113
78	6	0	-9.358926	8.754960	-1.450164	141	6	0	4.891224	8.570516	2.199622
79	6	0	-11.678422	10.141138	-2.162406	142	1	0	6.188837	8.660220	0.624388
80	1	0	-12.695220	8.228439	-1.977535	143	8	0	4.365460	7.905537	3.111473
81	6	0	-9.307639	10.127290	-1.693418	144	6	0	4.469318	9.979301	1.932597
82	1	0	-8.444229	8.222909	-1.147662	145	6	0	5.397981	10.988886	1.662089
83	6	0	-10.464082	10.819253	-2.054007	146	6	0	3.103550	10.280041	1.994046
84	1	0	-8.352453	10.664165	-1.596592	147	6	0	4.957577	12.293658	1.441524
85	6	0	6.153734	-3.539449	-1.469992	148	1	0	6.476262	10.769657	1.641061
86	6	0	7.335876	-3.225138	-0.772084	149	6	0	2.669945	11.585229	1.766694
87	6	0	6.120433	-3.535437	-2.864269	150	1	0	2.383458	9.481488	2.234027
88	6	0	8.461993	-2.892020	-1.499202	151	6	0	3.595437	12.591364	1.488574
89	1	0	7.346012	-3.262159	0.328737	152	1	0	5.688138	13.089254	1.233244
90	6	0	7.263764	-3.206625	-3.604440	153	1	0	1.596267	11.820519	1.812381
91	1	0	5.199750	-3.809623	-3.402423	154	1	0	3.251715	13.621406	1.311241
92	6	0	8.427293	-2.882011	-2.926700						

P2

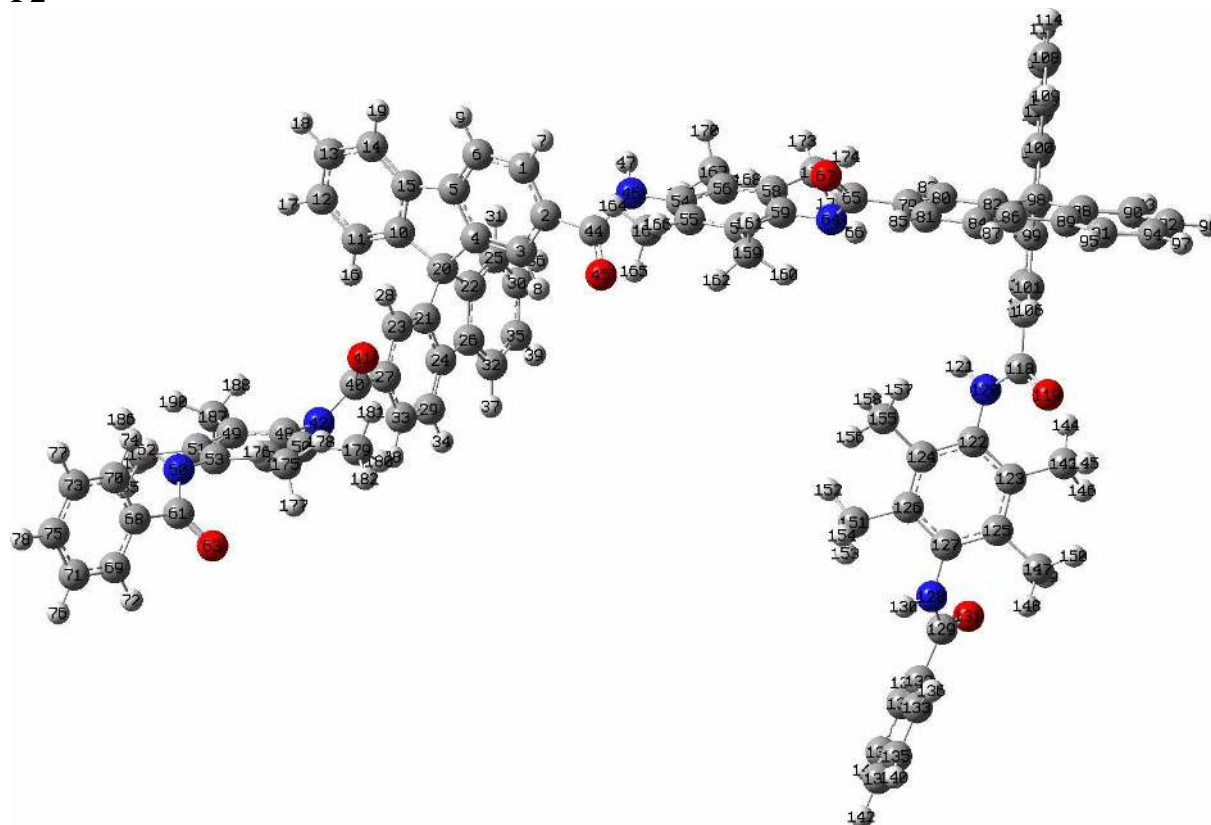


Figure S10. optimized structure of P2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.253479	-4.922101	1.660874
2	6	0	-2.820546	-3.596350	1.642304
3	6	0	-3.489053	-2.606255	2.388955
4	6	0	-4.569527	-2.980714	3.163582
5	6	0	-5.004174	-4.340403	3.193652
6	6	0	-4.353934	-5.303396	2.440133
7	1	0	-2.747806	-5.684584	1.047946
8	1	0	-3.150012	-1.559479	2.332238
9	1	0	-4.693656	-6.348904	2.446485
10	6	0	-6.432836	-3.146766	4.619192
11	6	0	-7.478034	-2.964273	5.505317
12	6	0	-8.253314	-4.075903	5.869953
13	6	0	-7.981178	-5.338756	5.353299
14	6	0	-6.922994	-5.534333	4.454823
15	6	0	-6.152040	-4.442970	4.090696
16	1	0	-7.702755	-1.971200	5.920348
17	1	0	-9.087488	-3.940578	6.574569
18	1	0	-8.601748	-6.197516	5.649867
19	1	0	-6.713206	-6.533828	4.048319
20	6	0	-5.451542	-2.133021	4.061306
21	6	0	-6.133025	-0.998134	3.319666
22	6	0	-4.670387	-1.405945	5.139744
23	6	0	-6.986272	-1.046821	2.234630
24	6	0	-5.773407	0.253852	3.904250
25	6	0	-3.855225	-1.917493	6.132113
26	6	0	-4.872560	0.002779	5.025971
27	6	0	-7.501396	0.162743	1.728309
28	1	0	-7.259957	-1.999300	1.753071
29	6	0	-6.268153	1.439420	3.386982
30	6	0	-3.233250	-1.025109	7.018979
31	1	0	-3.693575	-3.000572	6.230881
32	6	0	-4.253878	0.876420	5.904615
33	6	0	-7.139179	1.386694	2.290532

34	1	0	-5.982621	2.407491	3.822649
35	6	0	-3.428465	0.347886	6.906915
36	1	0	-2.582702	-1.422809	7.812234
37	1	0	-4.403782	1.962024	5.819640
38	1	0	-7.518057	2.330588	1.868319
39	1	0	-2.930685	1.031386	7.610884
40	6	0	-8.420399	0.077483	0.552494
41	8	0	-8.228405	-0.745588	-0.360682
42	7	0	-9.485280	0.972149	0.543996
43	1	0	-9.696754	1.440321	1.396888
44	6	0	-1.656447	-3.160356	0.812428
45	8	0	-1.663512	-2.073705	0.206307
46	7	0	-0.581375	-4.041165	0.758778
47	1	0	-0.555458	-4.774720	1.431418
48	6	0	-10.515314	0.987266	-0.424248
49	6	0	-11.864122	0.871976	0.002621
50	6	0	-10.225697	1.170990	-1.794325
51	6	0	-12.903362	1.027730	-0.920070
52	6	0	-11.267031	1.155119	-2.739044
53	6	0	-12.610796	1.126673	-2.305478
54	6	0	0.644734	-3.774369	0.107707
55	6	0	0.689021	-3.486981	-1.274477
56	6	0	1.851140	-3.853530	0.851216
57	6	0	1.919381	-3.198690	-1.891071
58	6	0	3.082144	-3.728061	0.199287
59	6	0	3.122973	-3.357784	-1.170009
60	7	0	-13.677957	1.138254	-3.232803
61	6	0	-13.904157	2.141226	-4.168109
62	1	0	-14.440746	0.537916	-3.011071
63	8	0	-13.117566	3.091015	-4.338395
64	7	0	4.375803	-3.100986	-1.774166
65	6	0	4.879313	-3.783757	-2.873966
66	1	0	5.021021	-2.593447	-1.210609
67	8	0	4.189398	-4.566149	-3.553414
68	6	0	-15.153928	2.015799	-4.977262
69	6	0	-15.852641	3.187807	-5.291440
70	6	0	-15.613880	0.780638	-5.443893
71	6	0	-17.017267	3.118776	-6.054090

72	1	0	-15.465464	4.158169	-4.941409	132	6	0	5.668171	9.899988	1.219503
73	6	0	-16.776887	0.719406	-6.211395	133	6	0	5.403677	10.386154	-0.064500
74	1	0	-15.057232	-0.144093	-5.228164	134	6	0	5.243293	10.620167	2.342624
75	6	0	-17.480955	1.885404	-6.512463	135	6	0	4.704601	11.582787	-0.221870
76	1	0	-17.566639	4.039991	-6.298325	136	1	0	5.757523	9.844009	-0.954676
77	1	0	-17.136125	-0.251855	-6.582377	137	6	0	4.540305	11.812407	2.178080
78	1	0	-18.399229	1.832642	-7.116153	138	1	0	5.481164	10.241097	3.349459
79	6	0	6.296378	-3.481286	-3.241388	139	6	0	4.268844	12.293082	0.896835
80	6	0	7.297768	-3.391942	-2.257578	140	1	0	4.500123	11.967246	-1.232049
81	6	0	6.604364	-3.319196	-4.593542	141	1	0	4.204777	12.375993	3.061181
82	6	0	8.592444	-3.120967	-2.656231	142	1	0	3.715292	13.235189	0.768424
83	1	0	7.064571	-3.553725	-1.194389	143	6	0	10.068974	4.570726	0.935168
84	6	0	7.915992	-3.044649	-5.001279	144	1	0	10.304710	3.649825	1.522999
85	1	0	5.803381	-3.419875	-5.344101	145	1	0	10.538818	4.461613	-0.076926
86	6	0	8.905890	-2.943052	-4.037771	146	1	0	10.541179	5.433285	1.467868
87	1	0	8.150313	-2.915243	-6.067667	147	6	0	9.044452	7.210614	0.523304
88	6	0	10.912572	-2.680025	-2.852592	148	1	0	8.602183	8.051897	-0.064827
89	6	0	10.335756	-2.671594	-4.158604	149	1	0	9.306712	7.603504	1.540073
90	6	0	12.264293	-2.446041	-2.683040	150	1	0	9.980726	6.896366	-0.001508
91	6	0	11.120613	-2.429763	-5.273662	151	6	0	4.349504	5.411041	0.809484
92	6	0	13.052209	-2.201757	-3.818658	152	1	0	3.832196	4.545877	1.294309
93	1	0	12.719490	-2.447066	-1.682092	153	1	0	4.106815	6.310278	1.428926
94	6	0	12.490511	-2.193846	-5.091497	154	1	0	3.916725	5.554188	-0.212544
95	1	0	10.681456	-2.420438	-6.281301	155	6	0	5.398033	2.724202	0.572577
96	1	0	14.128856	-2.011874	-3.693713	156	1	0	4.440843	3.014607	0.071784
97	1	0	13.124727	-1.998322	-5.969086	157	1	0	5.838074	1.901342	-0.044216
98	6	0	9.844674	-2.964671	-1.813553	158	1	0	5.157437	2.319995	1.587917
99	6	0	9.719731	-1.865372	-0.774974	159	6	0	1.935227	-2.746202	-3.305314
100	6	0	10.144811	-4.188798	-0.969314	160	1	0	2.811947	-2.086678	-3.518735
101	6	0	9.458153	-0.520265	-0.948789	161	1	0	2.000735	-3.635629	-3.984583
102	6	0	9.923039	-2.401867	0.532646	162	1	0	1.013587	-2.162723	-3.552147
103	6	0	10.363325	-5.496099	-1.362182	163	6	0	-0.553623	-3.465990	-2.087049
104	6	0	10.185958	-3.833365	0.412836	164	1	0	-1.323197	-4.169981	-1.685206
105	6	0	9.379204	0.302226	0.191712	165	1	0	-0.993776	-2.434788	-2.077318
106	1	0	9.324694	-0.079845	-1.949782	166	1	0	-0.349389	-3.767771	-3.144358
107	6	0	9.859414	-1.581995	1.647116	167	6	0	1.804131	-4.084813	2.318605
108	6	0	10.625166	-6.460084	-0.376252	168	1	0	2.723218	-3.695115	2.822798
109	1	0	10.334002	-5.781836	-2.423794	169	1	0	0.937662	-3.557700	2.790686
110	6	0	10.446035	-4.790869	1.379071	170	1	0	1.718392	-5.179006	2.537118
111	6	0	9.581919	-0.220054	1.468782	171	6	0	4.344593	-3.966966	0.946610
112	1	0	10.026602	-1.986872	2.655413	172	1	0	4.718249	-3.011198	1.392943
113	6	0	10.666098	-6.113734	0.970723	173	1	0	4.190121	-4.706859	1.771529
114	1	0	10.799903	-7.503473	-0.679212	174	1	0	5.146108	-4.389364	0.290514
115	1	0	10.481287	-4.522263	2.444307	175	6	0	-10.934866	1.187647	-4.185964
116	1	0	9.543930	0.436664	2.352017	176	1	0	-11.712914	0.672451	-4.801140
117	1	0	10.873966	-6.883999	1.728382	177	1	0	-10.870417	2.251247	-4.534669
118	6	0	9.103777	1.755878	-0.023790	178	1	0	-9.961126	0.675734	-4.387471
119	8	0	9.658119	2.390266	-0.939317	179	6	0	-8.827981	1.362699	-2.257555
120	7	0	8.209958	2.341763	0.865600	180	1	0	-8.198286	1.860064	-1.479491
121	1	0	7.658197	1.731227	1.426435	181	1	0	-8.366307	0.367073	-2.487339
122	6	0	7.724094	3.665946	0.760318	182	1	0	-8.790957	2.004254	-3.172854
123	6	0	8.604799	4.769376	0.787640	183	6	0	-14.313906	1.075102	-0.454076
124	6	0	6.323450	3.882035	0.682694	184	1	0	-14.381831	1.443599	0.599800
125	6	0	8.097814	6.074182	0.654993	185	1	0	-14.929447	1.775034	-1.072531
126	6	0	5.815871	5.184532	0.722615	186	1	0	-14.774494	0.056436	-0.503271
127	6	0	6.702424	6.291722	0.665206	187	6	0	-12.169497	0.599828	1.431509
128	7	0	6.165382	7.595306	0.561026	188	1	0	-11.413037	-0.083737	1.891804
129	6	0	6.428617	8.634118	1.446295	189	1	0	-12.188881	1.554935	2.014274
130	1	0	5.355775	7.676918	-0.013113	190	1	0	-13.160951	0.095031	1.546564
131	8	0	7.252346	8.533341	2.374397						

P3

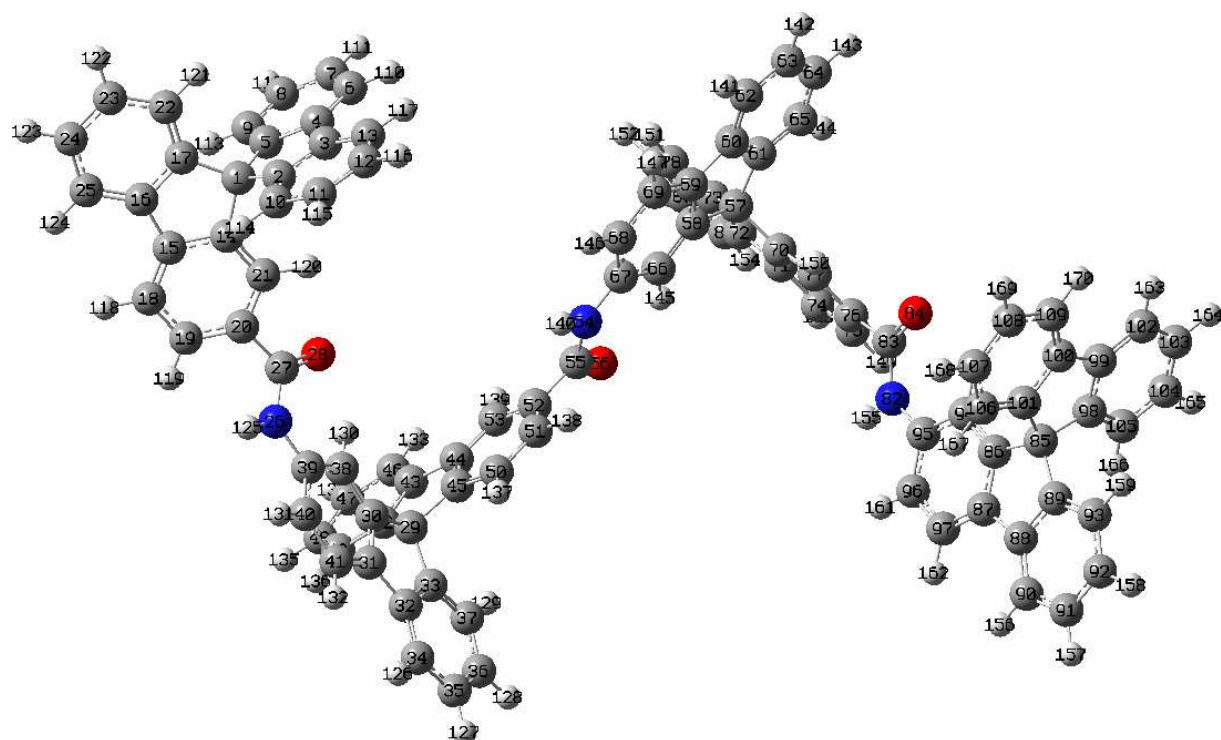


Figure S11. optimized structure of P3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-9.692153	-2.708078	-2.143437
2	6	0	-8.859746	-2.926483	-3.393226
3	6	0	-7.828505	-3.879155	-3.133326
4	6	0	-7.935798	-4.313933	-1.743146
5	6	0	-9.033886	-3.632360	-1.136461
6	6	0	-7.177978	-5.214884	-1.014042
7	6	0	-7.511782	-5.441587	0.328646
8	6	0	-8.581638	-4.776939	0.919332
9	6	0	-9.355468	-3.862368	0.187968
10	6	0	-8.984572	-2.353754	-4.644949
11	6	0	-8.078242	-2.726795	-5.649636
12	6	0	-7.072666	-3.654174	-5.396695
13	6	0	-6.938568	-4.241293	-4.130630
14	6	0	-9.711823	-1.259529	-1.692337
15	6	0	-11.055285	-0.777446	-1.650584
16	6	0	-11.950169	-1.856865	-2.058495
17	6	0	-11.163743	-3.011120	-2.354204
18	6	0	-11.324634	0.524056	-1.259944
19	6	0	-10.254978	1.360849	-0.916358
20	6	0	-8.942601	0.890449	-0.962266
21	6	0	-8.659532	-0.435195	-1.343597
22	6	0	-11.770179	-4.183390	-2.765823
23	6	0	-13.168161	-4.211771	-2.885639
24	6	0	-13.934668	-3.086747	-2.597509
25	6	0	-13.329430	-1.893638	-2.179178
26	7	0	-7.816825	3.053497	-1.084256
27	6	0	-7.790273	1.758893	-0.574805
28	8	0	-6.872221	1.334313	0.148334
29	6	0	-3.892042	5.212099	1.310877
30	6	0	-4.991454	5.034496	0.277820
31	6	0	-4.990212	6.136484	-0.626843
32	6	0	-3.920881	7.054066	-0.248389
33	6	0	-3.252959	6.524433	0.897375
34	6	0	-3.512946	8.253631	-0.807485
35	6	0	-2.433587	8.933337	-0.225763

36	6	0	-1.783325	8.416791	0.890271
37	6	0	-2.190016	7.202089	1.464118
38	6	0	-5.898215	4.002739	0.153248
39	6	0	-6.845732	4.051455	-0.904391
40	6	0	-6.839614	5.150739	-1.793365
41	6	0	-5.916198	6.188541	-1.653860
42	6	0	-4.412488	5.232870	2.735758
43	6	0	-3.793418	4.197264	3.498993
44	6	0	-2.870585	3.469571	2.631985
45	6	0	-2.911281	4.054544	1.329991
46	6	0	-4.110404	4.021244	4.835461
47	6	0	-5.050800	4.880910	5.420444
48	6	0	-5.654207	5.889938	4.676637
49	6	0	-5.338549	6.075337	3.321696
50	6	0	-2.124176	3.551951	0.310665
51	6	0	-1.297062	2.450387	0.575365
52	6	0	-1.263730	1.875078	1.845317
53	6	0	-2.047250	2.388534	2.893997
54	7	0	-0.417242	-0.324165	1.222175
55	6	0	-0.374777	0.711901	2.148052
56	8	0	0.335161	0.689720	3.168978
57	6	0	3.041630	-3.556920	3.075120
58	6	0	1.948441	-3.027039	2.162535
59	6	0	1.654349	-3.986540	1.150453
60	6	0	2.513292	-5.150221	1.341292
61	6	0	3.347552	-4.916908	2.476670
62	6	0	2.612538	-6.332870	0.627616
63	6	0	3.547059	-7.291827	1.042910
64	6	0	4.359892	-7.063679	2.148479
65	6	0	4.266202	-5.868222	2.878076
66	6	0	1.287072	-1.817949	2.223552
67	6	0	0.292438	-1.534224	1.249726
68	6	0	0.004788	-2.495422	0.251948
69	6	0	0.683396	-3.713954	0.202740
70	6	0	4.253482	-2.646055	3.132445
71	6	0	4.495213	-2.237008	4.479017
72	6	0	3.485279	-2.846914	5.339573
73	6	0	2.612590	-3.633317	4.528362
74	6	0	5.553897	-1.395960	4.780377
75	6	0	6.375504	-0.945889	3.738926
76	6	0	6.135780	-1.343163	2.423553

77	6	0	5.072400	-2.210267	2.108620	124	1	0	-13.939499	-1.008118	-1.951712
78	6	0	1.559014	-4.322539	5.099475	125	1	0	-8.533676	3.263528	-1.743694
79	6	0	1.368690	-4.231562	6.486907	126	1	0	-4.022649	8.666699	-1.689078
80	6	0	2.218990	-3.464875	7.277588	127	1	0	-2.100197	9.887081	-0.661194
81	6	0	3.289836	-2.762181	6.708052	128	1	0	-0.937864	8.963263	1.333973
82	7	0	7.295205	0.475037	1.286948	129	1	0	-1.669033	6.803945	2.346928
83	6	0	7.015839	-0.887890	1.304602	130	1	0	-5.881854	3.155028	0.858225
84	8	0	7.450562	-1.684548	0.455316	131	1	0	-7.569053	5.204881	-2.616225
85	6	0	10.585006	0.846273	-2.569985	132	1	0	-5.928807	7.033277	-2.358073
86	6	0	9.631790	1.299270	-1.477235	133	1	0	-3.636959	3.224979	5.427261
87	6	0	9.577025	2.723495	-1.440454	134	1	0	-5.311859	4.751193	6.481303
88	6	0	10.460009	3.255089	-2.472830	135	1	0	-6.390454	6.555174	5.151802
89	6	0	11.069354	2.159185	-3.156385	136	1	0	-5.821652	6.876275	2.743758
90	6	0	10.751382	4.559499	-2.835769	137	1	0	-2.141732	4.000418	-0.693470
91	6	0	11.654516	4.779278	-3.885145	138	1	0	-0.661584	2.056535	-0.232744
92	6	0	12.247880	3.711503	-4.550667	139	1	0	-1.991634	1.936463	3.895987
93	6	0	11.958618	2.386341	-4.189813	140	1	0	-1.071769	-0.228229	0.475617
94	6	0	8.892043	0.528149	-0.604774	141	1	0	1.974943	-6.517655	-0.248065
95	6	0	8.061410	1.179839	0.346058	142	1	0	3.636639	-8.234299	0.482587
96	6	0	8.013176	2.593417	0.372881	143	1	0	5.090130	-7.825681	2.458709
97	6	0	8.768363	3.360348	-0.515655	144	1	0	4.915743	-5.698148	3.748760
98	6	0	11.716265	-0.019242	-2.047424	145	1	0	1.528926	-1.091219	3.016642
99	6	0	11.708963	-1.285251	-2.707662	146	1	0	-0.765757	-2.294215	-0.508484
100	6	0	10.604826	-1.305255	-3.663512	147	1	0	0.444378	-4.444261	-0.584107
101	6	0	9.924050	-0.051861	-3.598565	148	1	0	5.748681	-1.083630	5.816161
102	6	0	12.653677	-2.247699	-2.393125	149	1	0	7.224751	-0.286579	3.975938
103	6	0	13.614909	-1.951848	-1.416475	150	1	0	4.916646	-2.530835	1.066504
104	6	0	13.622211	-0.717910	-0.774190	151	1	0	0.879513	-4.929879	4.484264
105	6	0	12.668126	0.263122	-1.085744	152	1	0	0.531974	-4.775244	6.950402
106	6	0	8.829714	0.192963	-4.406690	153	1	0	2.051804	-3.404755	8.363236
107	6	0	8.405268	-0.813278	-5.288221	154	1	0	3.957066	-2.155776	7.336551
108	6	0	9.067935	-2.034774	-5.351525	155	1	0	6.822551	1.036177	1.962052
109	6	0	10.178440	-2.292733	-4.535715	156	1	0	10.285624	5.406851	-2.313748
110	1	0	-6.330833	-5.741803	-1.475174	157	1	0	11.893794	5.810983	-4.182421
111	1	0	-6.915863	-6.153571	0.918978	158	1	0	12.954372	3.902022	-5.371959
112	1	0	-8.828248	-4.964825	1.974981	159	1	0	12.433332	1.549893	-4.722728
113	1	0	-10.197395	-3.341745	0.666565	160	1	0	8.944922	-0.572409	-0.651599
114	1	0	-9.776340	-1.621160	-4.857375	161	1	0	7.373222	3.114496	1.101650
115	1	0	-8.169621	-2.276443	-6.649203	162	1	0	8.714938	4.458091	-0.476059
116	1	0	-6.371471	-3.933833	-6.197069	163	1	0	12.650460	-3.225259	-2.895220
117	1	0	-6.142405	-4.973726	-3.936432	164	1	0	14.369571	-2.708928	-1.156948
118	1	0	-12.357773	0.897125	-1.215592	165	1	0	14.382990	-0.502810	-0.009380
119	1	0	-10.468128	2.390510	-0.589789	166	1	0	12.682365	1.234281	-0.570554
120	1	0	-7.617963	-0.793696	-1.346481	167	1	0	8.296420	1.153399	-4.362862
121	1	0	-11.174624	-5.078873	-2.995646	168	1	0	7.533924	-0.628553	-5.933674
122	1	0	-13.659943	-5.140364	-3.212326	169	1	0	8.718298	-2.812268	-6.046680
123	1	0	-15.029512	-3.129484	-2.697172	170	1	0	10.695801	-3.260933	-4.586766

P4

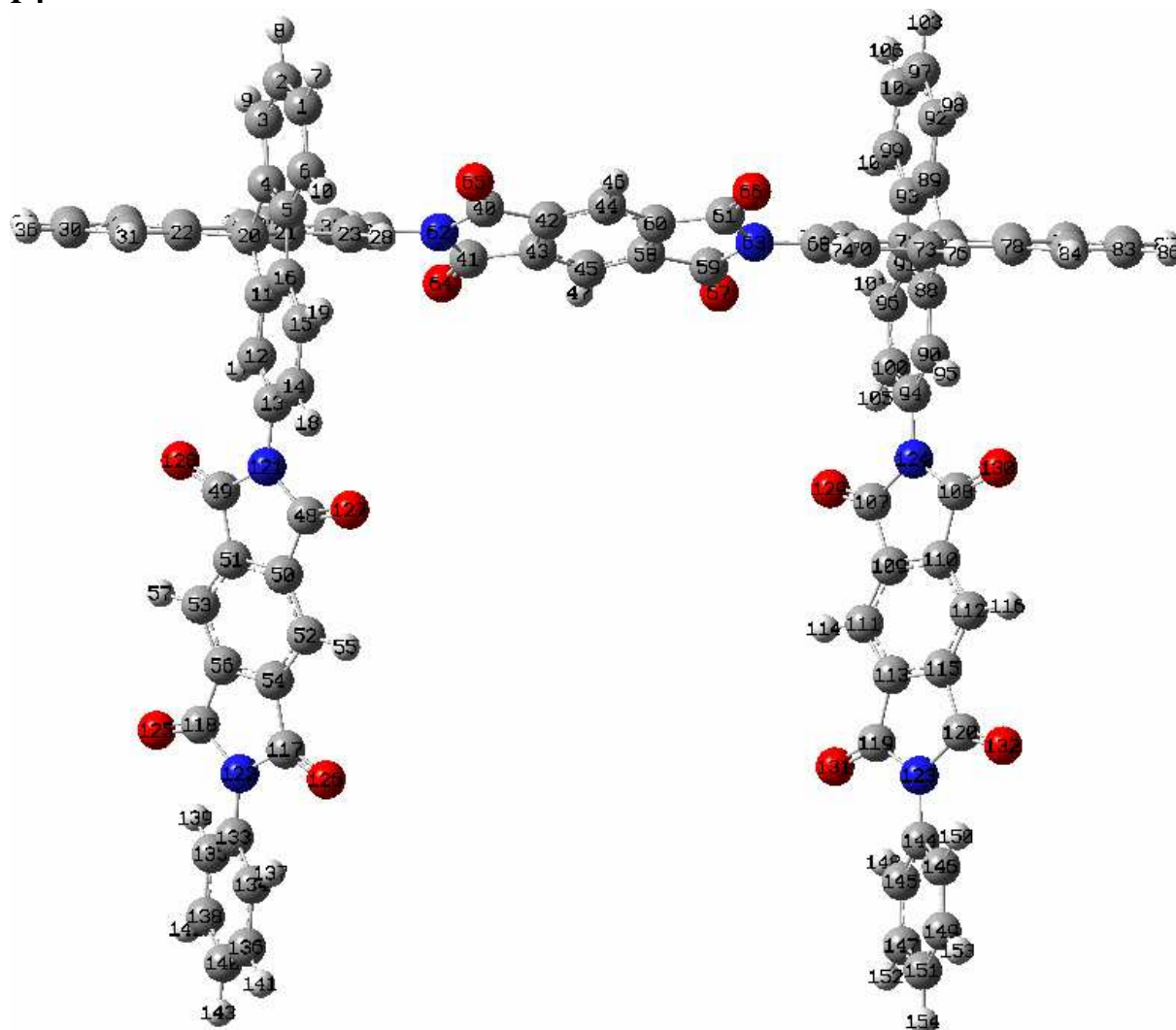


Figure S12. optimized structure of P4

Standard orientation:											
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)								
			X	Y	Z						
1	6	0	-8.641661	-6.989064	-2.830708	24	6	0	-7.290642	-3.957360	2.385815
2	6	0	-8.503397	-7.425189	-1.516874	25	6	0	-10.720228	-3.934757	1.125296
3	6	0	-8.376048	-6.508595	-0.461576	26	6	0	-8.740924	-3.941894	2.549983
4	6	0	-8.390681	-5.157339	-0.752138	27	6	0	-4.635171	-3.989674	1.503124
5	6	0	-8.532789	-4.709442	-2.100446	28	1	0	-5.463900	-4.018695	-0.534848
6	6	0	-8.657569	-5.620810	-3.135641	29	6	0	-6.267928	-3.955809	3.317425
7	1	0	-8.738240	-7.723252	-3.644357	30	6	0	-11.506322	-3.916245	2.287936
8	1	0	-8.491067	-8.502885	-1.295761	31	1	0	-11.196001	-3.937414	0.134025
9	1	0	-8.265656	-6.865248	0.572641	32	6	0	-9.524188	-3.923291	3.691886
10	1	0	-8.765087	-5.281791	-4.175548	33	6	0	-4.940572	-3.975030	2.877903
11	6	0	-8.363298	-2.786835	-0.768289	34	1	0	-6.486430	-3.939651	4.395350
12	6	0	-8.312522	-1.439308	-0.480049	35	6	0	-10.918740	-3.910542	3.548964
13	6	0	-8.415603	-0.509646	-1.549857	36	1	0	-12.602468	-3.904179	2.194191
14	6	0	-8.567131	-0.973606	-2.870937	37	1	0	-9.065225	-3.916719	4.690495
15	6	0	-8.613264	-2.343259	-3.149053	38	1	0	-4.133629	-3.959593	3.628868
16	6	0	-8.514359	-3.249957	-2.108875	39	1	0	-11.552093	-3.894001	4.448397
17	1	0	-8.210716	-1.093981	0.561456	40	6	0	-2.820582	-4.623654	-0.125898
18	1	0	-8.632944	-0.260378	-3.708962	41	6	0	-2.207952	-3.379935	1.769721
19	1	0	-8.727302	-2.686379	-4.187889	42	6	0	-1.339896	-4.376550	-0.188478
20	6	0	-8.272972	-3.967907	0.182014	43	6	0	-0.970826	-3.624810	0.953425
21	6	0	-6.988412	-3.974755	0.991969	44	6	0	-0.414702	-4.770337	-1.149444
22	6	0	-9.344252	-3.947495	1.255879	45	6	0	0.341509	-3.229401	1.190071
23	6	0	-5.684187	-3.990005	0.544495	46	1	0	-0.701901	-5.355382	-2.037257
						47	1	0	0.628716	-2.644276	2.077861
						48	6	0	-7.817367	1.854583	-2.171458
						49	6	0	-8.834477	1.497219	-0.085037
						50	6	0	-7.951291	3.183943	-1.484674
						51	6	0	-8.566554	2.968765	-0.227541
						52	6	0	-7.573006	4.449785	-1.919497

53	6	0	-8.834370	4.008944	0.656135	104	1	0	8.671362	-5.330898	4.233730
54	6	0	-7.841007	5.489945	-1.035951	105	1	0	8.671370	-0.313418	3.718630
55	1	0	-7.093599	4.617093	-2.896753	106	1	0	8.579255	-7.775974	3.726577
56	6	0	-8.456205	5.274768	0.221185	107	6	0	7.904680	1.808078	2.172048
57	1	0	-9.313159	3.841472	1.633753	108	6	0	8.860234	1.404050	0.065411
58	6	0	1.266713	-3.623251	0.229138	109	6	0	8.042055	3.125163	1.462368
59	6	0	2.747402	-3.376322	0.166535	110	6	0	8.620804	2.881899	0.193309
60	6	0	0.897629	-4.374995	-0.912797	111	6	0	7.695823	4.403244	1.888256
61	6	0	2.134723	-4.619983	-1.729137	112	6	0	8.882729	3.904812	-0.712105
62	7	0	-3.288500	-4.000477	1.071823	113	6	0	7.957766	5.426085	0.983013
63	7	0	3.215309	-3.999923	-1.030883	114	1	0	7.244526	4.592147	2.874942
64	8	0	-2.284764	-2.768378	2.834919	115	6	0	8.536606	5.182768	-0.286296
65	8	0	-3.504107	-5.241700	-0.940623	116	1	0	9.333430	3.715390	-1.698975
66	8	0	2.211486	-5.230769	-2.794757	117	6	0	-7.573444	6.961552	-1.177954
67	8	0	3.431191	-2.757572	0.980535	118	6	0	-8.589612	6.604342	0.908149
68	6	0	4.562494	-4.013240	-1.460454	119	6	0	7.718167	6.903769	1.110210
69	6	0	5.610275	-4.016847	-0.500457	120	6	0	8.673624	6.499854	-0.995995
70	6	0	4.869397	-4.026432	-2.834871	121	7	0	-8.362019	0.878061	-1.283141
71	6	0	6.915046	-4.033990	-0.946254	122	7	0	-8.043187	7.580794	0.020295
72	1	0	5.388498	-3.990640	0.578625	123	7	0	8.166649	7.497964	-0.108854
73	6	0	6.197236	-4.048468	-3.272763	124	7	0	8.409766	0.809537	1.283989
74	1	0	4.063223	-4.038589	-3.586720	125	8	0	-9.073386	6.818448	2.019171
75	6	0	7.218742	-4.051084	-2.339844	126	8	0	-7.053142	7.530094	-2.137359
76	1	0	6.417106	-4.062549	-4.350440	127	8	0	-7.337015	1.639774	-3.284022
77	6	0	9.271080	-4.066880	-1.207863	128	8	0	-9.359031	0.928366	0.871058
78	6	0	8.669120	-4.070486	-2.502555	129	8	0	7.453751	1.619289	3.301284
79	6	0	10.646902	-4.081996	-1.075840	130	8	0	9.351853	0.814677	-0.895973
80	6	0	9.453531	-4.089066	-3.643680	131	8	0	7.232552	7.494920	2.074104
81	6	0	11.434178	-4.100609	-2.237671	132	8	0	9.131244	6.689951	-2.122423
82	1	0	11.121666	-4.077791	-0.084092	133	6	0	-7.975035	8.967219	0.290866
83	6	0	10.847905	-4.104181	-3.499323	134	6	0	-8.029119	9.906082	-0.762221
84	1	0	8.995624	-4.090436	-4.642795	135	6	0	-7.851935	9.432905	1.618038
85	1	0	12.530250	-4.110512	-2.142829	136	6	0	-7.957422	11.268006	-0.484111
86	1	0	11.482214	-4.117248	-4.398140	137	1	0	-8.111016	9.571186	-1.808772
87	6	0	8.198575	-4.046691	-0.134971	138	6	0	-7.789616	10.799912	1.872446
88	6	0	8.319736	-2.859485	0.803646	139	1	0	-7.821080	8.723794	2.460887
89	6	0	8.287090	-5.230006	0.810778	140	6	0	-7.839754	11.721505	0.828329
90	6	0	8.298993	-1.513931	0.502956	141	1	0	-7.995790	11.989020	-1.314817
91	6	0	8.465893	-3.313317	2.147913	142	1	0	-7.698399	11.149579	2.912084
92	6	0	8.236419	-6.583212	0.533476	143	1	0	-7.786737	12.799445	1.038681
93	6	0	8.445740	-4.772771	2.154084	144	6	0	8.114756	8.881351	-0.397690
94	6	0	8.431832	-0.576678	1.562988	145	6	0	8.211168	9.833955	0.639946
95	1	0	8.195436	-1.176867	-0.541011	146	6	0	7.965747	9.330404	-1.727950
96	6	0	8.594395	-2.399607	3.178511	147	6	0	8.155044	11.192845	0.344012
97	6	0	8.343364	-7.492629	1.597206	148	1	0	8.314015	9.512519	1.688876
98	1	0	8.115539	-6.946813	-0.497229	149	6	0	7.919729	10.694549	-2.000515
99	6	0	8.550157	-5.677159	3.197682	150	1	0	7.901738	8.610139	-2.559387
100	6	0	8.581636	-1.031960	2.887381	151	6	0	8.011669	11.629777	-0.971485
101	1	0	8.705163	-2.735288	4.220096	152	1	0	8.226509	11.924715	1.162953
102	6	0	8.497380	-7.047438	2.906242	153	1	0	7.808024	11.031043	-3.042488
103	1	0	8.304380	-8.571754	1.386408	154	1	0	7.971237	12.705387	-1.196039

PIM1

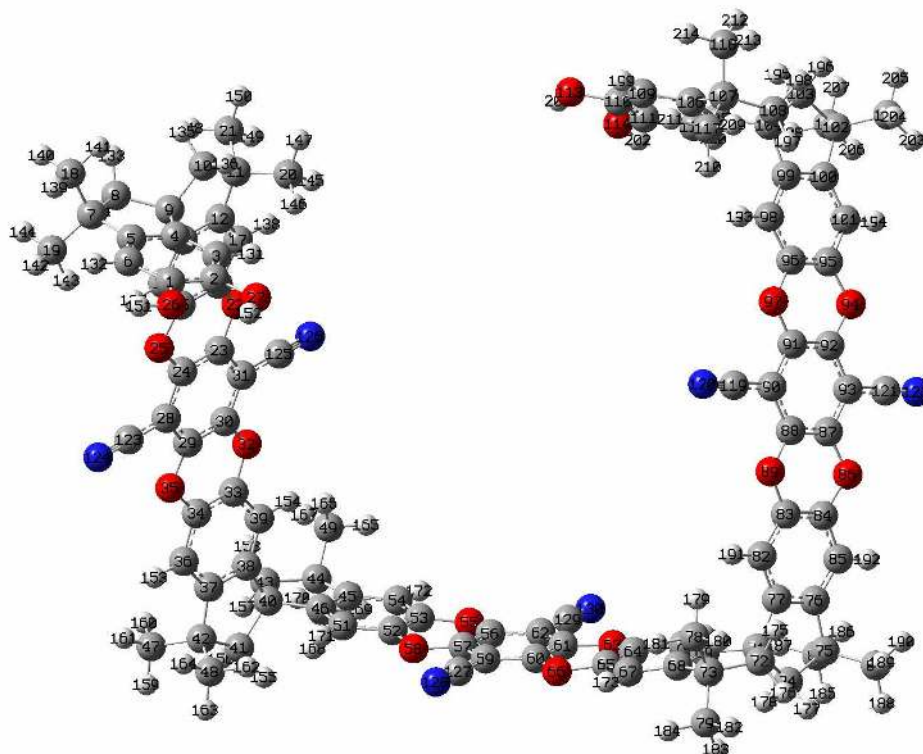


Figure S13. optimized structure of P2

Standard orientation:											
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)								
			X	Y	Z						
1	6	0	-10.002625	5.607662	5.835551	34	6	0	-7.816972	-4.059607	-1.572541
2	6	0	-8.719819	5.546592	5.252529	35	8	0	-8.690878	-3.134973	-0.996366
3	6	0	-8.563300	5.712243	3.865297	36	6	0	-8.073494	-5.411646	-1.298341
4	6	0	-9.694728	5.932883	3.094856	37	6	0	-7.232993	-6.353477	-1.874562
5	6	0	-10.976311	5.997857	3.682153	38	6	0	-6.152899	-5.966438	-2.698851
6	6	0	-11.141130	5.835106	5.049340	39	6	0	-5.895478	-4.629466	-2.968008
7	6	0	-12.043421	6.257480	2.654345	40	6	0	-5.395552	-7.162498	-3.208424
8	6	0	-11.267604	6.362889	1.317400	41	6	0	-6.138692	-8.376077	-2.599668
9	6	0	-9.762619	6.144312	1.607044	42	6	0	-7.313643	-7.850021	-1.738020
10	6	0	-8.886898	7.339991	1.161322	43	6	0	-5.360933	-7.194468	-4.755587
11	6	0	-7.846231	6.830485	0.133207	44	6	0	-3.881298	-7.176302	-5.213707
12	6	0	-8.144537	5.361371	0.000226	45	6	0	-3.095853	-7.150329	-3.930271
13	6	0	-9.219094	4.974487	0.832245	46	6	0	-3.946905	-7.141719	-2.802548
14	6	0	-9.665900	3.660887	0.866665	47	6	0	-8.640648	-8.369360	-2.265387
15	6	0	-9.013649	2.732809	0.040860	48	6	0	-7.143710	-8.268292	-0.286894
16	6	0	-7.948132	3.115847	-0.781273	49	6	0	-3.592837	-5.938505	-6.046913
17	6	0	-7.493352	4.442875	-0.810794	50	6	0	-3.554107	-8.421069	-6.021381
18	6	0	-12.777327	7.554453	2.950790	51	6	0	-3.433643	-7.127767	-1.513091
19	6	0	-13.038708	5.110123	2.606164	52	6	0	-2.037677	-7.123277	-1.371340
20	6	0	-6.433150	7.047624	0.648709	53	6	0	-1.194818	-7.124858	-2.488619
21	6	0	-8.016457	7.538675	-1.200202	54	6	0	-1.715249	-7.136475	-3.791643
22	8	0	-7.289457	2.216605	-1.624319	55	8	0	0.197748	-7.130211	-2.378651
23	6	0	-7.644335	0.887997	-1.430446	56	6	0	0.669338	-6.944688	-1.084980
24	6	0	-8.714795	0.503444	-0.605556	57	6	0	-0.176130	-6.948495	0.036382
25	8	0	-9.499571	1.422578	0.078222	58	8	0	-1.549348	-7.134060	-0.062136
26	8	0	-10.054831	5.438429	7.205355	59	6	0	0.339546	-6.776745	1.334536
27	8	0	-7.577727	5.335234	5.987580	60	6	0	1.730784	-6.617622	1.474863
28	6	0	-9.056252	-0.852186	-0.445312	61	6	0	2.575780	-6.610252	0.353231
29	6	0	-8.304168	-1.809194	-1.152231	62	6	0	2.058190	-6.765102	-0.946306
30	6	0	-7.234542	-1.424936	-1.976136	63	8	0	3.953834	-6.466931	0.454782
31	6	0	-6.880577	-0.070377	-2.121776	64	6	0	4.404745	-6.145097	1.737593
32	8	0	-6.479787	-2.340330	-2.699501	65	6	0	3.563417	-6.156727	2.855962
33	6	0	-6.749390	-3.676325	-2.392553	66	8	0	2.208345	-6.485508	2.772929
						67	6	0	4.050805	-5.848790	4.135257
						68	6	0	5.398093	-5.537055	4.250017
						69	6	0	6.246186	-5.519558	3.120200
						70	6	0	5.764999	-5.821074	1.853791
						71	6	0	7.657047	-5.158977	3.498786

72	6	0	7.602873	-4.952412	5.031782	149	1	0	-7.294540	7.128917	-1.947338
73	6	0	6.147476	-5.187458	5.507414	150	1	0	-7.824690	8.631879	-1.078687
74	6	0	8.657420	-6.262089	3.076719	151	1	0	-10.986069	5.437558	7.467057
75	6	0	9.700166	-5.637441	2.116434	152	1	0	-7.836751	5.204964	6.913054
76	6	0	9.292896	-4.192170	2.015782	153	1	0	-8.915831	-5.696060	-0.651975
77	6	0	8.143649	-3.922975	2.792162	154	1	0	-5.060357	-4.309776	-3.607927
78	6	0	5.579817	-3.927687	6.140131	155	1	0	-5.436275	-8.975130	-1.967790
79	6	0	6.087339	-6.330449	6.506807	156	1	0	-6.524780	-9.045969	-3.406846
80	6	0	9.644835	-6.308880	0.754211	157	1	0	-5.870581	-8.111493	-5.141214
81	6	0	11.101592	-5.764381	2.689800	158	1	0	-5.902173	-6.306170	-5.167278
82	6	0	7.598604	-2.648085	2.853727	159	1	0	-8.672039	-9.482848	-2.189244
83	6	0	8.231916	-1.636154	2.116301	160	1	0	-8.780357	-8.078852	-3.333969
84	6	0	9.366399	-1.904347	1.341811	161	1	0	-9.483307	-7.945121	-1.667677
85	6	0	9.914954	-3.194364	1.278961	162	1	0	-6.166913	-7.905982	0.115000
86	8	0	10.023520	-0.916426	0.604787	163	1	0	-7.174270	-9.381273	-0.203974
87	6	0	9.358355	0.302917	0.562934	164	1	0	-7.965925	-7.839134	0.335170
88	6	0	8.223165	0.573162	1.343668	165	1	0	-2.512086	-5.907118	-6.326491
89	8	0	7.675125	-0.358634	2.216390	166	1	0	-3.839485	-5.012371	-5.473888
90	6	0	7.585495	1.826665	1.287946	167	1	0	-4.204824	-5.955370	-6.980584
91	6	0	8.130044	2.805929	0.436443	168	1	0	-3.766942	-9.342349	-5.428318
92	6	0	9.264626	2.534770	-0.346002	169	1	0	-2.473862	-8.421364	-6.304879
93	6	0	9.892547	1.276109	-0.302093	170	1	0	-4.169242	-8.443978	-6.952900
94	8	0	9.836752	3.478668	-1.189181	171	1	0	-4.080601	-7.122845	-0.623918
95	6	0	9.101466	4.660321	-1.313751	172	1	0	-1.039572	-7.138165	-4.658636
96	6	0	7.970899	4.930270	-0.534797	173	1	0	3.376849	-5.862543	5.003517
97	8	0	7.491916	4.039319	0.429537	174	1	0	6.410512	-5.814041	0.963620
98	6	0	7.260015	6.132022	-0.675616	175	1	0	7.928321	-3.913199	5.287979
99	6	0	7.722788	7.044561	-1.613405	176	1	0	8.294620	-5.662124	5.548674
100	6	0	8.866144	6.772619	-2.397908	177	1	0	9.169885	-6.691468	3.972493
101	6	0	9.566659	5.582549	-2.263569	178	1	0	8.113073	-7.094656	2.564857
102	6	0	9.174653	7.909668	-3.334321	179	1	0	5.627125	-3.072165	5.424062
103	6	0	8.069803	8.955355	-3.042434	180	1	0	6.164112	-3.662456	7.053808
104	6	0	7.144498	8.395905	-1.934996	181	1	0	4.513796	-4.090593	6.430384
105	6	0	5.715209	8.318756	-2.395277	182	1	0	6.675950	-6.070648	7.419324
106	6	0	4.863429	9.076742	-1.563792	183	1	0	6.507641	-7.264206	6.062715
107	6	0	5.627483	9.737237	-0.448272	184	1	0	5.028671	-6.523161	6.805794
108	6	0	7.096190	9.303122	-0.681314	185	1	0	9.918928	-7.387105	0.848329
109	6	0	3.501714	9.153657	-1.811224	186	1	0	10.361580	-5.816009	0.053830
110	6	0	2.981356	8.455405	-2.914890	187	1	0	8.617887	-6.236986	0.321654
111	6	0	3.835944	7.700651	-3.745487	188	1	0	11.376231	-6.841864	2.791015
112	6	0	5.212394	7.629967	-3.489321	189	1	0	11.160615	-5.283248	3.695191
113	8	0	1.629221	8.556879	-3.136966	190	1	0	11.839046	-5.268310	2.013504
114	8	0	3.235331	7.063215	-4.813947	191	1	0	6.706197	-2.419579	3.454233
115	6	0	10.550602	8.486700	-3.047057	192	1	0	10.807007	-3.388264	0.666706
116	6	0	9.107991	7.449016	-4.780923	193	1	0	6.372227	6.327683	-0.056616
117	6	0	5.134306	9.251183	0.904502	194	1	0	10.457129	5.355636	-2.866499
118	6	0	5.496684	11.249041	-0.524118	195	1	0	7.474784	9.155378	-3.968416
119	6	0	6.436907	2.097256	2.073732	196	1	0	8.530914	9.921197	-2.720427
120	7	0	5.495131	2.318573	2.718632	197	1	0	7.477772	8.743362	0.208878
121	6	0	11.033261	1.000091	-1.097445	198	1	0	7.745337	10.202117	-0.820759
122	7	0	11.968107	0.773521	-1.750576	199	1	0	2.827453	9.739656	-1.171100
123	6	0	-10.131456	-1.241664	0.392693	200	1	0	5.871522	7.039795	-4.141682
124	7	0	-11.012891	-1.561284	1.080268	201	1	0	1.406682	7.993777	-3.894856
125	6	0	-5.795909	0.316155	-2.948863	202	1	0	3.889804	6.470234	-5.208671
126	7	0	-4.906157	0.632627	-3.627115	203	1	0	11.335164	7.709183	-3.211897
127	6	0	-0.514356	-6.775854	2.466264	204	1	0	10.615697	8.840041	-1.990299
128	7	0	-1.214665	-6.775122	3.394378	205	1	0	10.752112	9.349403	-3.726586
129	6	0	2.910566	-6.751885	-2.079106	206	1	0	9.871704	6.655907	-4.967545
130	7	0	3.609609	-6.740567	-3.008104	207	1	0	9.307929	8.308381	-5.465065
131	1	0	-7.558111	5.662353	3.422685	208	1	0	8.098082	7.033575	-5.013850
132	1	0	-12.137564	5.882703	5.510123	209	1	0	5.728848	9.724828	1.722157
133	1	0	-11.436956	7.365485	0.853396	210	1	0	5.235831	8.141987	0.983817
134	1	0	-11.634047	5.589024	0.597624	211	1	0	4.058902	9.520282	1.039505
135	1	0	-9.517445	8.141444	0.703938	212	1	0	5.864922	11.626368	-1.507860
136	1	0	-8.366911	7.780727	2.048506	213	1	0	6.093539	11.726371	0.289784
137	1	0	-10.498671	3.341988	1.510000	214	1	0	4.426714	11.546838	-0.406803
138	1	0	-6.653763	4.727141	-1.460647						
139	1	0	-13.295335	7.484790	3.937633						
140	1	0	-13.539351	7.752844	2.159252						
141	1	0	-12.062831	8.411284	2.983967						
142	1	0	-13.555915	5.009303	3.590665						
143	1	0	-12.518694	4.148742	2.377657						
144	1	0	-13.804576	5.299682	1.816236						
145	1	0	-5.691920	6.627317	-0.073098						
146	1	0	-6.294072	6.545069	1.636223						
147	1	0	-6.235196	8.139499	0.771683						
148	1	0	-9.052314	7.397731	-1.591219						

[ⁱ] Thiemann, F., Piehler, T. Haase, D., Saak, W., Lützen, A., *Eur. J. Org. Chem.* **2005**, 1991-2001

[ⁱⁱ] **Gaussian 03**, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, *Gaussian, Inc.*, Wallingford CT, **2004**.