Supporting Information for

ortho-Phenylene Oligomers with Terminal Push–Pull Substitution

Jian He, Sanyo M. Mathew, Sarah D. Cornett, Stephan C. Grundy, and C. Scott Hartley*

Department of Chemistry & Biochemistry, Miami University, Oxford, OH 45056

Supplemental Figures

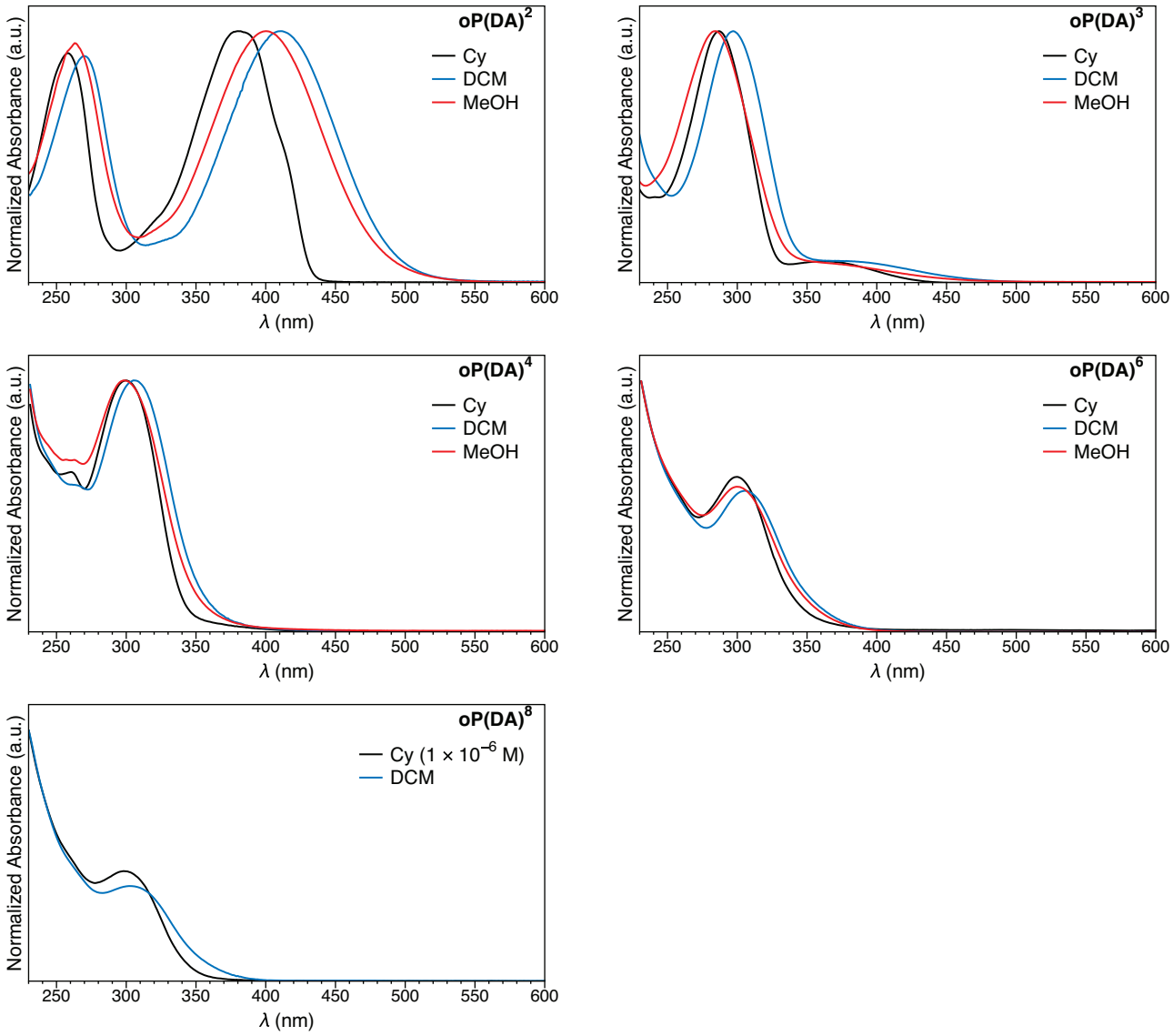


Fig. S1 UV/vis spectra of **oP(DA)^n** in cyclohexane, dichloromethane, and methanol.

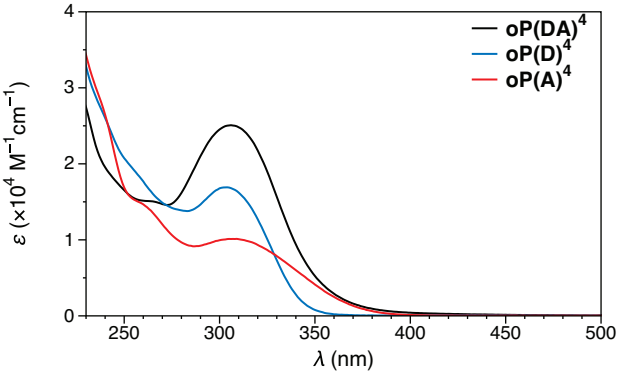


Fig. S2 UV/vis spectra of **oP(D)^4** and **oP(A)^4**.

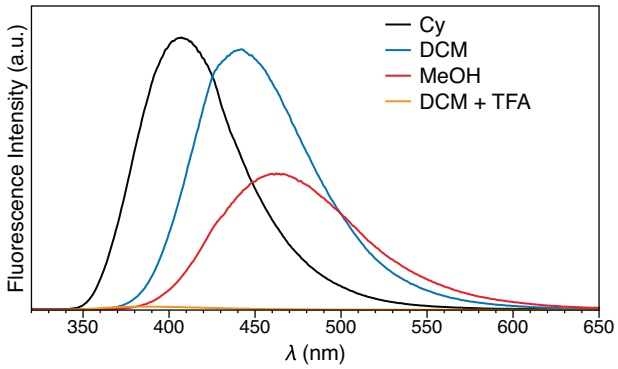


Fig. S3 Fluorescence spectra of **oP(D)^4**. The spectra are taken at identical concentrations and instrumental settings.

NMR Spectra of oP(DA)^6

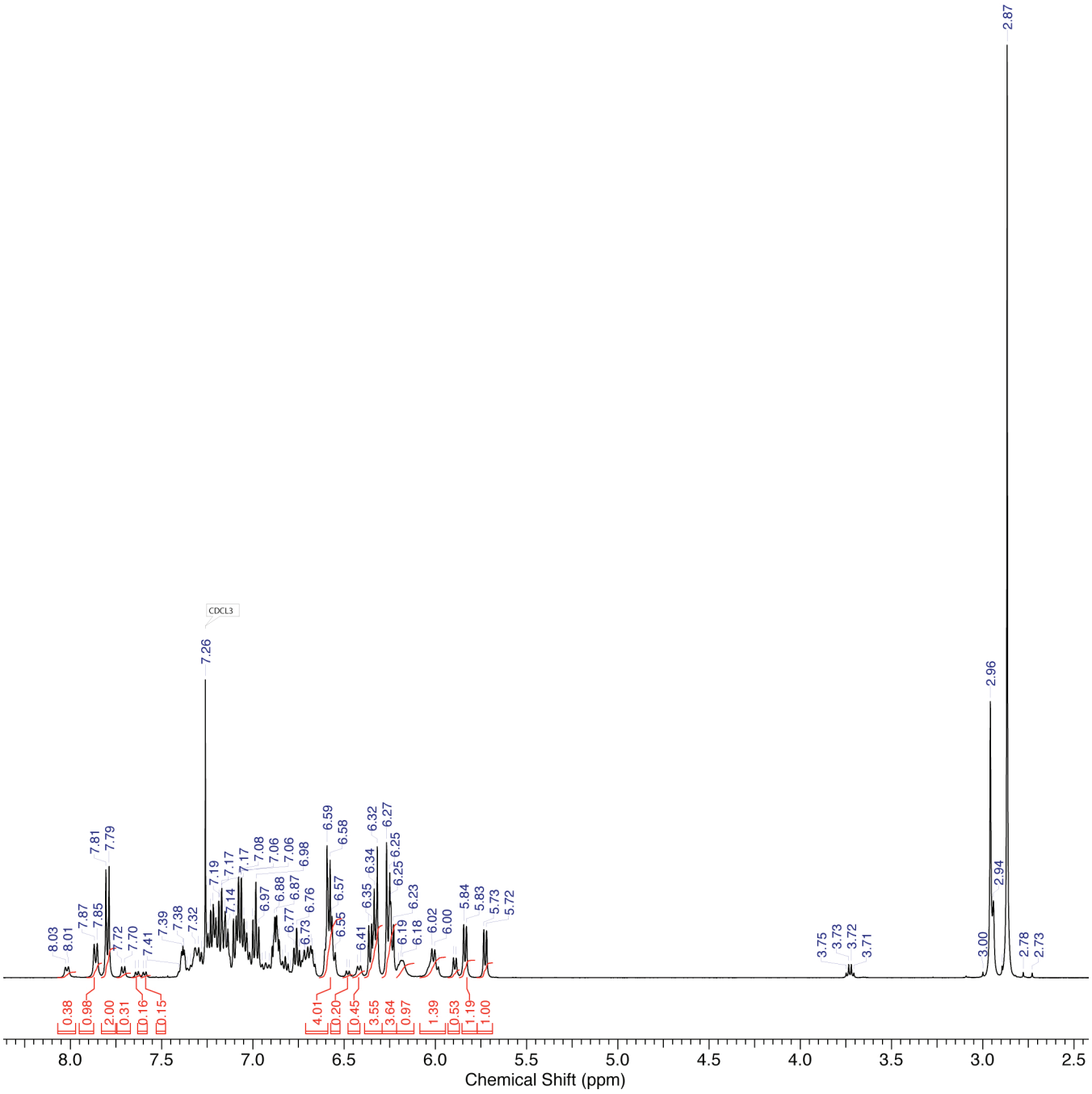


Fig. S4 ^{1}H NMR spectrum (500 MHz, 0 °C, $CDCl_3$) of **oP(DA)^6**.

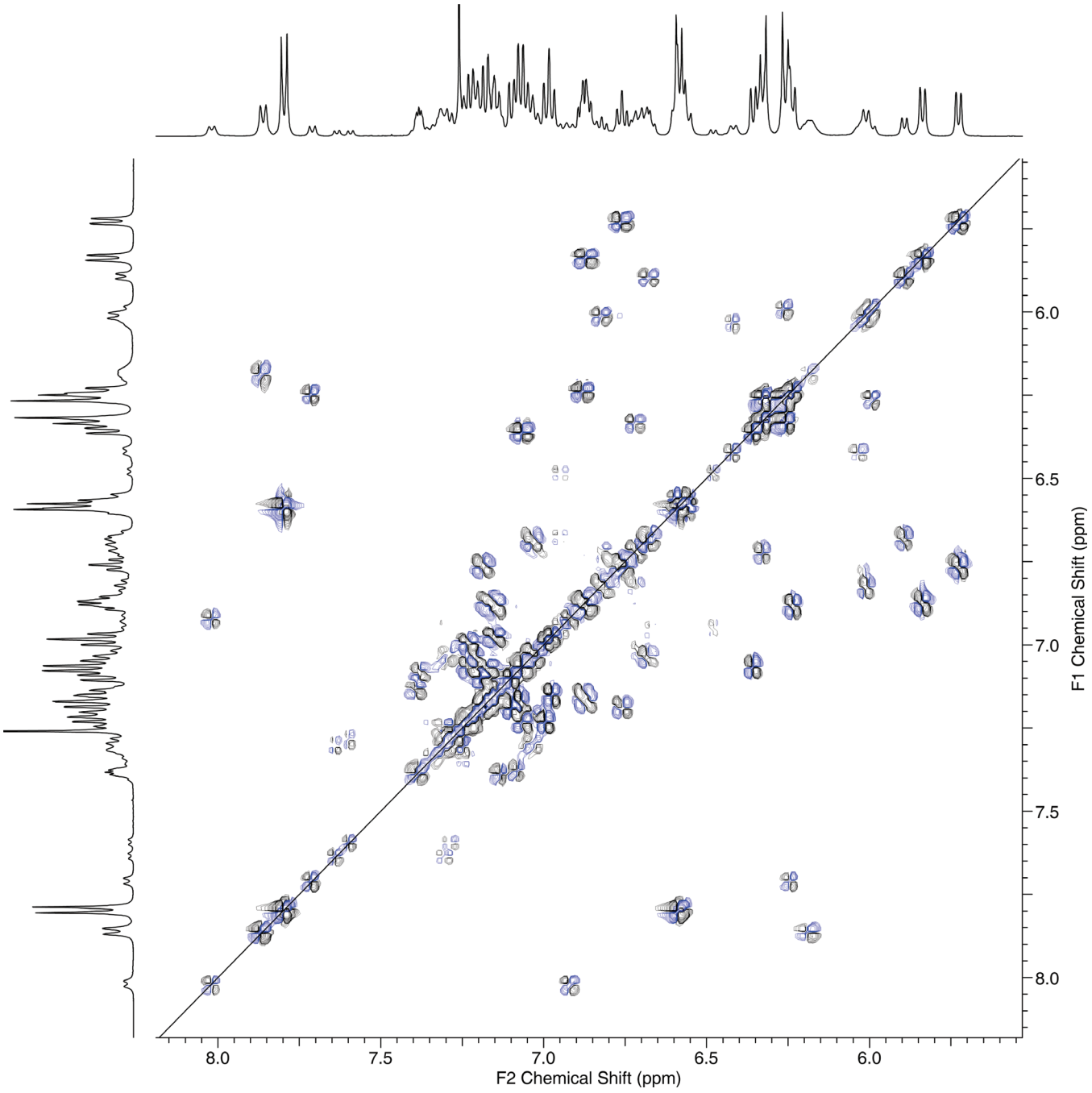


Fig. S5 DQFCOSY spectrum (500 MHz, 0 °C, $CDCl_3$) of **oP(DA)^6**.

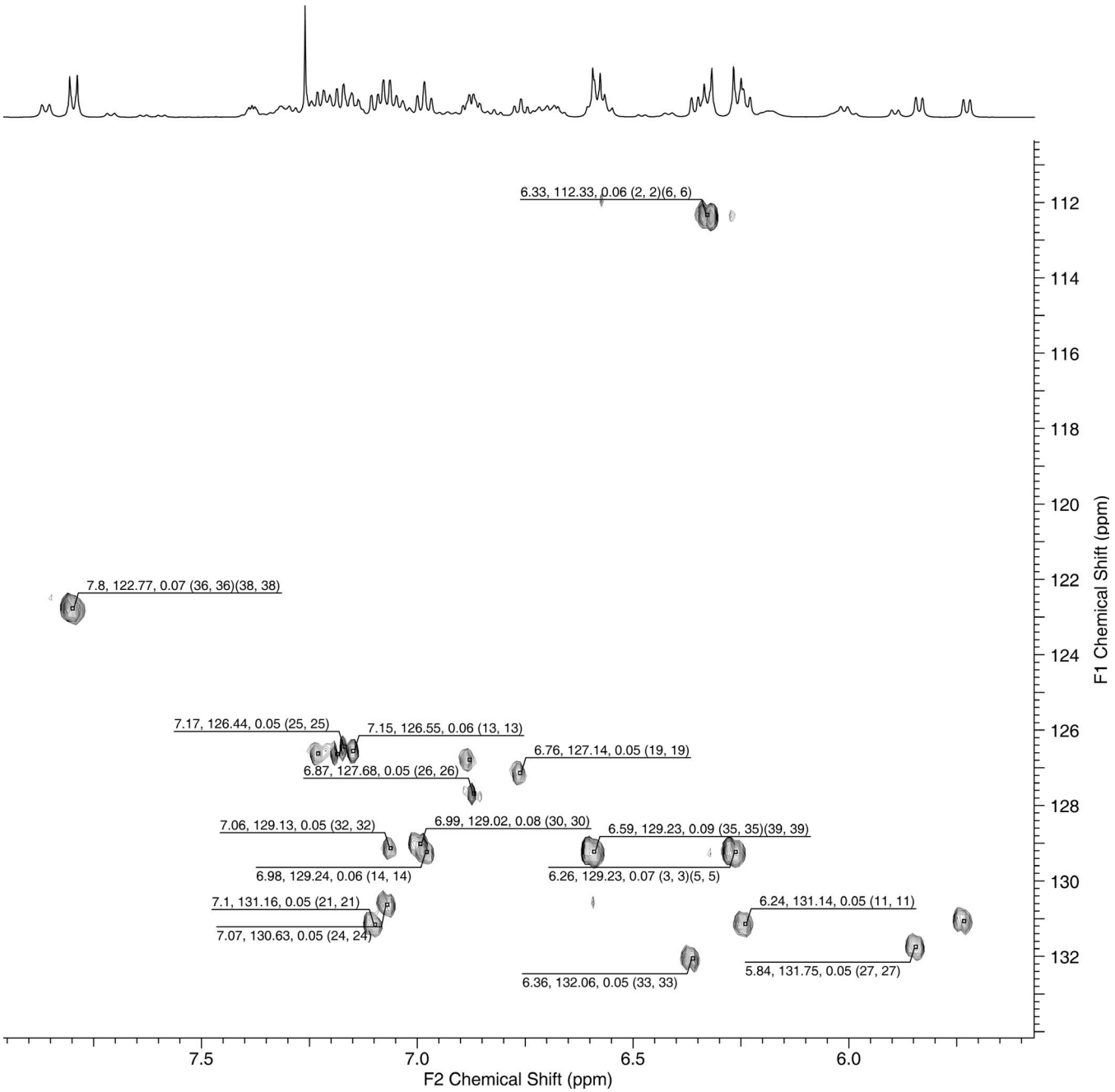


Fig. S6 HMQC spectrum (500 MHz, 0 °C, $CDCl_3$) of **oP(DA)^6** (aromatic region).

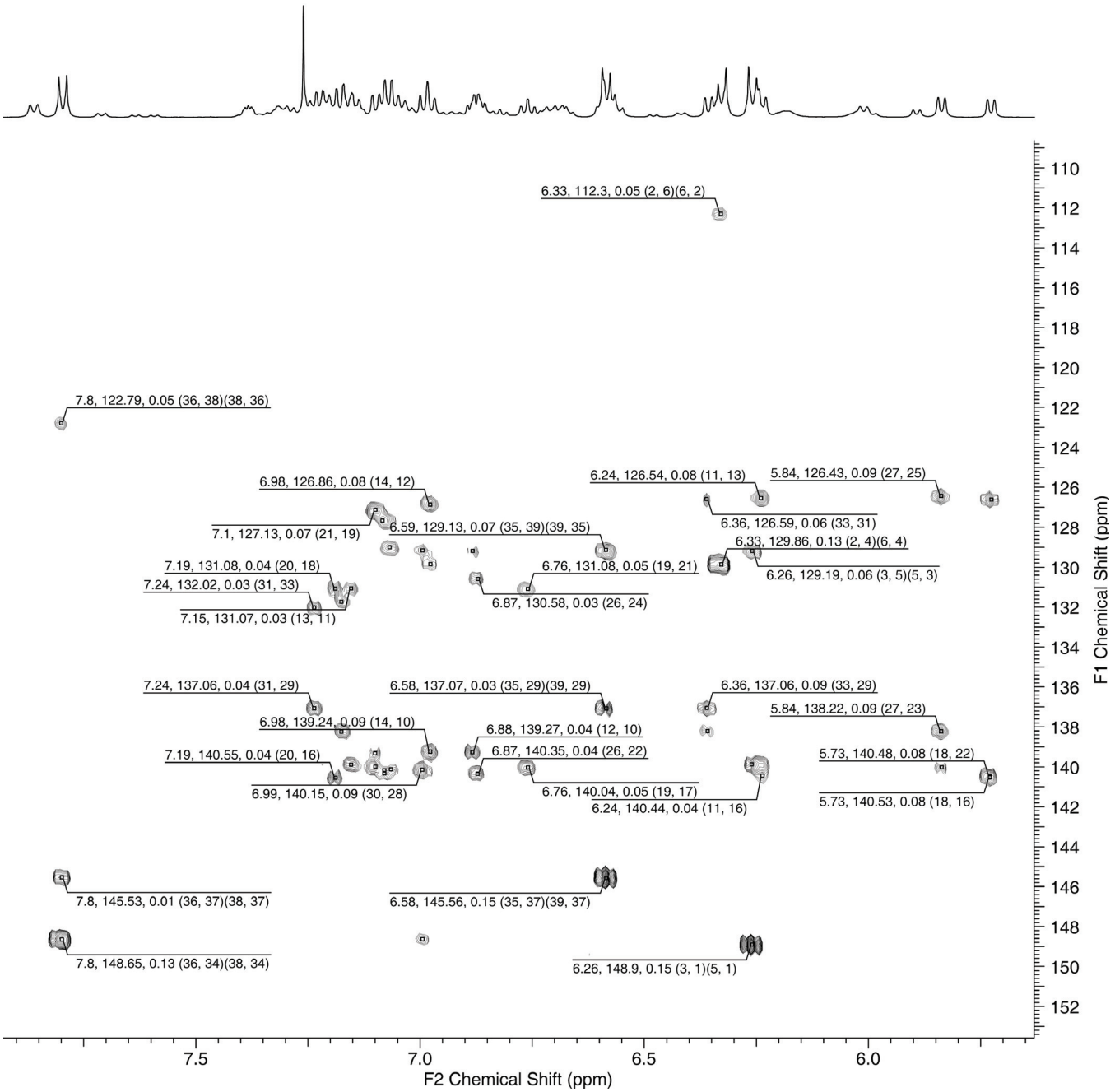


Fig. S7 HMBC spectrum (500 MHz, 0 °C, $CDCl_3$) of **oP(DA)^6** (aromatic region).

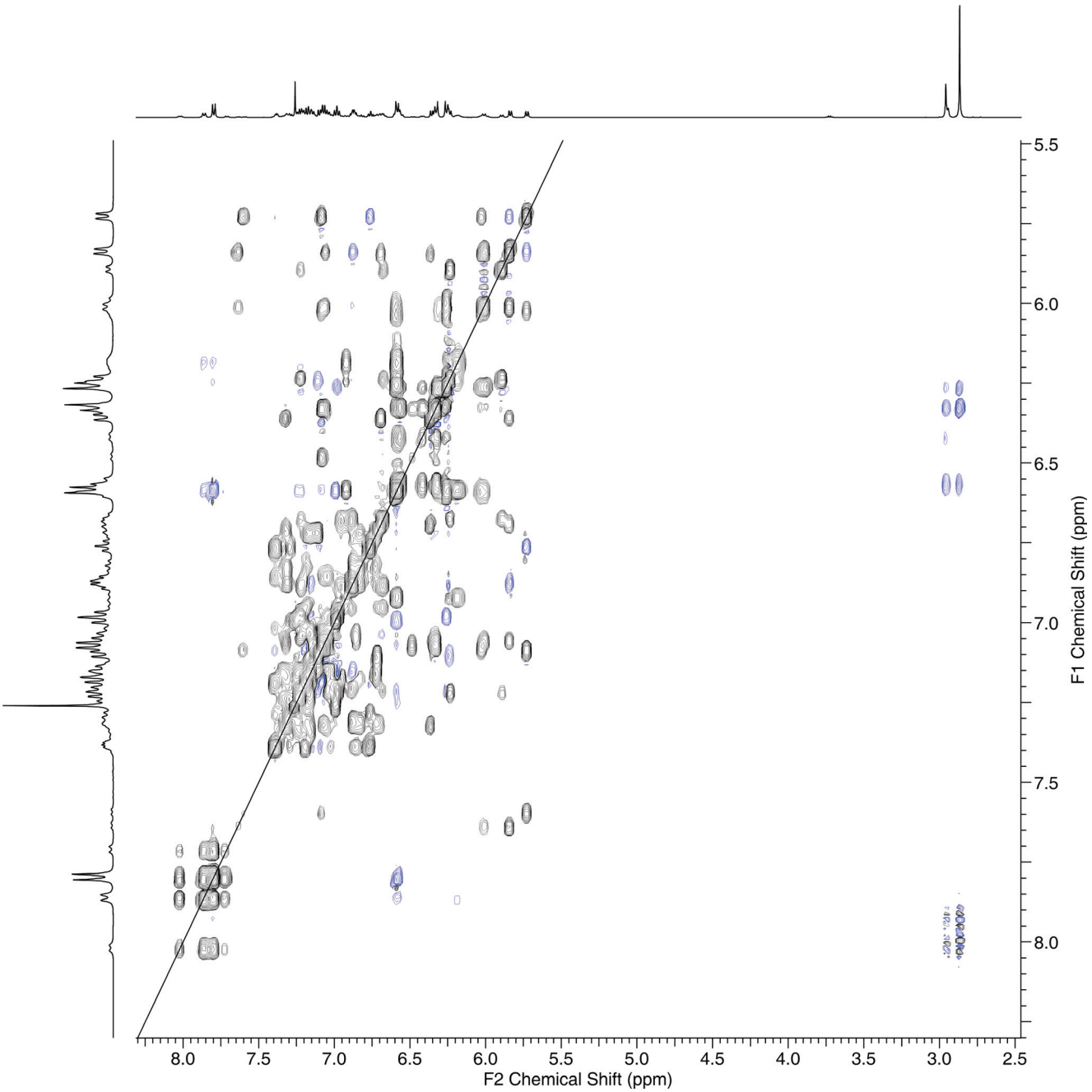


Fig. S8 EXSY spectrum (500 MHz, 0 °C, $CDCl_3$) of **oP(DA)^6**.

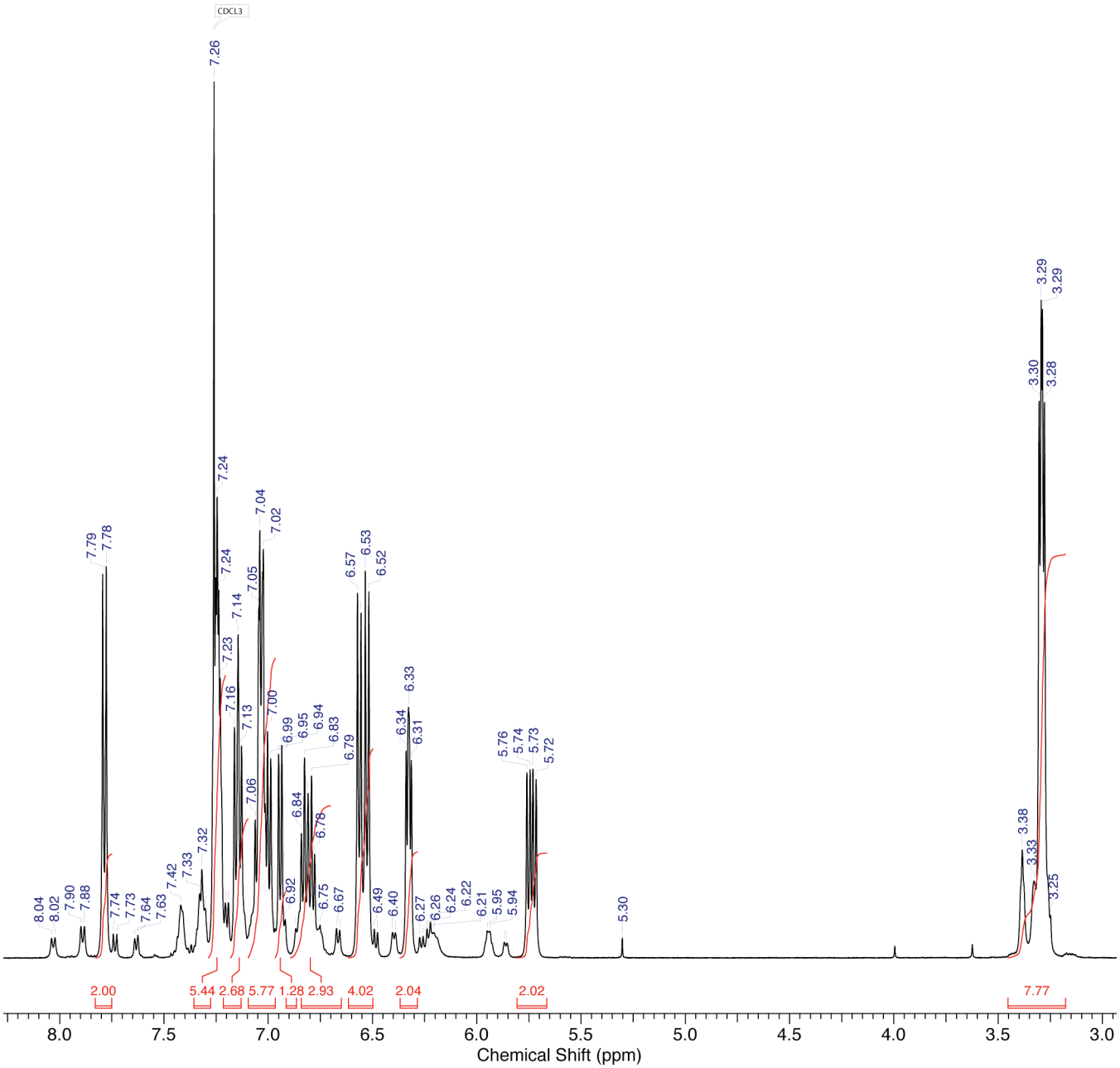


Fig. S9 ^{1}H NMR spectrum (500 MHz, 0 °C, $CDCl_3$) of **oP(DA)^{6}** + TFA.

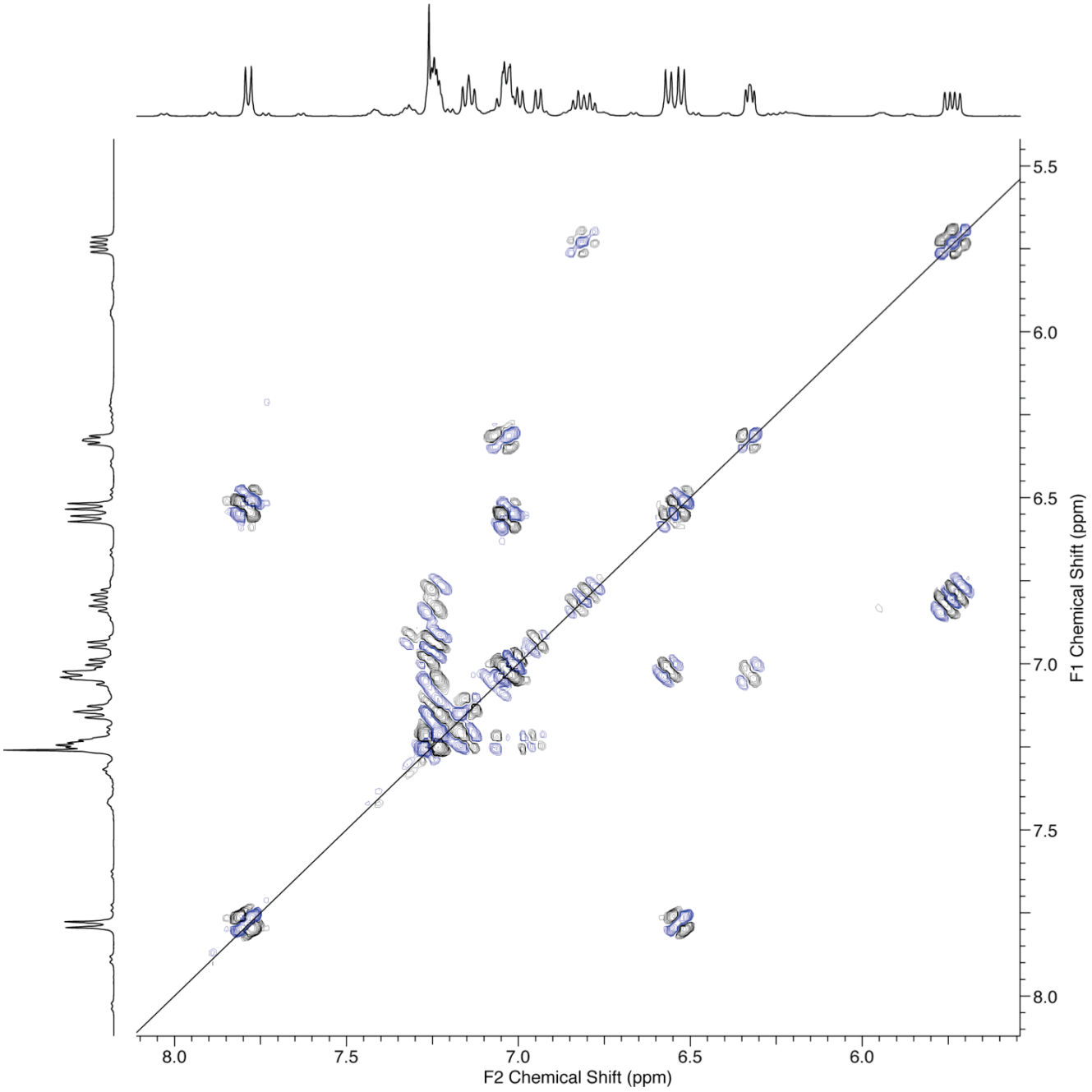


Fig. S10 DQFCOSY spectrum (500 MHz, 0 °C, $CDCl_3$) of **oP(DA)^6** + TFA.

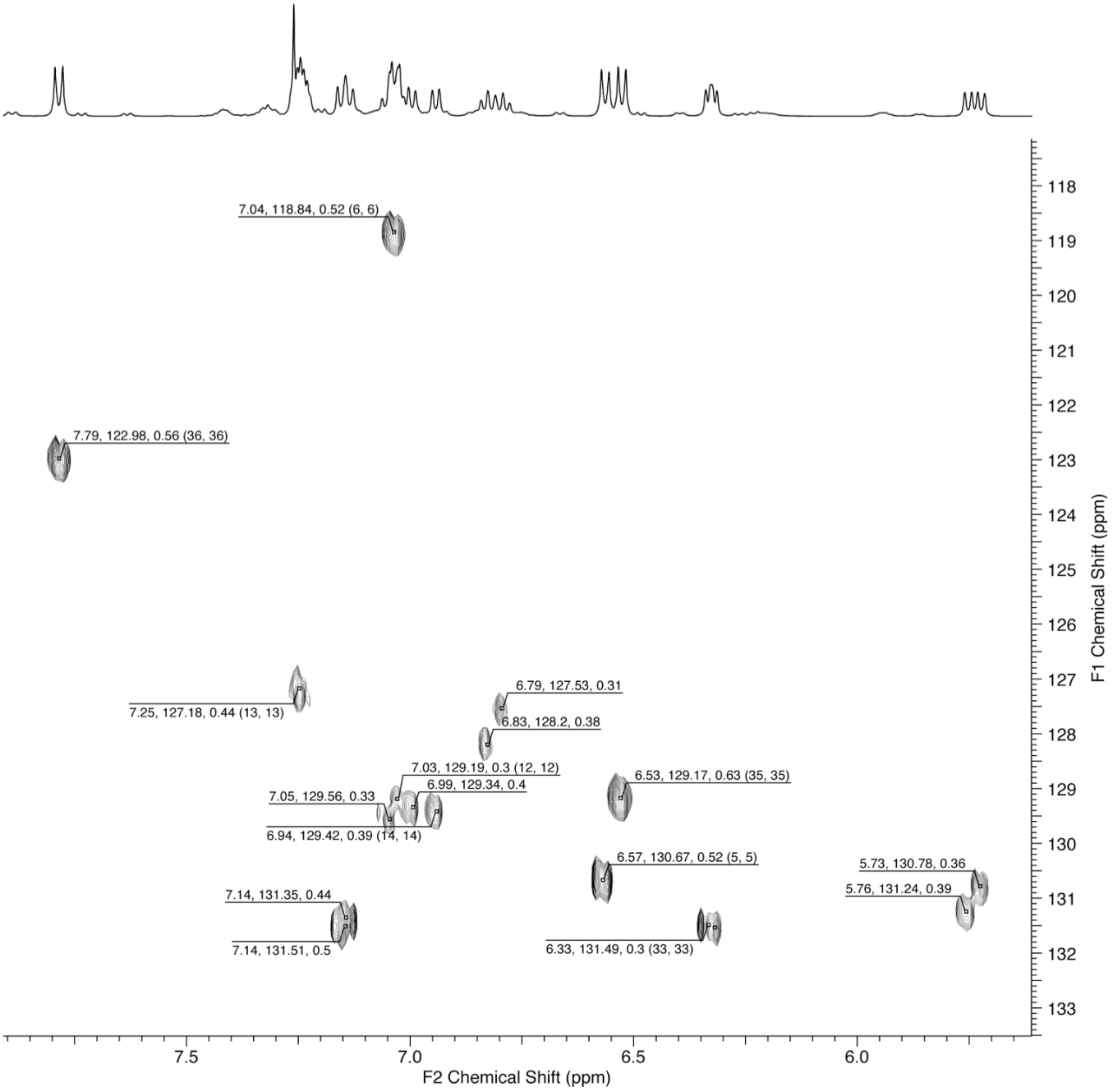


Fig. S11 HMQC spectrum (500 MHz, 0 °C, $CDCl_3$) of **oP(DA)^6** + TFA.

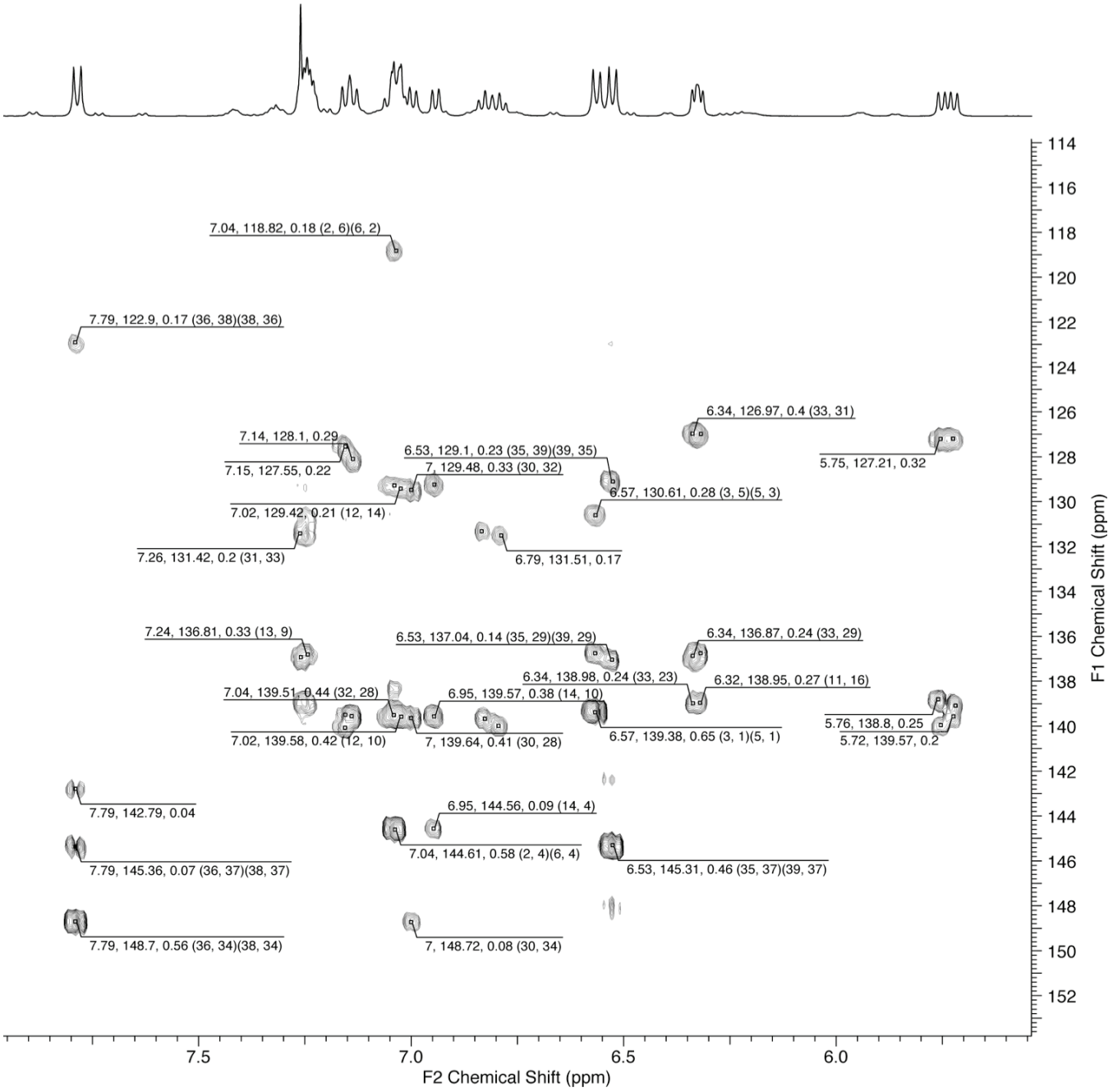


Fig. S12 HMBC spectrum (500 MHz, 0 °C, $CDCl_3$) of **oP(DA)^6** + TFA.

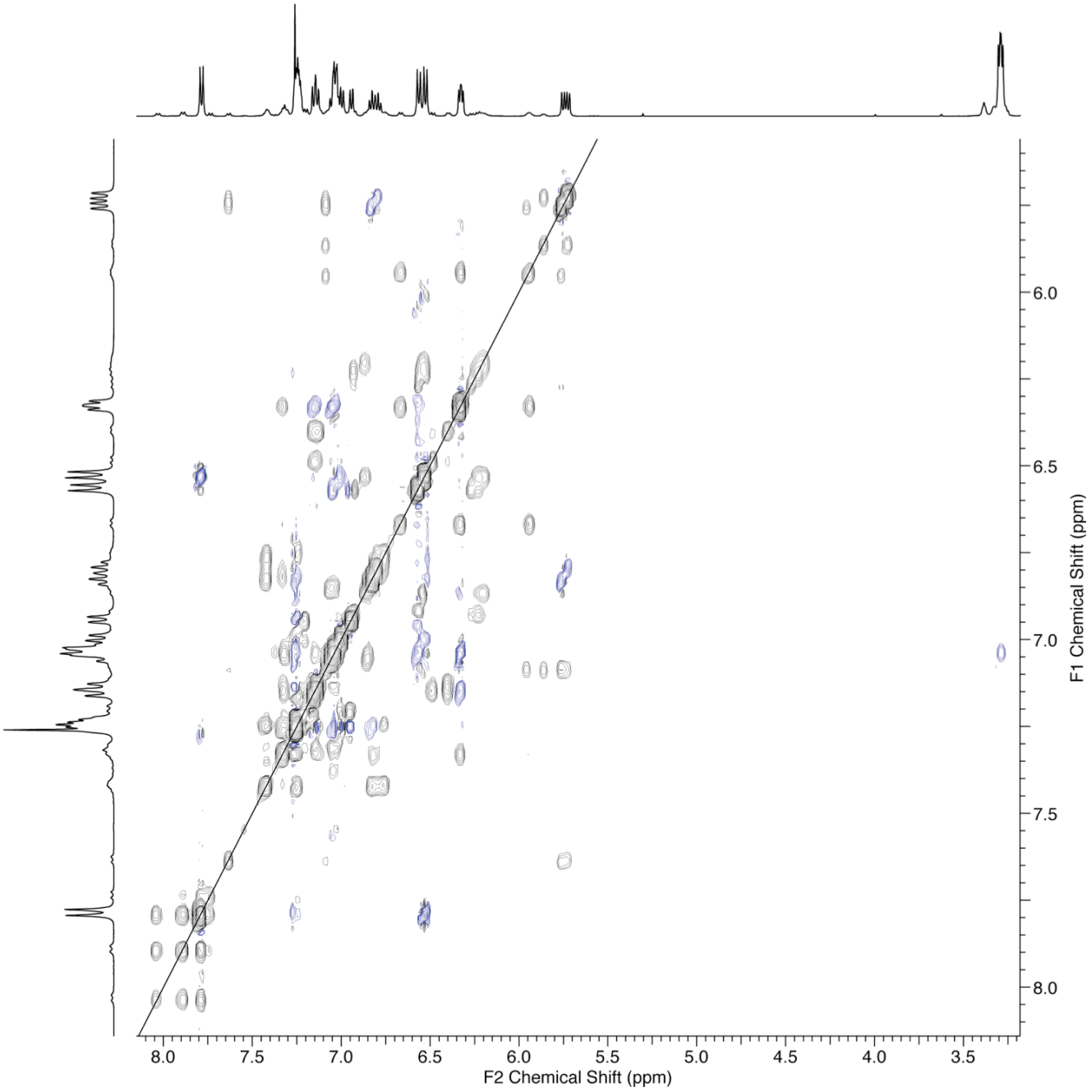


Fig. S13 EXSY spectrum (500 MHz, 0 °C, $CDCl_3$) of **oP(DA)^6** + TFA.

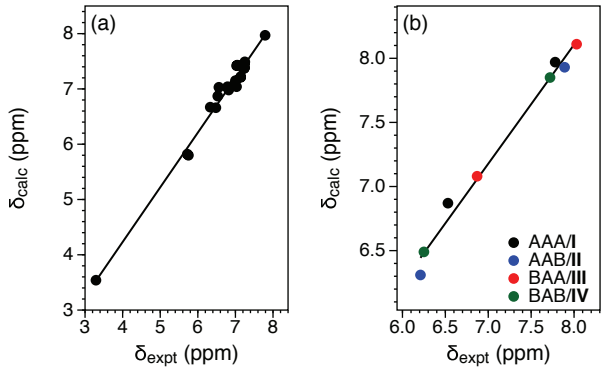


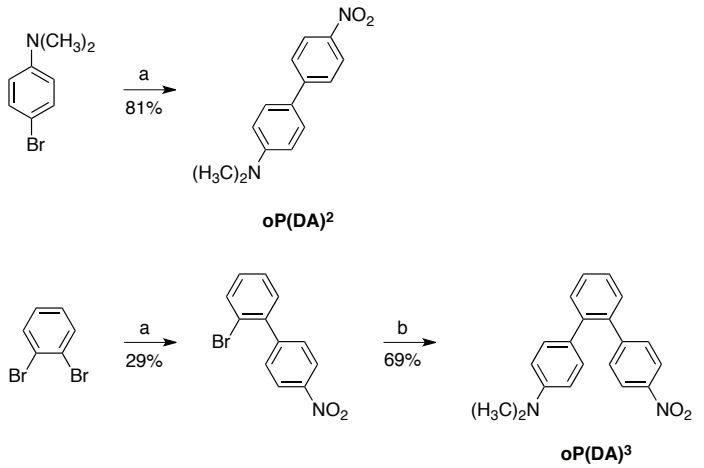
Fig. S14 Calculated (GIAO/PCM/WP04/6-31G(d)//B3LYP/6-31+G(d,p)) vs experimental chemical shifts for **oP(DA)^6** + TFA. (a) Calculated for AAA geometry vs **I**. (b) H_a and H_b for all four conformers.

Data for Optimized Geometries

Table S1 Energies and zero-point energy corrections for all optimized geometries (B3LYP/6-31+G(d,p)).

Compound	Imag. Freq.	Energy (E_h)	ZPC (E_h)	Total (E_h)
oP(DA)^6 AAA	0	−1726.081719	0.578929	−1725.502789
oP(DA)^6 AAB	0	−1726.082441	0.579103	−1725.503338
oP(DA)^6 BAA	0	−1726.081146	0.579011	−1725.502134
oP(DA)^6 BAB	0	−1726.081374	0.579179	−1725.502196
[oP(DA)^6 + H$^+$] AAA	0	−1726.455757	0.593752	−1725.862005
[oP(DA)^6 + H$^+$] AAB	0	−1726.455561	0.593940	−1725.861621
[oP(DA)^6 + H$^+$] BAA	0	−1726.455415	0.593884	−1725.861531
[oP(DA)^6 + H$^+$] BAB	0	−1726.455866	0.594051	−1725.861814
oP(DA)^8	0	−2188.204903	0.739974	−2187.464929
oP(DA)^8 + H$^+$	0	−2188.580514	0.754913	−2187.825601

Synthesis of oP(DA)^2 and oP(DA)^3



Scheme S1 Reagents and conditions: (a) 4-nitrophenylboronic acid pinacol ester, $Pd(PPh_3)_4$, Na_2CO_3(aq), toluene, EtOH; (b) 4-dimethylaminophenylboronic acid, $Pd(OAc)_2$, SPhos, K_3PO_4, THF, water.

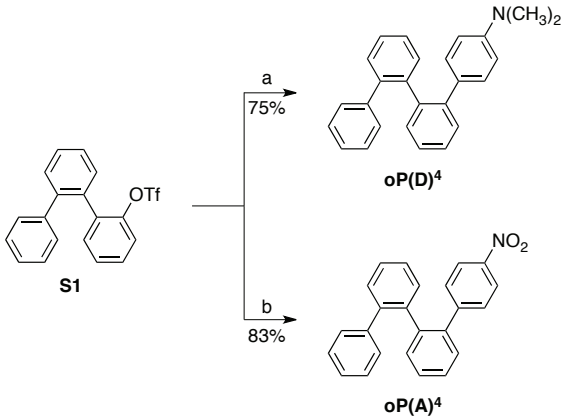
***N*,*N*-Dimethyl-4-(4-nitrophenyl)aniline (oP(DA)^2):** A Schlenk tube was charged with 4-bromo-*N*,*N*-dimethylaniline (200 mg, 1.0 mmol), 4-nitrophenylboronic acid pinacol ester (249 mg, 1.0 mmol),

and $Pd(PPh_3)_4$ (23 mg, 0.02 mmol), then evacuated and backfilled with argon (3×). Degassed toluene (4.0 mL), ethanol (0.6 mL), and 2 M Na_2CO_3(aq) (2.0 mL) were added under the positive pressure of argon. The mixture was heated at 100 °C for 24 h, then diluted with EtOAc (10mL), washed with brine (10 mL). The aqueous layer extracted with EtOAc (3 × 10 mL). The organic layers were dried over $MgSO_4$, filtered, and concentrated. The crude product was purified by flash chromatography (3:1 hexanes:EtOAc) and then recrystallized from abs. ethanol to afford 197 mg (81%) of **oP(DA)²** as deep red solid: m.p. 249.4°C; ^{1}H NMR (CDCl3, 500 MHz) δ 3.05 (s, 6H), 6.84 (m, 2H), 7.58 (m, 2H), 7.69 (m, 2H), 8.25 (m, 2H). The ^{1}H NMR spectrum is in agreement with previous reports.[1] Prior to UV/vis and fluorescence spectroscopy, the compound was again recrystallized from EtOH.

2-Bromo-4'-nitrobiphenyl: The same procedure as for **oP(DA)²** was used with 1,2-dibromobenzene (236 mg, 1.0 mmol) and 4-nitrophenylboronic acid pinacol ester (249 mg, 1.0 mmol) as starting materials. The crude product was purified by flash chromatography (6:1 hexanes:EtOAc) to afford 80 mg (29%) of 2-bromo-4'-nitrobiphenyl as a yellow solid: ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.28 (td, 1H, *J* = 7.7, 1.8 Hz), 7.32 (dd, 1H, *J* = 7.6, 1.4 Hz), 7.43 (td, 1H, *J* = 7.3, 1.0 Hz), 7.60 (m, 2H), 7.72 (dd, 1H, *J* = 8.0, 1.0 Hz), 8.30 (m, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 122.2, 123.4, 127.8, 130.1, 130.6, 131.0, 133.6, 140.5, 147.4, 147.6; MS (APCI) calc'd for $C_{12}H_9BrNO_2$ ($M+H^+$) 277.9, found 277.9.

oP(DA)³: A Schlenk vacuum tube was charged with 2-bromo-4'-nitrobiphenyl (276 mg, 1.0 mmol), 4-(dimethylamino)phenylboronic acid (198 mg, 1.2 mmol), $Pd(OAc)_2$ (44.9 mg, 0.20 mol), SPhos (98.5 mg, 0.24 mmol), and K_3PO_4 (849 mg, 4.0 mmol), then evacuated and backfilled with argon (3×). Anhydrous THF (2.0 mL) was added followed by water (0.5 mL). The reaction mixture was degassed by three freeze-pump-thaw cycles, then sealed and heated at 90 °C overnight. The reaction mixture was then cooled, diluted with EtOAc (20 mL), and washed with water, acidifying the aqueous layer with 1 M HCl (15 mL). The aqueous layer was extracted with EtOAc, and the combined organic layers washed with water and brine, dried over $MgSO_4$, filtered, and concentrated. The crude product was purified by flash chromatography (12:1 hexane:EtOAc) to afford 219 mg (69%) of **oP(DA)³** as red solid, which was recrystallized from abs. ethanol prior to further analysis: m.p. 140.7 °C; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 2.95 (s, 6H), 6.61 (m, 2H), 6.97 (m, 2H), 7.35 (d, 2H, *J* = 7.8 Hz), 7.40 (s, 2H), 7.47 (s, 2H), 8.11 (m, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 40.5, 112.2, 123.4, 127.0, 128.3, 128.9, 130.4, 130.7, 130.8, 130.9, 138.1, 141.1, 146.4, 149.4, 149.6; MS (ESI) calc'd for $C_{20}H_{19}N_2O_2$ ($M+H^+$) 319.1, found 319.2; HRMS (ESI) calc'd for $C_{20}H_{19}N_2O_2$ ($M+H^+$) 319.1447, found 319.1439.

Synthesis of oP(D)[4] and oP(A)[4]



Scheme S2 Reagents and conditions: (a) 4-dimethylaminophenylboronic acid, $Pd(OAc)_2$, SPhos, K_3PO_4, THF, water; (b) 4-nitrophenylboronic acid, $Pd(OAc)_2$, SPhos, K_3PO_4, THF, water.

oP(D)[4]: The same procedure as for **oP(DA)[3]** was used with **S1**[2] (100 mg, 0.264 mmol) instead of 2-bromo-4'-nitrobiphenyl as starting material. Purification by flash chromatography (4:1 hexane: EtOAc) and recrystallization from hexanes/CH_2Cl_2 gave 69.6 mg (0.199 mmol, 75%) of **oP(D)[4]** as a white solid: m.p. 128.5 °C; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 2.89 (s, 6H), 6.42 (m, 2H), 6.55 (m, 2H), 6.70 (m, 2H), 7.01 (t, 2H, *J* = 7.3 Hz), 7.07 (t, 1H, *J* = 7.3 Hz), 7.16 (dd, 1H, *J* = 7.3, 1.4 Hz), 7.2–7.4 (m, 7H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 40.7, 112.1, 125.8, 126.1, 127.0, 127.2, 127.3, 129.2, 129.7, 129.95, 129.99, 131.64, 131.65, 139.6, 140.6, 141.0, 141.2, 149.0; MS (MALDI) calc'd for $C_{26}H_{24}N$ ($M+H^+$) 350.19, found 349.87; HRMS (ESI) calc'd for $C_{26}H_{24}N$ ($M+H^+$) 350.1909, found 350.1919.

oP(A)[4]: The same procedure as for **oP(DA)[3]** was used with **S1** (100 mg, 0.264 mmol) and 4-nitrophenylboronic acid as starting materials. Purification by flash chromatography (7:3 hexanes:CH_2Cl_2) and recrystallization from abs. ethanol gave 77.4 mg (0.220 mmol, 83%) of **oP(A)[4]** as an off-white solid: m.p. 136.6 °C; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 6.51 (d, 2H, *J* = 7.0 Hz), 6.65 (d, 2H, *J* = 8.5 Hz), 6.98 (t, 2H, *J* = 7.6 Hz), 7.0–7.2 (m, 3H), 7.35–7.55 (m, 6H), 7.81 (d, 2H, *J* = 8.5 Hz); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 122.6, 126.2, 127.6, 127.7, 127.8, 128.2, 128.7, 129.2, 129.6, 129.8, 130.1, 131.6, 132.0, 138.8, 139.0, 140.3, 140.4, 140.7, 146.0, 147.8; MS (MALDI) calc'd for $C_{24}H_{17}CuNO_2$ ($M+Cu^+$)[3] 414.67, found 413.82; HRMS (ESI) calc'd for $C_{26}H_{23}NNa$ ($M+Na^+$) 374.1157, found 374.1157.

NMR Spectra

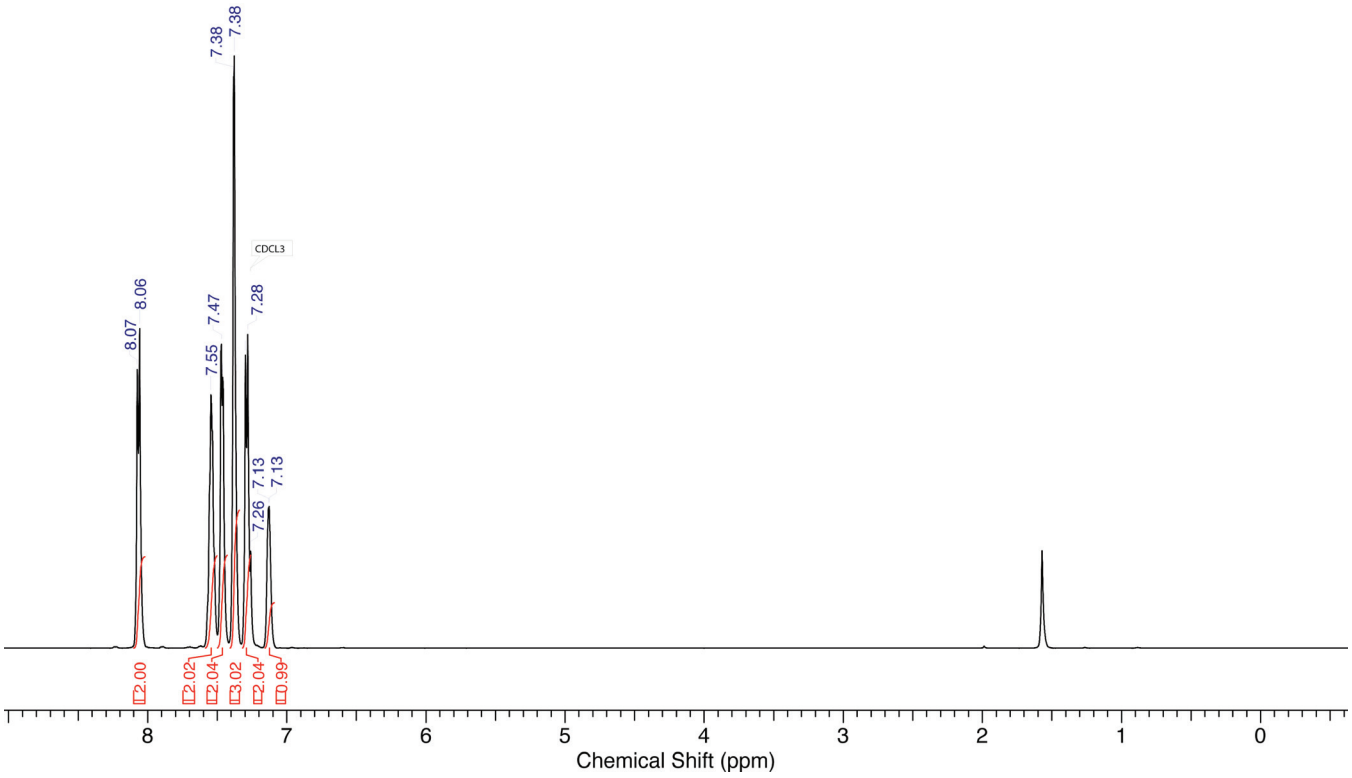


Fig. S15 ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **oP(A)^3-OTf**.

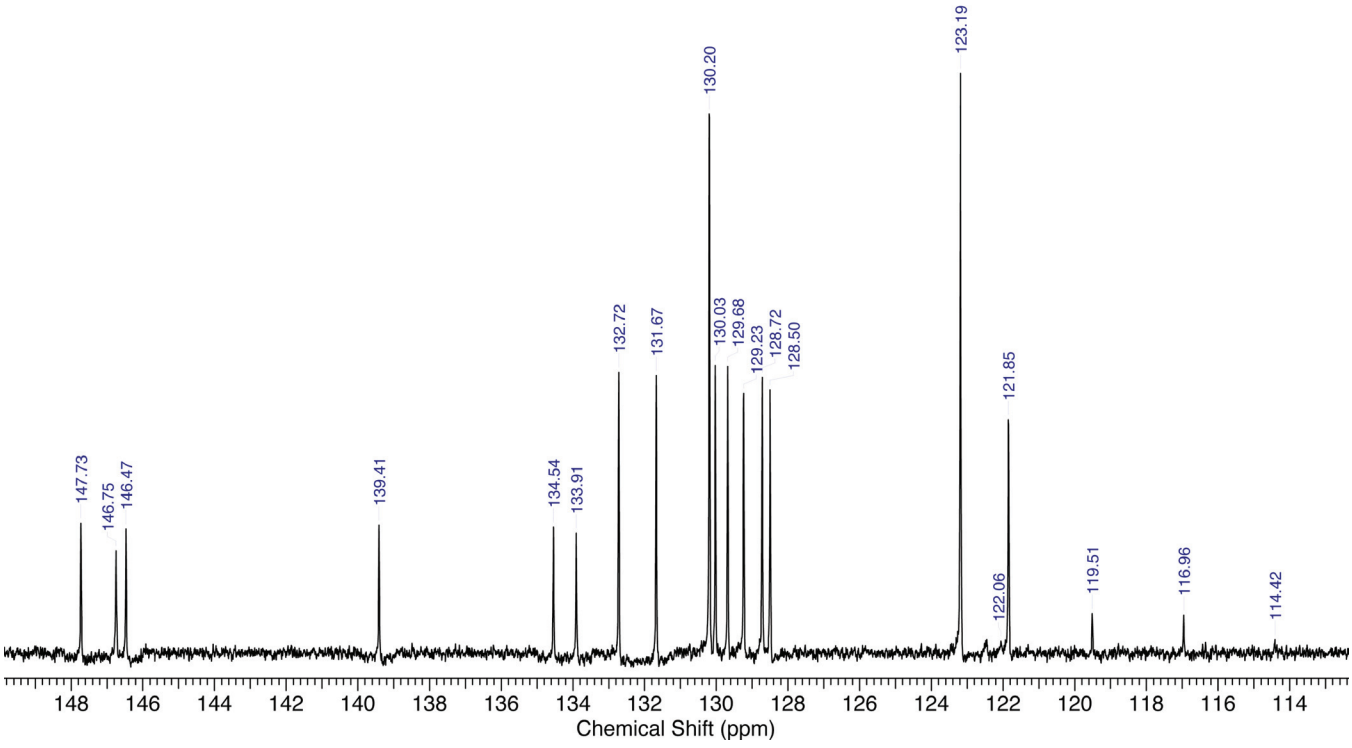


Fig. S16 ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **oP(A)^3-OTf**.

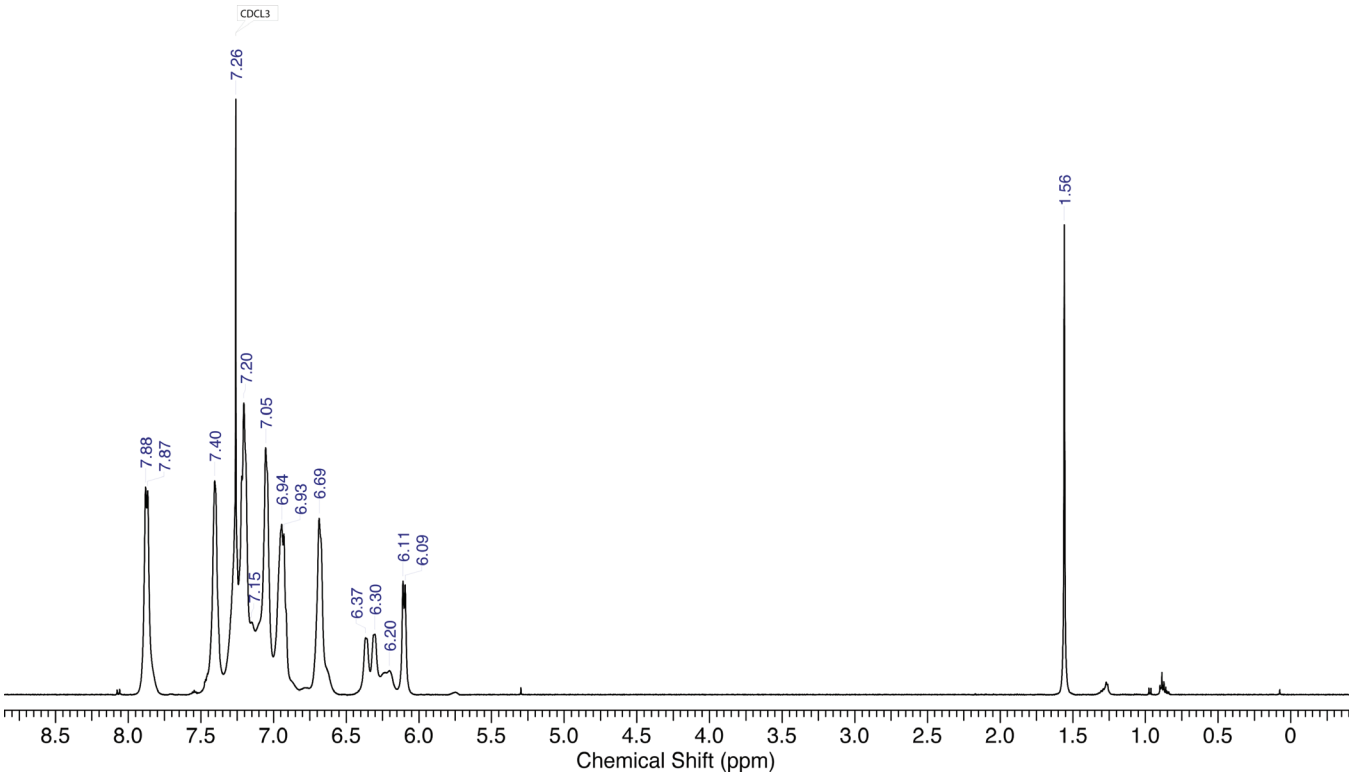


Fig. S17 ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **oP(A)^5-OTf**.

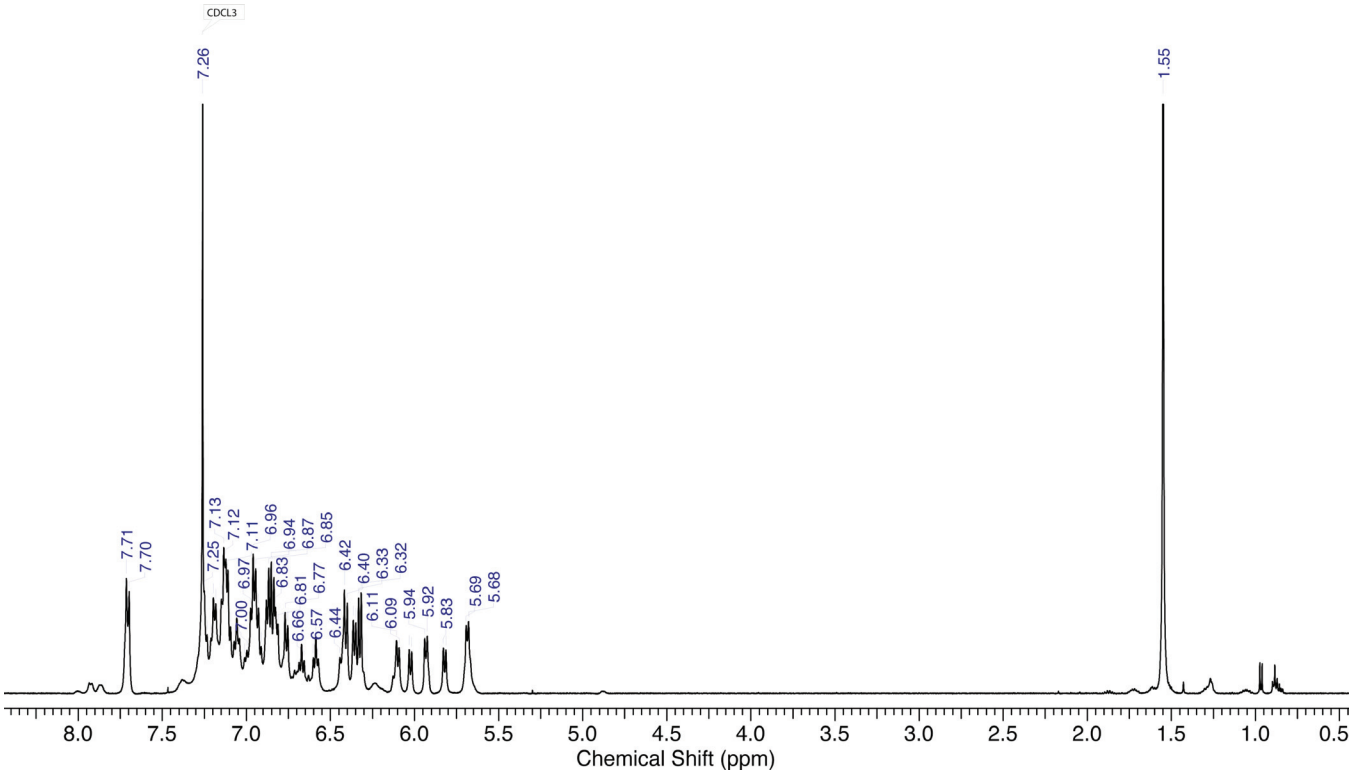


Fig. S18 ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **oP(A)^7-OTf**.

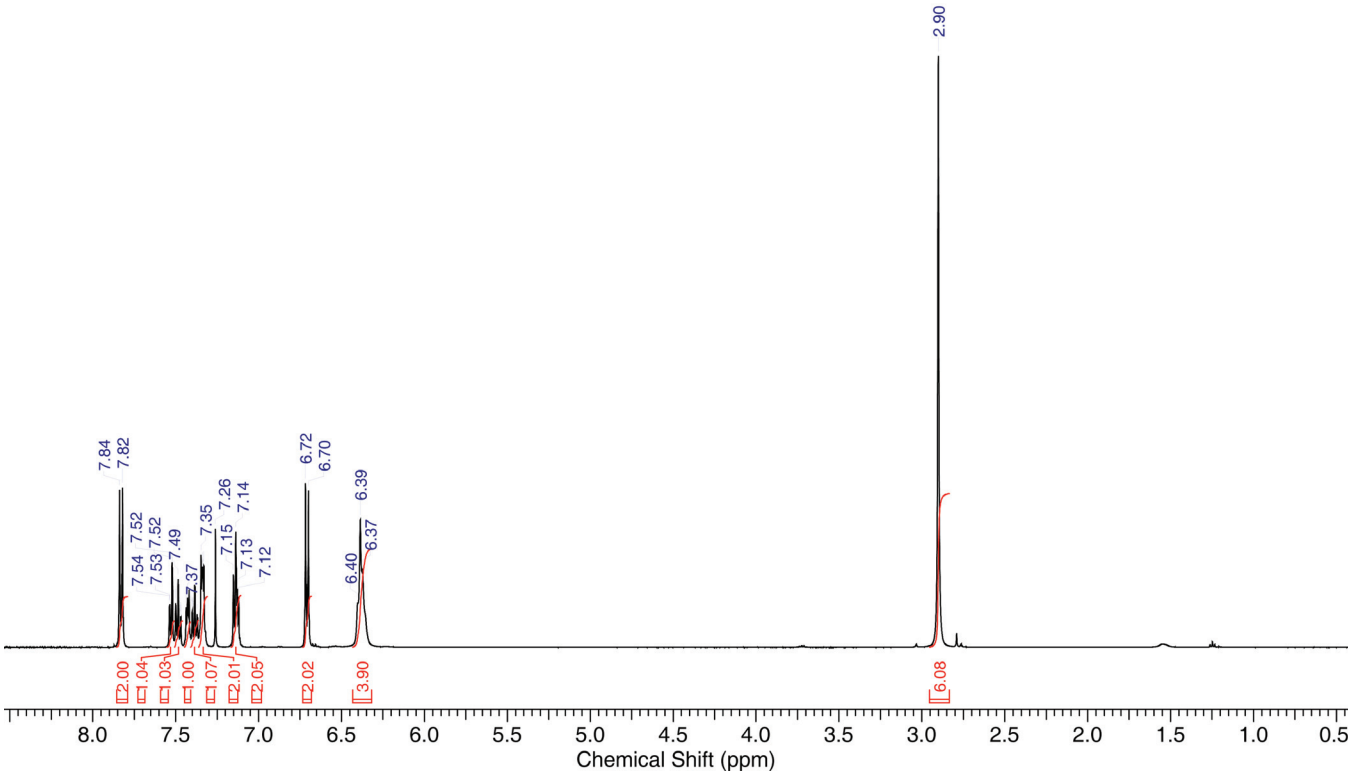


Fig. S19 ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **oP(DA)^4**.

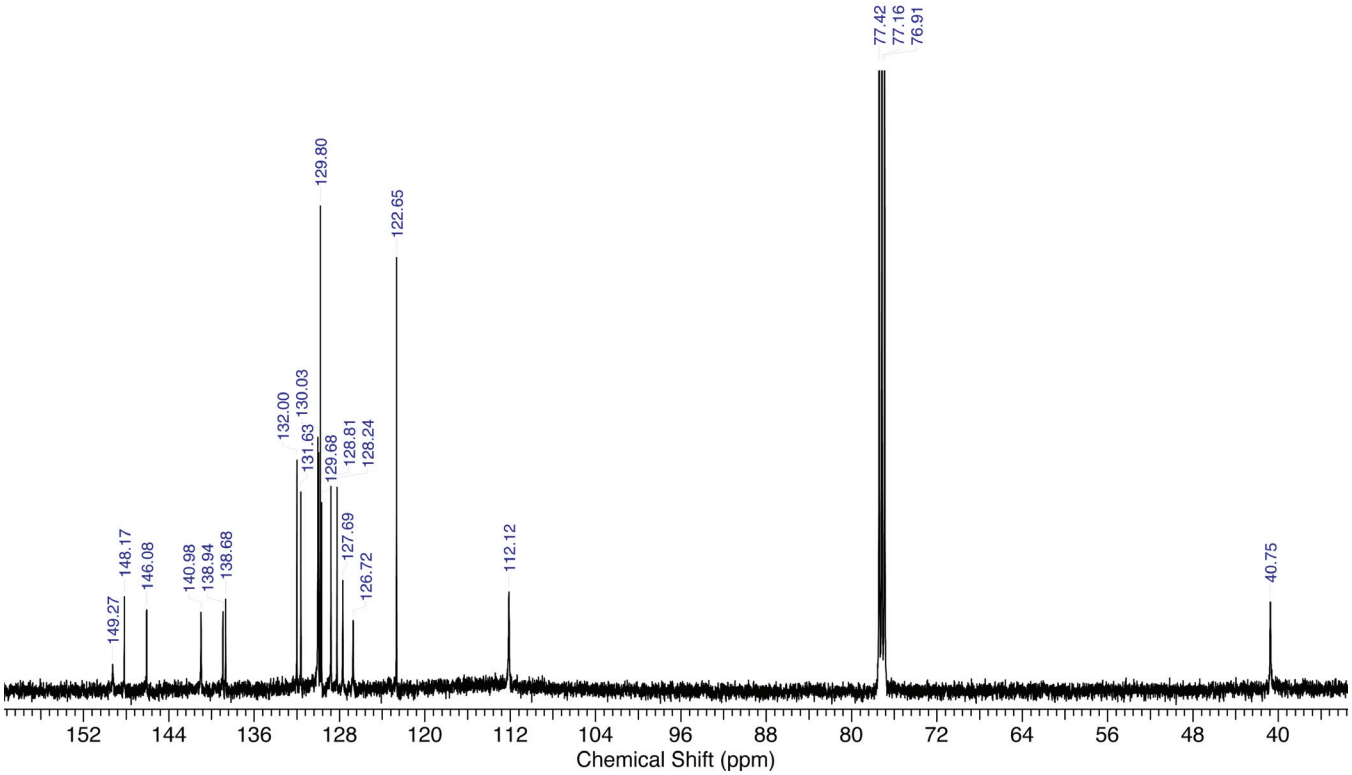


Fig. S20 ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **oP(DA)^4**.

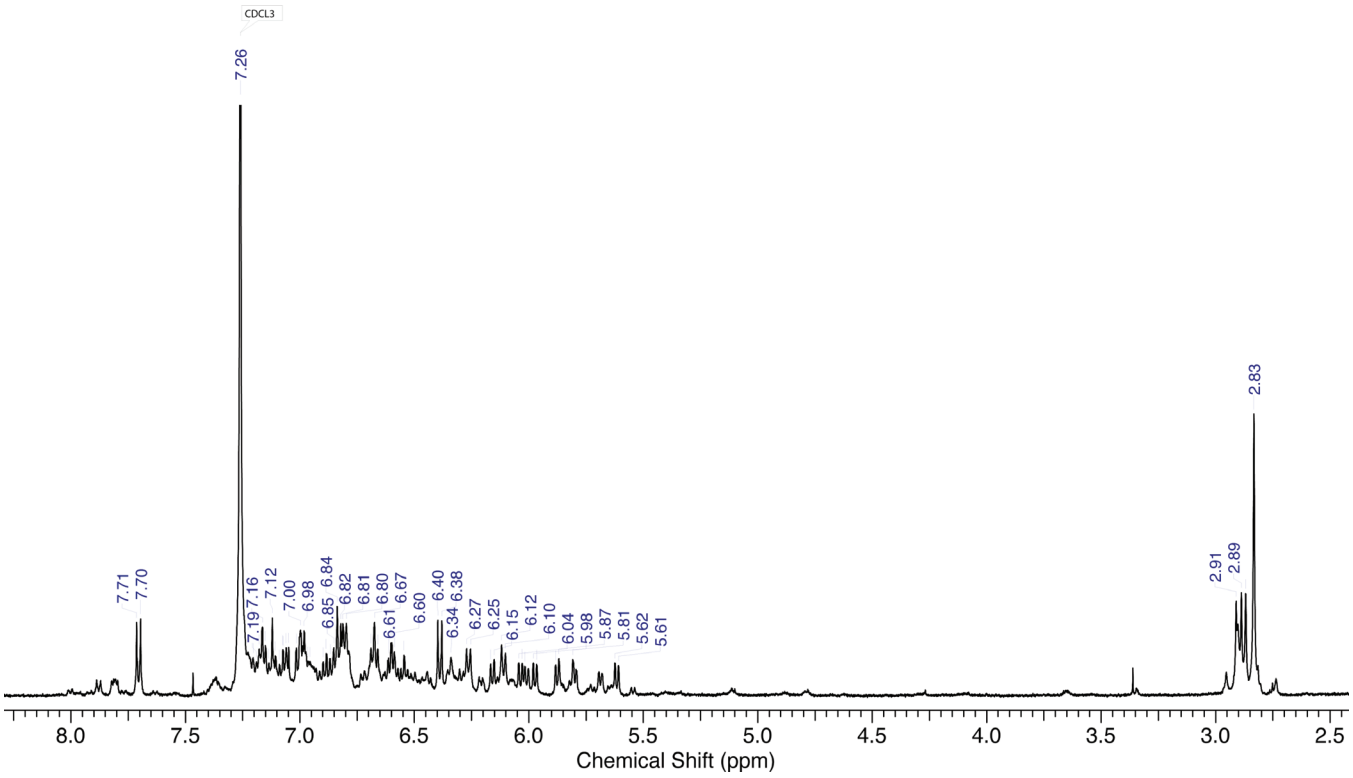


Fig. S21 ^{1}H NMR spectrum (500 MHz, 0 °C, $CDCl_3$) of **oP(DA)^{8}**.

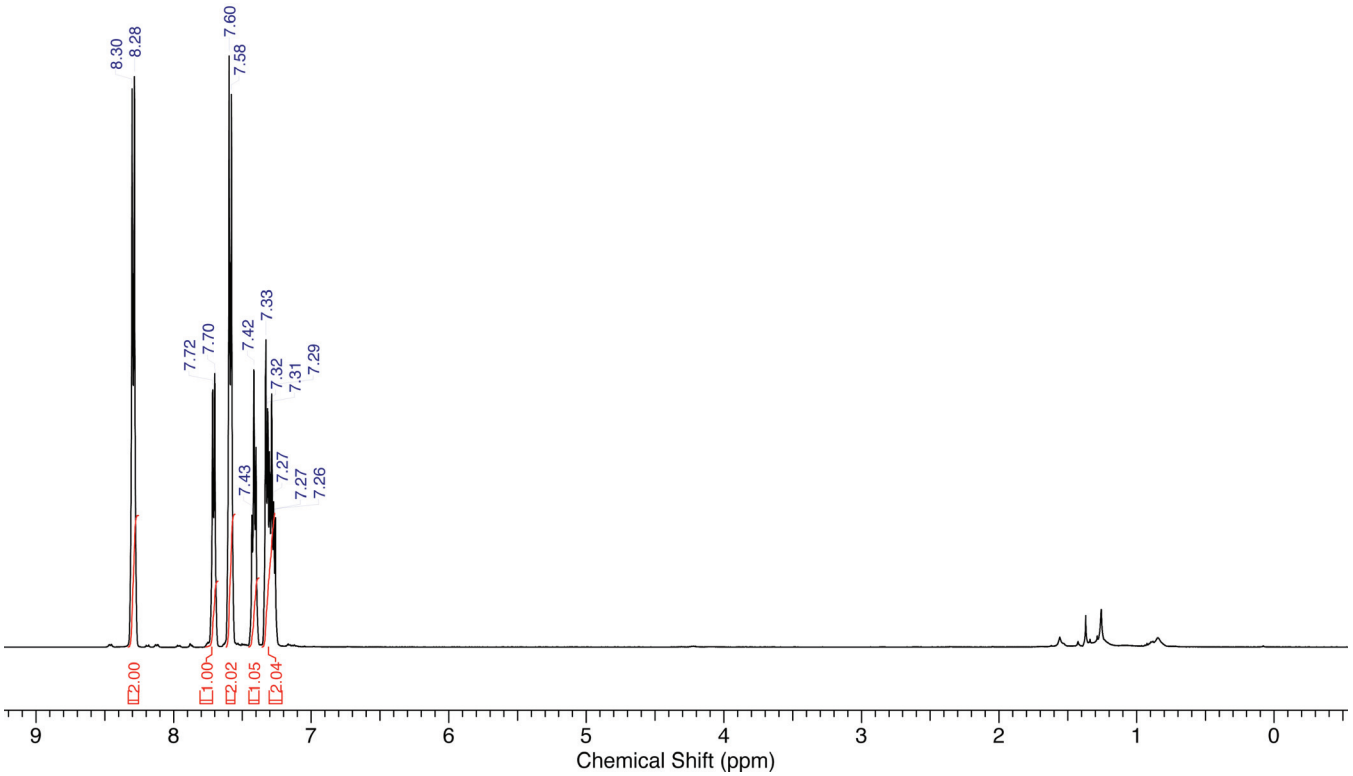


Fig. S22 ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of 2-bromo-4'-nitrobiphenyl.

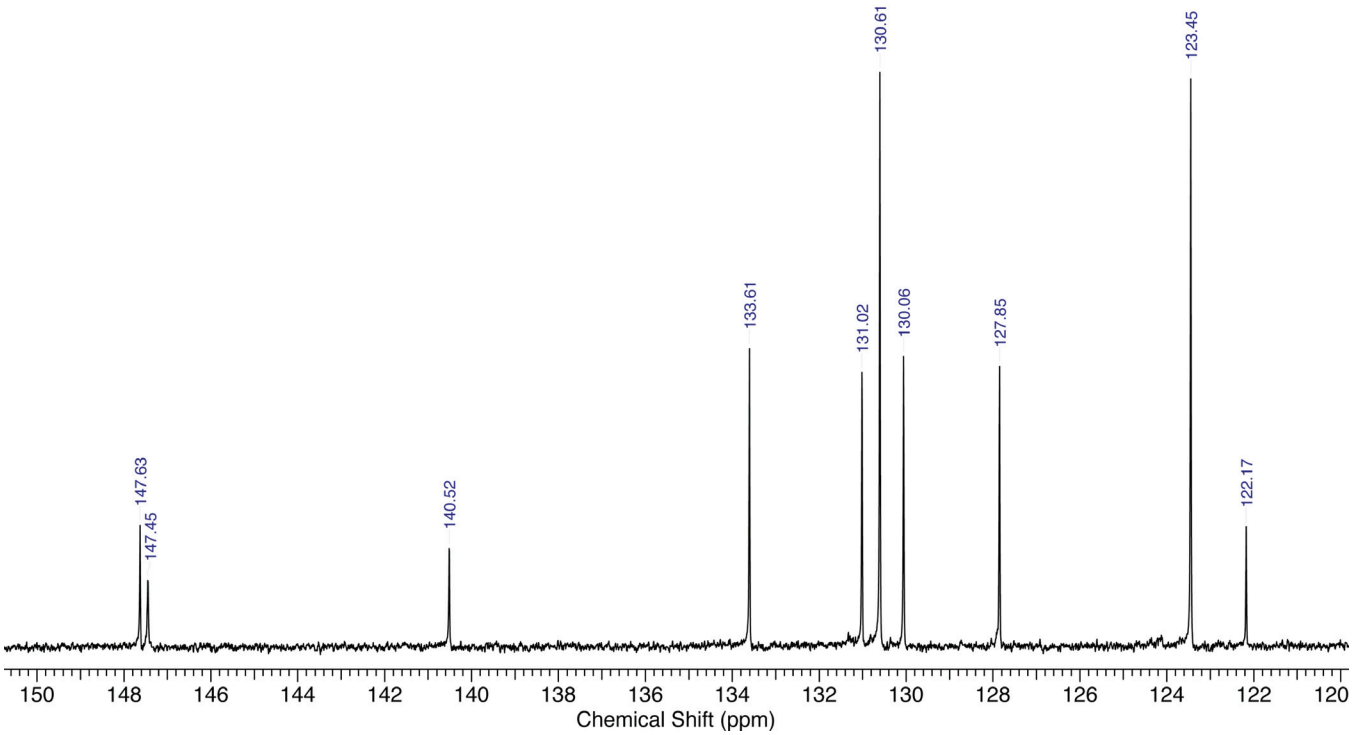


Fig. S23 ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of 2-bromo-4'-nitrobiphenyl.

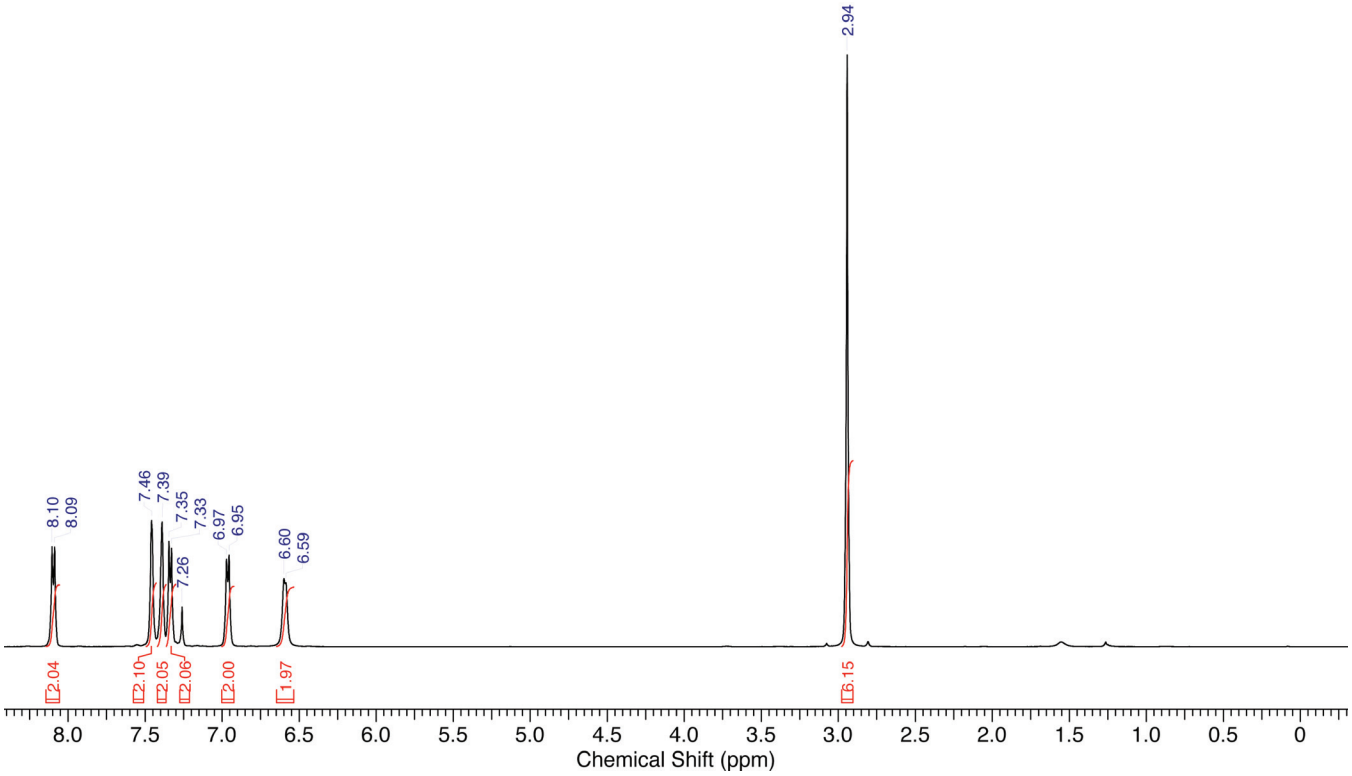


Fig. S24 ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **oP(DA)^3**.

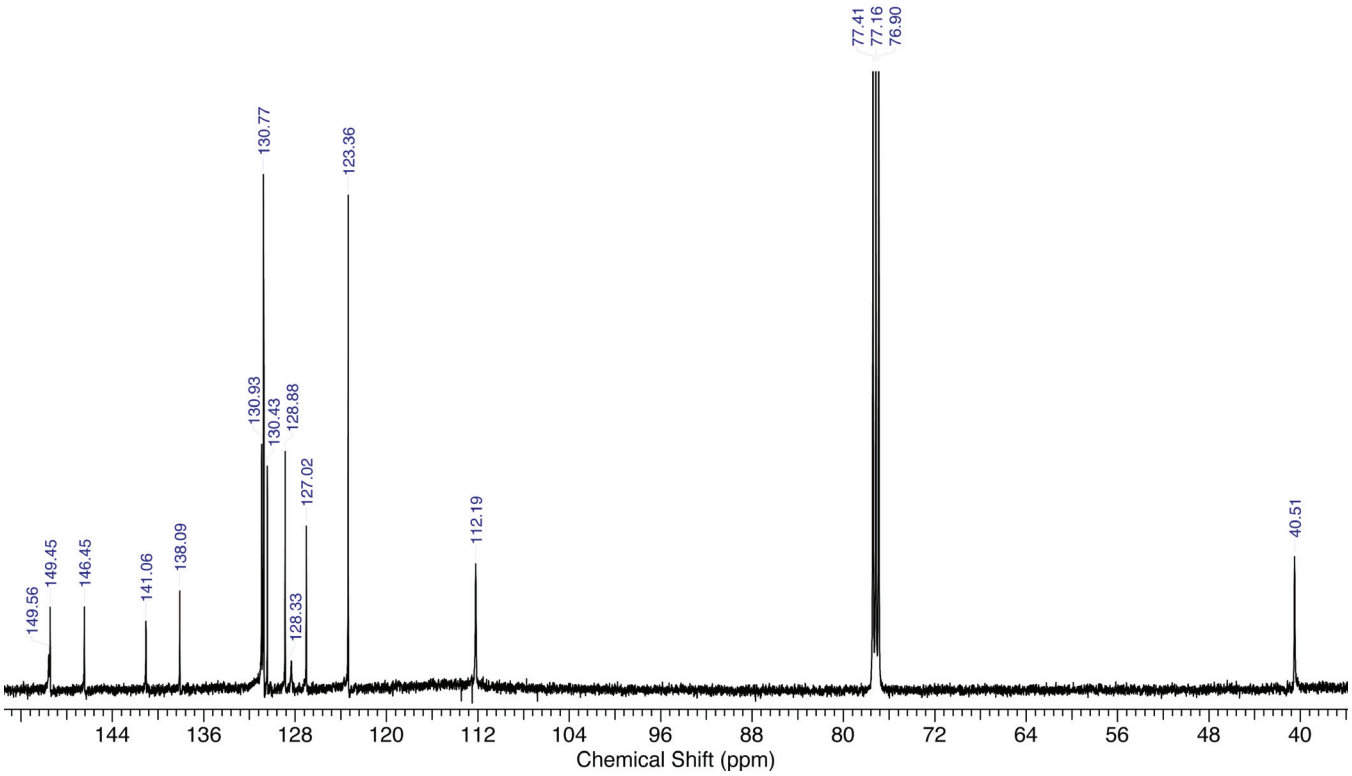


Fig. S25 ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **oP(DA)^3**.

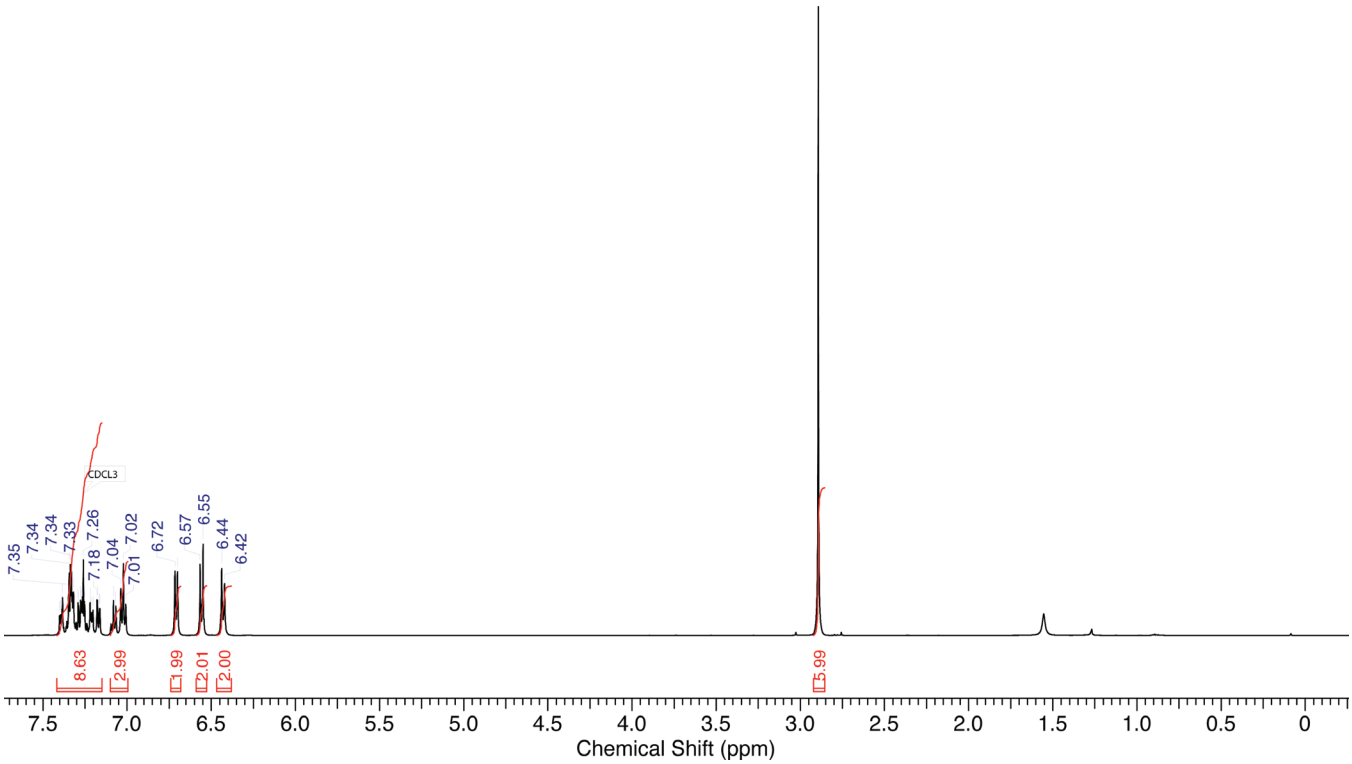


Fig. S26 ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **oP(D)^4**.

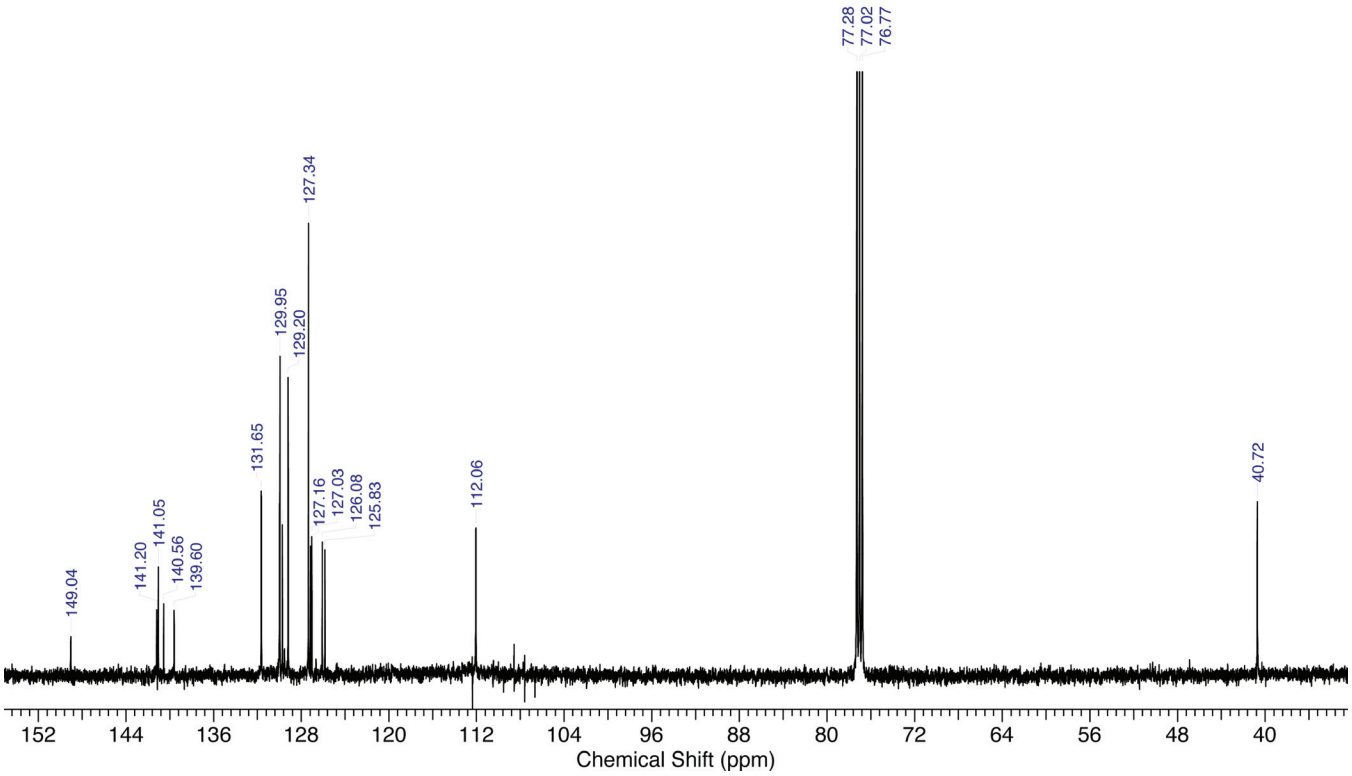


Fig. S27 ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **oP(D)^4**.

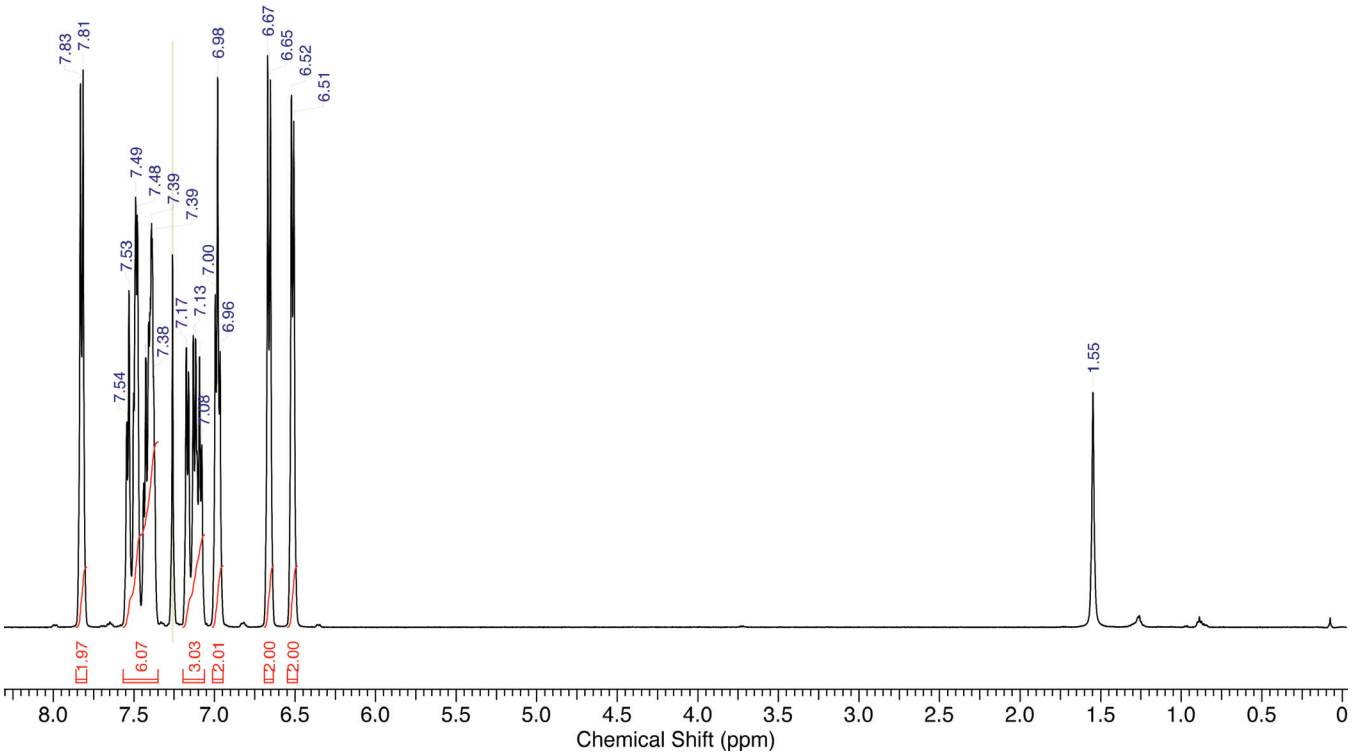


Fig. S28 ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **oP(A)^4**.

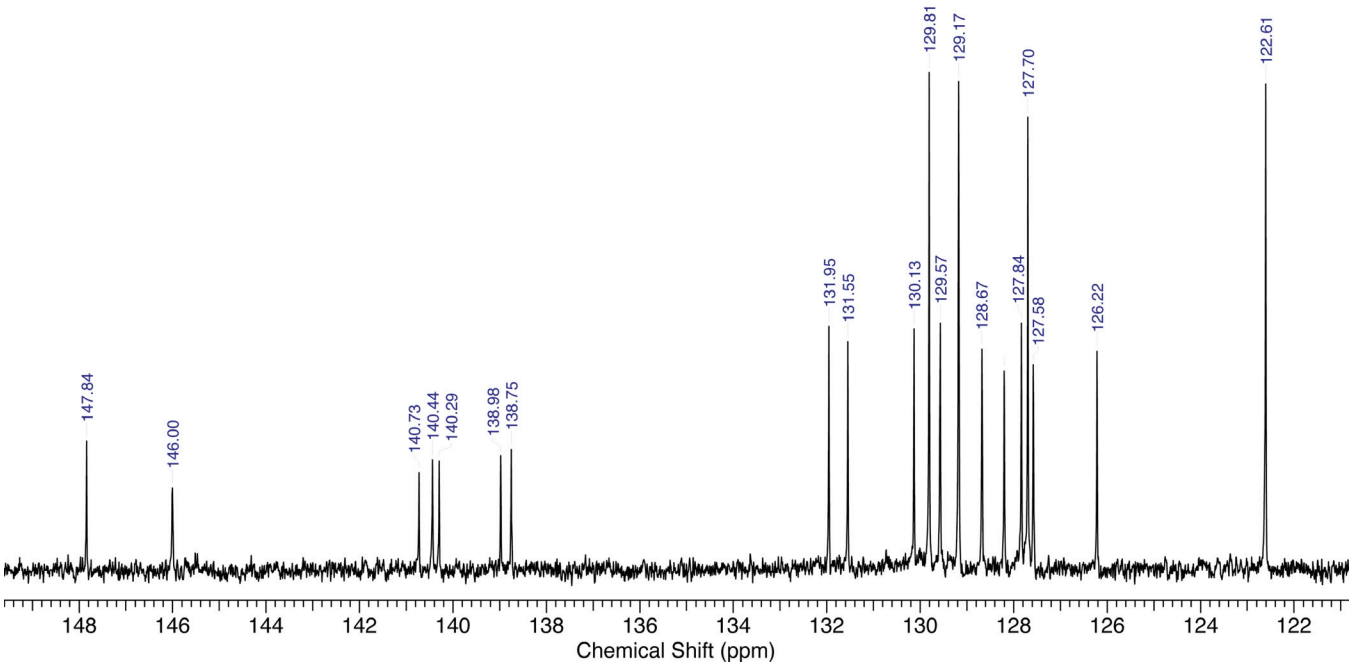


Fig. S29 ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **oP(A)^4**.

Cartesian Coordinates for Optimized Geometries

Table S2 Optimized Cartesian coordinates for **oP(DA)^6** AAA.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-4.121640	0.624171	1.721276
2	6	0	-4.120165	-0.074728	0.891464
3	6	0	-4.064498	-1.907289	-1.216763
4	6	0	-3.487679	0.284496	-0.314725
5	6	0	-4.715953	-1.320886	1.055271
6	6	0	-4.678166	-2.226829	-0.005064
7	6	0	-3.474470	-0.655050	-1.363027
8	1	0	-5.194374	-1.601281	1.985517
9	1	0	-3.009058	-0.400958	-2.307558
10	1	0	-4.062334	-2.628564	-2.024621
11	6	0	-2.924424	1.654500	-0.479138
12	6	0	-2.105345	4.327092	-0.858978
13	6	0	-3.730852	2.735078	-0.072496
14	6	0	-1.662628	1.928802	-1.065820
15	6	0	-1.286657	3.269202	-1.252311
16	6	0	-3.334331	4.057978	-0.256271
17	1	0	-4.706842	2.527370	0.355710
18	1	0	-0.318925	3.476615	-1.697602
19	1	0	-3.988257	4.867825	0.053661
20	1	0	-1.780442	5.351150	-1.018075
21	6	0	-0.724676	0.871996	-1.570833
22	6	0	0.921444	-1.098791	-2.733868
23	6	0	-0.560695	0.784530	-2.965632
24	6	0	-0.005598	-0.021032	-0.742181
25	6	0	0.795325	-1.004005	-1.348784
26	6	0	0.249206	-0.188324	-3.549914
27	1	0	-1.105881	1.480917	-3.597173
28	1	0	1.346722	-1.688582	-0.712073
29	1	0	0.344809	-0.237744	-4.630872
30	1	0	1.553122	-1.868332	-3.167485
31	6	0	-0.087949	-0.023322	0.757107
32	6	0	-0.344161	-0.203299	3.562450
33	6	0	-0.788583	-1.080146	1.363737
34	6	0	0.541876	0.936845	1.583961

35	6	0	0.375676	0.838003	2.977619
36	6	0	-0.917088	-1.181127	2.748557
37	1	0	-1.253124	-1.826824	0.726708
38	1	0	0.853067	1.582278	3.609158
39	1	0	-1.468302	-2.009914	3.183240
40	1	0	-0.441719	-0.256419	4.643113
41	6	0	1.386046	2.068734	1.076210
42	6	0	2.856650	4.330828	0.254066
43	6	0	0.900799	3.372216	1.277205
44	6	0	2.662834	1.894974	0.479871
45	6	0	3.364786	3.046529	0.070336
46	6	0	1.617787	4.497933	0.874401
47	1	0	-0.073083	3.495195	1.741388
48	1	0	4.352841	2.924013	-0.362992
49	1	0	1.210840	5.490979	1.042206
50	1	0	3.436461	5.193106	-0.063258
51	6	0	3.333344	0.576423	0.306283
52	6	0	4.754776	-1.897894	-0.028714
53	6	0	4.021551	0.272016	-0.880342
54	6	0	3.390970	-0.385734	1.327899
55	6	0	4.080286	-1.585939	1.175128
56	6	0	4.715973	-0.921717	-1.052041
57	1	0	3.999079	0.978179	-1.705582
58	1	0	2.904666	-0.192256	2.277573
59	1	0	4.097047	-2.275339	2.010019
60	1	0	5.219604	-1.092196	-1.995545
61	7	0	-5.301026	-3.547265	0.157984
62	8	0	-5.256060	-4.328598	-0.795474
63	8	0	-5.834025	-3.804084	1.240793
64	7	0	5.412280	-3.112414	-0.203729
65	6	0	6.315127	-3.270718	-1.333892
66	1	0	6.718908	-4.284470	-1.326994
67	1	0	5.783734	-3.137114	-2.282054
68	1	0	7.158321	-2.561058	-1.310610
69	6	0	5.632759	-3.970100	0.951089
70	1	0	4.682152	-4.249394	1.416879
71	1	0	6.117988	-4.890645	0.622427
72	1	0	6.266751	-3.498983	1.720099

Table S3 Optimized Cartesian coordinates for **oP(DA)^6** AAB.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	5.340972	0.455659	-1.186562
2	6	0	4.670981	-0.264481	-0.727251
3	6	0	2.937704	-2.129946	0.419434
4	6	0	3.387443	0.146884	-0.317881
5	6	0	5.091263	-1.583415	-0.578528
6	6	0	4.213911	-2.503366	-0.004587
7	6	0	2.531550	-0.809668	0.256997
8	1	0	6.073633	-1.904983	-0.901665
9	1	0	1.545667	-0.515026	0.593688
10	1	0	2.285313	-2.865630	0.872622
11	6	0	2.993386	1.579609	-0.455827
12	6	0	2.438774	4.336807	-0.622854
13	6	0	3.897291	2.540531	0.034475
14	6	0	1.774742	2.015696	-1.041938
15	6	0	1.534156	3.399091	-1.117834
16	6	0	3.629639	3.905657	-0.037341
17	1	0	4.815390	2.200375	0.504481
18	1	0	0.624384	3.745449	-1.593267
19	1	0	4.343577	4.621378	0.359536
20	1	0	2.215100	5.396576	-0.703352
21	6	0	0.796477	1.070720	-1.670588
22	6	0	-0.925782	-0.723200	-3.014139
23	6	0	1.282682	0.151167	-2.619470
24	6	0	-0.598766	1.099709	-1.414148
25	6	0	-1.431048	0.192631	-2.093440
26	6	0	0.442614	-0.736197	-3.287020

27	1	0	2.343277	0.149710	-2.848632
28	1	0	-2.495301	0.208875	-1.880442
29	1	0	0.855180	-1.426523	-4.017076
30	1	0	-1.597460	-1.412806	-3.516836
31	6	0	-1.277954	2.128614	-0.553916
32	6	0	-2.588660	4.209310	0.836247
33	6	0	-2.008546	3.122388	-1.232452
34	6	0	-1.251797	2.155841	0.857638
35	6	0	-1.893933	3.216318	1.524525
36	6	0	-2.660680	4.152432	-0.556685
37	1	0	-2.042164	3.087979	-2.318100
38	1	0	-1.861613	3.238115	2.610379
39	1	0	-3.209531	4.906081	-1.114089
40	1	0	-3.078592	5.009306	1.383853
41	6	0	-0.576754	1.128800	1.716918
42	6	0	0.730100	-0.616302	3.504840
43	6	0	0.539735	1.545599	2.463151
44	6	0	-1.061878	-0.195135	1.881883
45	6	0	-0.380800	-1.042923	2.779522
46	6	0	1.194498	0.690729	3.348952
47	1	0	0.903056	2.560172	2.327837
48	1	0	-0.763925	-2.047118	2.934850
49	1	0	2.057358	1.042325	3.906772
50	1	0	1.219505	-1.296980	4.195566
51	6	0	-2.271632	-0.732737	1.198402
52	6	0	-4.608970	-1.870471	-0.023278
53	6	0	-2.257739	-2.015385	0.625081
54	6	0	-3.493226	-0.041154	1.158539
55	6	0	-4.632178	-0.587287	0.572365
56	6	0	-3.384707	-2.577117	0.032668
57	1	0	-1.335501	-2.589595	0.623596
58	1	0	-3.571433	0.940323	1.613040
59	1	0	-5.545881	-0.006455	0.592794
60	1	0	-3.300026	-3.568626	-0.394425
61	7	0	4.645347	-3.897636	0.159442
62	8	0	3.851219	-4.692080	0.669693
63	8	0	5.779312	-4.200076	-0.221871
64	7	0	-5.732189	-2.406432	-0.646819
65	6	0	-5.741746	-3.820723	-0.990786
66	1	0	-6.682182	-4.058456	-1.490616
67	1	0	-4.931650	-4.060192	-1.687462
68	1	0	-5.641409	-4.475705	-0.110013
69	6	0	-7.021376	-1.757591	-0.460443
70	1	0	-6.992352	-0.722363	-0.815715
71	1	0	-7.772811	-2.284326	-1.051007
72	1	0	-7.349585	-1.750420	0.591933

Table S4 Optimized Cartesian coordinates for **oP(DA)^6** BAA.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.111275	-2.639073	0.550663
2	6	0	-2.105182	-2.205749	0.589911
3	6	0	-4.657794	-1.070251	0.633941
4	6	0	-2.288791	-0.950269	1.200404
5	6	0	-3.166720	-2.891196	0.007530
6	6	0	-4.434818	-2.310983	0.035815
7	6	0	-3.583797	-0.398895	1.211507
8	1	0	-3.025419	-3.852334	-0.471078
9	1	0	-3.756954	0.558720	1.687517
10	1	0	-5.656875	-0.652519	0.648267
11	6	0	-1.139310	-0.277949	1.871381
12	6	0	1.008740	0.851001	3.309769
13	6	0	-0.374375	-1.045826	2.770686
14	6	0	-0.806667	1.087696	1.687791
15	6	0	0.267618	1.624284	2.417161
16	6	0	0.684368	-0.494039	3.488898
17	1	0	-0.645657	-2.084998	2.932378
18	1	0	0.528832	2.666571	2.262392

19	1	0	1.247215	-1.109805	4.183985
20	1	0	1.836557	1.296015	3.853411
21	6	0	-1.599836	2.022755	0.825274
22	6	0	-3.251431	3.820708	-0.586640
23	6	0	-2.361367	3.000078	1.493342
24	6	0	-1.628686	1.982291	-0.586129
25	6	0	-2.480778	2.876530	-1.262569
26	6	0	-3.178495	3.895209	0.805451
27	1	0	-2.322079	3.034304	2.578780
28	1	0	-2.513495	2.836342	-2.347796
29	1	0	-3.759075	4.632520	1.352176
30	1	0	-3.892090	4.497938	-1.143971
31	6	0	-0.830357	1.042047	-1.445163
32	6	0	0.423727	-0.657865	-3.313229
33	6	0	-1.560505	0.085363	-2.174565
34	6	0	0.570024	1.142596	-1.655635
35	6	0	1.162008	0.283910	-2.601920
36	6	0	-0.950494	-0.765370	-3.093493
37	1	0	-2.631515	0.015953	-2.008705
38	1	0	2.226333	0.373344	-2.789123
39	1	0	-1.544540	-1.494052	-3.637418
40	1	0	0.918941	-1.295812	-4.039574
41	6	0	1.437427	2.173186	-0.997000
42	6	0	3.050160	4.245013	0.057668
43	6	0	1.041058	3.521980	-1.055838
44	6	0	2.692264	1.861870	-0.403525
45	6	0	3.466984	2.916902	0.116704
46	6	0	1.826098	4.550781	-0.538439
47	1	0	0.104792	3.771074	-1.541251
48	1	0	4.411325	2.675066	0.595567
49	1	0	1.485532	5.579695	-0.610008
50	1	0	3.675096	5.030056	0.474196
51	6	0	3.259033	0.485775	-0.304152
52	6	0	4.436473	-2.122820	-0.083095
53	6	0	4.585913	0.238082	-0.693157
54	6	0	2.541411	-0.603304	0.213474
55	6	0	3.107910	-1.868627	0.332624
56	6	0	5.167406	-1.023564	-0.589802
57	1	0	5.180636	1.049199	-1.105077
58	1	0	1.520949	-0.460274	0.549642
59	1	0	2.504872	-2.660817	0.758656
60	1	0	6.193219	-1.145437	-0.914785
61	7	0	-5.563327	-3.025283	-0.577283
62	8	0	-6.673583	-2.489376	-0.540958
63	8	0	-5.338478	-4.121814	-1.095988
64	7	0	4.992699	-3.397213	-0.011181
65	6	0	6.426898	-3.554295	-0.198177
66	1	0	6.679602	-4.614173	-0.137834
67	1	0	6.733755	-3.200941	-1.188261
68	1	0	7.019147	-3.012864	0.557791
69	6	0	4.299477	-4.431383	0.740798
70	1	0	3.298826	-4.607423	0.332344
71	1	0	4.855549	-5.366484	0.655437
72	1	0	4.195109	-4.186835	1.810886

Table S5 Optimized Cartesian coordinates for **oP(DA)^6** BAB.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.041864	-1.824071	3.162552
2	6	0	3.138422	-1.747734	2.083963
3	6	0	3.412638	-1.524073	-0.686788
4	6	0	2.201482	-0.988229	1.356138
5	6	0	4.202281	-2.384364	1.450990
6	6	0	4.325398	-2.262695	0.066860
7	6	0	2.358417	-0.889360	-0.037421
8	1	0	4.930187	-2.961140	2.008060
9	1	0	1.644797	-0.322702	-0.622532
10	1	0	3.528033	-1.456543	-1.760906

11	6	0	1.052071	-0.357176	2.067742
12	6	0	-1.146425	0.652827	3.513065
13	6	0	0.308973	-1.175224	2.939131
14	6	0	0.677907	1.004567	1.915738
15	6	0	-0.422066	1.477293	2.653769
16	6	0	-0.779743	-0.685769	3.656920
17	1	0	0.581848	-2.222258	3.030511
18	1	0	-0.697268	2.521578	2.567980
19	1	0	-1.334910	-1.345169	4.317533
20	1	0	-1.984823	1.059647	4.070966
21	6	0	1.483813	1.990680	1.125750
22	6	0	3.124168	3.937467	-0.102758
23	6	0	2.855666	2.099304	1.427349
24	6	0	0.927864	2.883861	0.176545
25	6	0	1.767720	3.850688	-0.407737
26	6	0	3.673748	3.049754	0.823733
27	1	0	3.279146	1.433162	2.172014
28	1	0	1.334499	4.544984	-1.122671
29	1	0	4.726051	3.104694	1.086443
30	1	0	3.741354	4.693915	-0.578671
31	6	0	-0.529855	2.950662	-0.201428
32	6	0	-3.244047	3.373832	-0.849354
33	6	0	-1.268467	4.004922	0.369484
34	6	0	-1.169257	2.100067	-1.137328
35	6	0	-2.525087	2.337993	-1.437803
36	6	0	-2.610077	4.219353	0.063309
37	1	0	-0.766989	4.666126	1.071414
38	1	0	-3.014227	1.698170	-2.164332
39	1	0	-3.149425	5.040919	0.525920
40	1	0	-4.286591	3.526584	-1.112779
41	6	0	-0.462382	1.030563	-1.915322
42	6	0	0.844069	-0.800932	-3.630186
43	6	0	0.683021	1.392432	-2.648817
44	6	0	-0.968612	-0.291192	-2.056383
45	6	0	-0.288954	-1.179605	-2.913215
46	6	0	1.334697	0.498966	-3.497686
47	1	0	1.052116	2.408246	-2.572455
48	1	0	-0.656606	-2.197918	-2.996738
49	1	0	2.210348	0.820814	-4.053850
50	1	0	1.339962	-1.516349	-4.280075
51	6	0	-2.189301	-0.799439	-1.368403
52	6	0	-4.531800	-1.862706	-0.097523
53	6	0	-3.171127	-1.495822	-2.092837
54	6	0	-2.402835	-0.662007	0.011686
55	6	0	-3.531734	-1.182390	0.636641
56	6	0	-4.311472	-2.016244	-1.485921
57	1	0	-3.052416	-1.623550	-3.165606
58	1	0	-1.666442	-0.151557	0.621940
59	1	0	-3.623969	-1.055900	1.707823
60	1	0	-5.031460	-2.536909	-2.104990
61	7	0	5.443372	-2.930979	-0.613153
62	8	0	5.528594	-2.812255	-1.837870
63	8	0	6.237185	-3.575017	0.077978
64	7	0	-5.685476	-2.345055	0.514753
65	6	0	-6.545157	-3.261106	-0.219250
66	1	0	-7.408666	-3.511365	0.399291
67	1	0	-6.923270	-2.794442	-1.134937
68	1	0	-6.034395	-4.197625	-0.497267
69	6	0	-5.750879	-2.387188	1.967311
70	1	0	-5.629419	-1.385639	2.392949
71	1	0	-6.734009	-2.752941	2.268444
72	1	0	-4.985303	-3.044218	2.412126

Table S6 Optimized Cartesian coordinates for [**oP(DA)^6** + H^+] AAA.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	4.024258	0.543504	-1.837561
2	6	0	4.034183	-0.126468	-0.984080

3	6	0	4.027093	-1.878412	1.193422
4	6	0	3.466043	0.292836	0.234077
5	6	0	4.583029	-1.397110	-1.128242
6	6	0	4.561945	-2.263580	-0.035798
7	6	0	3.484473	-0.602489	1.320054
8	1	0	5.012139	-1.725378	-2.067001
9	1	0	3.086408	-0.294766	2.279609
10	1	0	4.050176	-2.567536	2.028697
11	6	0	2.932842	1.678287	0.369941
12	6	0	2.181891	4.378587	0.707486
13	6	0	3.737880	2.730749	-0.106260
14	6	0	1.703298	1.996459	1.002235
15	6	0	1.362985	3.349299	1.169615
16	6	0	3.374532	4.066195	0.054596
17	1	0	4.690808	2.491960	-0.568305
18	1	0	0.425740	3.591324	1.661312
19	1	0	4.029726	4.852948	-0.306712
20	1	0	1.889588	5.413542	0.857804
21	6	0	0.774016	0.974406	1.588177
22	6	0	-0.806770	-0.947285	2.923186
23	6	0	0.631906	0.980919	2.988797
24	6	0	0.054161	0.012410	0.838460
25	6	0	-0.705457	-0.946354	1.532690
26	6	0	-0.146924	0.038351	3.658033
27	1	0	1.179942	1.724372	3.560448
28	1	0	-1.229074	-1.702609	0.954334
29	1	0	-0.215987	0.061764	4.741477
30	1	0	-1.393011	-1.709706	3.428711
31	6	0	0.098345	-0.099279	-0.658126
32	6	0	0.284655	-0.480645	-3.452512
33	6	0	0.736813	-1.226640	-1.205616
34	6	0	-0.502934	0.829710	-1.540755
35	6	0	-0.371055	0.632833	-2.928139
36	6	0	0.827119	-1.427617	-2.582511
37	1	0	1.196083	-1.941426	-0.529548
38	1	0	-0.816761	1.360183	-3.601422
39	1	0	1.337976	-2.304097	-2.969669
40	1	0	0.364808	-0.607456	-4.528052
41	6	0	-1.297991	2.021473	-1.097818
42	6	0	-2.707578	4.368256	-0.391803
43	6	0	-0.783859	3.297247	-1.377034
44	6	0	-2.567819	1.928913	-0.473322
45	6	0	-3.242553	3.111691	-0.116230
46	6	0	-1.474196	4.460275	-1.036797
47	1	0	0.187886	3.370676	-1.854410
48	1	0	-4.225541	3.043266	0.340622
49	1	0	-1.046463	5.430451	-1.270194
50	1	0	-3.259119	5.263522	-0.122177
51	6	0	-3.278264	0.641933	-0.234995
52	6	0	-4.757512	-1.698781	0.185179
53	6	0	-3.928859	0.405772	0.989235
54	6	0	-3.391703	-0.337746	-1.240647
55	6	0	-4.123894	-1.506348	-1.040845
56	6	0	-4.670483	-0.755533	1.204684
57	1	0	-3.838314	1.128566	1.792551
58	1	0	-2.911350	-0.181562	-2.198646
59	1	0	-4.194721	-2.233381	-1.844124
60	1	0	-5.158151	-0.914014	2.164567
61	7	0	5.112911	-3.620438	-0.184898
62	8	0	5.065941	-4.369141	0.793136
63	8	0	5.578956	-3.932924	-1.282024
64	7	0	-5.560490	-2.932305	0.430720
65	6	0	-6.780125	-3.029150	-0.457589
66	1	0	-7.371423	-3.892416	-0.148515
67	1	0	-7.354201	-2.108966	-0.353793
68	1	0	-6.449999	-3.148581	-1.488537
69	6	0	-4.735381	-4.198018	0.387703
70	1	0	-3.898921	-4.086662	1.076764
71	1	0	-5.367477	-5.038500	0.678252
72	1	0	-4.366108	-4.338410	-0.627165
73	1	0	-5.908167	-2.845775	1.390328

Table S7 Optimized Cartesian coordinates for [**oP(DA)^6** + H^+] AAB.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	5.379662	0.512875	-1.079687
2	6	0	4.703429	-0.226728	-0.662639
3	6	0	2.959281	-2.144480	0.377325
4	6	0	3.410654	0.161871	-0.262520
5	6	0	5.126456	-1.550489	-0.559121
6	6	0	4.242556	-2.495883	-0.041403
7	6	0	2.551558	-0.820559	0.260922
8	1	0	6.116413	-1.854834	-0.876388
9	1	0	1.559787	-0.540298	0.592014
10	1	0	2.307588	-2.903769	0.791040
11	6	0	3.000293	1.593596	-0.357965
12	6	0	2.405385	4.347698	-0.442903
13	6	0	3.878359	2.550507	0.182976
14	6	0	1.786401	2.033061	-0.952602
15	6	0	1.524800	3.414193	-0.987454
16	6	0	3.590498	3.913419	0.151513
17	1	0	4.794346	2.209490	0.656119
18	1	0	0.624302	3.765704	-1.477198
19	1	0	4.287238	4.625849	0.582525
20	1	0	2.170991	5.406533	-0.496751
21	6	0	0.839907	1.099112	-1.643908
22	6	0	-0.814560	-0.641565	-3.143414
23	6	0	1.368909	0.216559	-2.605834
24	6	0	-0.566292	1.113266	-1.449161
25	6	0	-1.361939	0.237206	-2.210951
26	6	0	0.565999	-0.645835	-3.346753
27	1	0	2.437354	0.229842	-2.791242
28	1	0	-2.438538	0.266635	-2.066301
29	1	0	1.014969	-1.301154	-4.086898
30	1	0	-1.458274	-1.298369	-3.721924
31	6	0	-1.297077	2.104214	-0.586148
32	6	0	-2.708073	4.122582	0.806688
33	6	0	-2.058088	3.076956	-1.264213
34	6	0	-1.288036	2.126356	0.826534
35	6	0	-1.980165	3.154209	1.495812
36	6	0	-2.759143	4.073880	-0.587708
37	1	0	-2.066987	3.060798	-2.350543
38	1	0	-1.951598	3.177122	2.581875
39	1	0	-3.321927	4.815956	-1.146184
40	1	0	-3.229359	4.902587	1.353369
41	6	0	-0.579832	1.128160	1.692579
42	6	0	0.759725	-0.576042	3.507357
43	6	0	0.516982	1.577298	2.446835
44	6	0	-1.010553	-0.211663	1.860548
45	6	0	-0.321892	-1.044021	2.764529
46	6	0	1.181621	0.744162	3.346353
47	1	0	0.854579	2.599890	2.310709
48	1	0	-0.669277	-2.061969	2.916190
49	1	0	2.024634	1.125034	3.914327
50	1	0	1.261768	-1.235226	4.208434
51	6	0	-2.200193	-0.789690	1.174545
52	6	0	-4.451764	-1.986002	0.018837
53	6	0	-2.118204	-2.058130	0.573339
54	6	0	-3.447564	-0.136296	1.169355
55	6	0	-4.574314	-0.723830	0.596767
56	6	0	-3.235933	-2.662112	-0.001847
57	1	0	-1.165989	-2.575858	0.539382
58	1	0	-3.545032	0.838429	1.631597
59	1	0	-5.521870	-0.194434	0.623644
60	1	0	-3.141205	-3.642984	-0.463468
61	7	0	4.668578	-3.899888	0.066989
62	8	0	3.852548	-4.713633	0.508843
63	8	0	5.811564	-4.183187	-0.291376
64	7	0	-5.640128	-2.654955	-0.587058
65	6	0	-6.708231	-2.992020	0.428771
66	1	0	-7.490065	-3.572070	-0.063836

67	1	0	-6.248351	-3.566032	1.232575
68	1	0	-7.119105	-2.063003	0.821520
69	6	0	-6.208750	-1.904603	-1.769150
70	1	0	-5.405163	-1.729064	-2.483524
71	1	0	-7.001080	-2.505892	-2.217488
72	1	0	-6.610338	-0.955055	-1.418259
73	1	0	-5.294800	-3.548393	-0.950222

Table S8 Optimized Cartesian coordinates for [**oP(DA)^6** + H^+] BAA.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.174710	-2.642649	0.533784
2	6	0	-2.147338	-2.163214	0.579901
3	6	0	-4.648016	-0.922990	0.658108
4	6	0	-2.272154	-0.908721	1.205716
5	6	0	-3.240280	-2.795529	-0.004831
6	6	0	-4.480298	-2.160852	0.039114
7	6	0	-3.542157	-0.304312	1.236964
8	1	0	-3.147308	-3.757062	-0.494513
9	1	0	-3.673971	0.650934	1.730469
10	1	0	-5.629416	-0.465579	0.687698
11	6	0	-1.088581	-0.293707	1.875123
12	6	0	1.101391	0.732261	3.334981
13	6	0	-0.351690	-1.103772	2.762293
14	6	0	-0.703800	1.062218	1.713607
15	6	0	0.389982	1.545767	2.453306
16	6	0	0.726458	-0.603344	3.491151
17	1	0	-0.674889	-2.128536	2.921575
18	1	0	0.679137	2.584817	2.328707
19	1	0	1.248357	-1.243874	4.196489
20	1	0	1.930923	1.143806	3.902213
21	6	0	-1.470891	2.045709	0.881173
22	6	0	-3.079003	3.929125	-0.468435
23	6	0	-2.184615	3.036834	1.581078
24	6	0	-1.526685	2.034475	-0.529363
25	6	0	-2.355802	2.970689	-1.176168
26	6	0	-2.979087	3.973876	0.923149
27	1	0	-2.129935	3.048486	2.666174
28	1	0	-2.412134	2.951571	-2.261038
29	1	0	-3.524015	4.720119	1.493187
30	1	0	-3.705457	4.638382	-1.000719
31	6	0	-0.773226	1.088255	-1.421610
32	6	0	0.402700	-0.585077	-3.369230
33	6	0	-1.532329	0.144968	-2.137029
34	6	0	0.618840	1.181102	-1.683333
35	6	0	1.172401	0.340712	-2.668534
36	6	0	-0.961300	-0.692009	-3.094096
37	1	0	-2.597211	0.080188	-1.936573
38	1	0	2.224234	0.448714	-2.914529
39	1	0	-1.581318	-1.402015	-3.633073
40	1	0	0.859663	-1.198075	-4.140814
41	6	0	1.516704	2.190038	-1.034752
42	6	0	3.221841	4.205768	-0.003227
43	6	0	1.164055	3.550080	-1.080401
44	6	0	2.772070	1.847826	-0.465240
45	6	0	3.601897	2.866724	0.038862
46	6	0	1.994440	4.547590	-0.572206
47	1	0	0.226854	3.831465	-1.545027
48	1	0	4.548775	2.597077	0.497936
49	1	0	1.685829	5.586793	-0.631240
50	1	0	3.877113	4.970439	0.402032
51	6	0	3.278580	0.449965	-0.360250
52	6	0	4.305895	-2.140553	-0.109406
53	6	0	4.590106	0.148648	-0.768387
54	6	0	2.499760	-0.588874	0.184239
55	6	0	3.003781	-1.880208	0.315098
56	6	0	5.109436	-1.141350	-0.648394
57	1	0	5.207733	0.926293	-1.205216

58	1	0	1.492500	-0.382624	0.523831
59	1	0	2.376948	-2.651946	0.750961
60	1	0	6.124020	-1.349036	-0.982738
61	7	0	-5.642619	-2.819190	-0.583710
62	8	0	-6.726800	-2.239769	-0.526343
63	8	0	-5.456954	-3.909266	-1.128190
64	7	0	4.874221	-3.515424	0.006290
65	6	0	5.006957	-3.983579	1.437073
66	1	0	5.522215	-4.945265	1.445341
67	1	0	5.573312	-3.235997	1.991556
68	1	0	4.009769	-4.087131	1.862354
69	6	0	4.150218	-4.528827	-0.850201
70	1	0	4.123343	-4.156219	-1.873655
71	1	0	4.684114	-5.478849	-0.796882
72	1	0	3.136547	-4.644244	-0.469271
73	1	0	5.826253	-3.449682	-0.365866

Table S9 Optimized Cartesian coordinates for [**oP(DA)^6** + H^+] BAB.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.041864	-1.824071	3.162552
2	6	0	3.138422	-1.747734	2.083963
3	6	0	3.412638	-1.524073	-0.686788
4	6	0	2.201482	-0.988229	1.356138
5	6	0	4.202281	-2.384364	1.450990
6	6	0	4.325398	-2.262695	0.066860
7	6	0	2.358417	-0.889360	-0.037421
8	1	0	4.930187	-2.961140	2.008060
9	1	0	1.644797	-0.322702	-0.622532
10	1	0	3.528033	-1.456543	-1.760906
11	6	0	1.052071	-0.357176	2.067742
12	6	0	-1.146425	0.652827	3.513065
13	6	0	0.308973	-1.175224	2.939131
14	6	0	0.677907	1.004567	1.915738
15	6	0	-0.422066	1.477293	2.653769
16	6	0	-0.779743	-0.685769	3.656920
17	1	0	0.581848	-2.222258	3.030511
18	1	0	-0.697268	2.521578	2.567980
19	1	0	-1.334910	-1.345169	4.317533
20	1	0	-1.984823	1.059647	4.070966
21	6	0	1.483813	1.990680	1.125750
22	6	0	3.124168	3.937467	-0.102758
23	6	0	2.855666	2.099304	1.427349
24	6	0	0.927864	2.883861	0.176545
25	6	0	1.767720	3.850688	-0.407737
26	6	0	3.673748	3.049754	0.823733
27	1	0	3.279146	1.433162	2.172014
28	1	0	1.334499	4.544984	-1.122671
29	1	0	4.726051	3.104694	1.086443
30	1	0	3.741354	4.693915	-0.578671
31	6	0	-0.529855	2.950662	-0.201428
32	6	0	-3.244047	3.373832	-0.849354
33	6	0	-1.268467	4.004922	0.369484
34	6	0	-1.169257	2.100067	-1.137328
35	6	0	-2.525087	2.337993	-1.437803
36	6	0	-2.610077	4.219353	0.063309
37	1	0	-0.766989	4.666126	1.071414
38	1	0	-3.014227	1.698170	-2.164332
39	1	0	-3.149425	5.040919	0.525920
40	1	0	-4.286591	3.526584	-1.112779
41	6	0	-0.462382	1.030563	-1.915322
42	6	0	0.844069	-0.800932	-3.630186
43	6	0	0.683021	1.392432	-2.648817
44	6	0	-0.968612	-0.291192	-2.056383
45	6	0	-0.288954	-1.179605	-2.913215
46	6	0	1.334697	0.498966	-3.497686
47	1	0	1.052116	2.408246	-2.572455
48	1	0	-0.656606	-2.197918	-2.996738

49	1	0	2.210348	0.820814	-4.053850
50	1	0	1.339962	-1.516349	-4.280075
51	6	0	-2.189301	-0.799439	-1.368403
52	6	0	-4.531800	-1.862706	-0.097523
53	6	0	-3.171127	-1.495822	-2.092837
54	6	0	-2.402835	-0.662007	0.011686
55	6	0	-3.531734	-1.182390	0.636641
56	6	0	-4.311472	-2.016244	-1.485921
57	1	0	-3.052416	-1.623550	-3.165606
58	1	0	-1.666442	-0.151557	0.621940
59	1	0	-3.623969	-1.055900	1.707823
60	1	0	-5.031460	-2.536909	-2.104990
61	7	0	5.443372	-2.930979	-0.613153
62	8	0	5.528594	-2.812255	-1.837870
63	8	0	6.237185	-3.575017	0.077978
64	7	0	-5.685476	-2.345055	0.514753
65	6	0	-6.545157	-3.261106	-0.219250
66	1	0	-7.408666	-3.511365	0.399291
67	1	0	-6.923270	-2.794442	-1.134937
68	1	0	-6.034395	-4.197625	-0.497267
69	6	0	-5.750879	-2.387188	1.967311
70	1	0	-5.629419	-1.385639	2.392949
71	1	0	-6.734009	-2.752941	2.268444
72	1	0	-4.985303	-3.044218	2.412126

Table S10 Optimized Cartesian coordinates for **oP(DA)^8**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.469327	1.188483	2.715026
2	6	0	-1.728081	0.139679	2.608955
3	6	0	-2.325644	-2.542148	2.335792
4	6	0	-1.858720	-0.388042	1.311428
5	6	0	-1.892222	-0.644006	3.749148
6	6	0	-2.177488	-2.002789	3.612495
7	6	0	-2.202212	-1.754881	1.174642
8	1	0	-1.781323	-0.197855	4.733075
9	1	0	-2.580674	-3.592422	2.223787
10	6	0	-1.714129	0.576254	0.169612
11	6	0	-1.695789	2.493256	-1.904414
12	6	0	-2.682082	1.596111	0.097043
13	6	0	-0.677619	0.556846	-0.796477
14	6	0	-0.709715	1.511690	-1.829836
15	6	0	-2.682279	2.547927	-0.920488
16	1	0	-3.467717	1.615954	0.846326
17	1	0	0.083455	1.494630	-2.570582
18	1	0	-3.453583	3.312191	-0.948524
19	1	0	-1.677970	3.218432	-2.712879
20	6	0	0.443252	-0.441649	-0.851887
21	6	0	2.467226	-2.382214	-1.198848
22	6	0	0.439383	-1.324667	-1.947256
23	6	0	1.523007	-0.506717	0.063022
24	6	0	2.502862	-1.499177	-0.121283
25	6	0	1.434578	-2.282455	-2.130350
26	1	0	-0.383578	-1.267452	-2.653199
27	1	0	3.329753	-1.544609	0.580421
28	1	0	1.392280	-2.950726	-2.985783
29	1	0	3.252171	-3.123575	-1.316812
30	6	0	1.703136	0.394246	1.251080
31	6	0	2.069821	1.901756	3.612447
32	6	0	1.549206	-0.182396	2.523845
33	6	0	2.102287	1.749785	1.167103
34	6	0	2.247204	2.485075	2.358513
35	6	0	1.736026	0.549704	3.695232
36	1	0	1.256686	-1.226115	2.586573
37	1	0	2.542819	3.528308	2.288475
38	1	0	1.605667	0.069694	4.660845
39	1	0	2.206725	2.495080	4.512200
40	6	0	2.401620	2.475106	-0.112244

41	6	0	2.851565	4.018603	-2.429865
42	6	0	1.548232	3.533835	-0.465954
43	6	0	3.534588	2.205413	-0.924218
44	6	0	3.721523	2.987231	-2.081882
45	6	0	1.760394	4.303916	-1.608304
46	1	0	0.686622	3.735884	0.163189
47	1	0	4.599226	2.803949	-2.694396
48	1	0	1.077495	5.112189	-1.853374
49	1	0	3.040236	4.608136	-3.322800
50	6	0	4.573242	1.186650	-0.603628
51	6	0	6.679769	-0.692349	-0.069305
52	6	0	5.099449	0.357984	-1.608687
53	6	0	5.142056	1.059626	0.674053
54	6	0	6.165744	0.153748	0.940790
55	6	0	6.122094	-0.553080	-1.361609
56	1	0	4.686201	0.409285	-2.612043
57	1	0	4.796890	1.694706	1.482353
58	1	0	6.569599	0.120799	1.945030
59	1	0	6.475415	-1.163790	-2.183261
60	7	0	7.676567	-1.628974	0.198771
61	6	0	8.369596	-2.257372	-0.916008
62	1	0	9.094190	-2.973967	-0.525465
63	1	0	7.670040	-2.812672	-1.549320
64	1	0	8.905316	-1.532554	-1.550957
65	6	0	8.392023	-1.553166	1.463785
66	1	0	7.702695	-1.653847	2.308222
67	1	0	9.100990	-2.380967	1.520968
68	1	0	8.949171	-0.609602	1.586132
69	6	0	-2.470752	-2.450354	-0.127062
70	6	0	-3.585443	-2.173195	-0.958897
71	6	0	-1.605461	-3.494822	-0.492529
72	6	0	-3.754486	-2.926016	-2.137098
73	6	0	-1.800702	-4.245128	-1.650720
74	1	0	-0.748137	-3.700964	0.140539
75	6	0	-2.878899	-3.952136	-2.485845
76	1	0	-4.619555	-2.729381	-2.763246
77	1	0	-1.108749	-5.043827	-1.900902
78	1	0	-3.049882	-4.525987	-3.391953
79	6	0	-4.643994	-1.176006	-0.632959
80	6	0	-5.122137	-0.305892	-1.631487
81	6	0	-5.248618	-1.126779	0.637432
82	6	0	-6.160927	0.584422	-1.380687
83	1	0	-4.655386	-0.310134	-2.610914
84	6	0	-6.288354	-0.241544	0.906881
85	1	0	-4.912357	-1.796587	1.419807
86	6	0	-6.732034	0.607004	-0.108152
87	1	0	-6.522856	1.260974	-2.144927
88	1	0	-6.761209	-0.207418	1.880608
89	1	0	-2.297466	-2.635542	4.487245
90	7	0	-7.827952	1.545241	0.168875
91	8	0	-8.315713	1.545102	1.301946
92	8	0	-8.200130	2.284410	-0.746310

Table S11 Optimized Cartesian coordinates for [**oP(DA)^{8}** + H^{+}].

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.444666	1.253678	2.710432
2	6	0	-1.675999	0.196759	2.618845
3	6	0	-2.222958	-2.498636	2.386431
4	6	0	-1.778420	-0.357105	1.329166
5	6	0	-1.842457	-0.567768	3.771094
6	6	0	-2.102526	-1.933594	3.654860
7	6	0	-2.096660	-1.732374	1.211120
8	1	0	-1.760626	-0.100956	4.748089
9	1	0	-2.466597	-3.553126	2.291691
10	6	0	-1.644732	0.591483	0.174219
11	6	0	-1.678969	2.466505	-1.942867
12	6	0	-2.597085	1.627706	0.115644

13	6	0	-0.647869	0.537553	-0.831913
14	6	0	-0.707211	1.470883	-1.885023
15	6	0	-2.622934	2.558301	-0.920553
16	1	0	-3.358721	1.670540	0.887915
17	1	0	0.052454	1.425158	-2.659662
18	1	0	-3.386499	3.330216	-0.937161
19	1	0	-1.687145	3.169902	-2.770214
20	6	0	0.452676	-0.478444	-0.917189
21	6	0	2.414077	-2.476807	-1.332942
22	6	0	0.461038	-1.285352	-2.072029
23	6	0	1.493684	-0.652914	0.029810
24	6	0	2.438126	-1.674607	-0.194178
25	6	0	1.424183	-2.266260	-2.292598
26	1	0	-0.339432	-1.156939	-2.793568
27	1	0	3.218970	-1.819448	0.547423
28	1	0	1.379547	-2.877260	-3.189153
29	1	0	3.157241	-3.258350	-1.468182
30	6	0	1.671048	0.134159	1.295643
31	6	0	2.062621	1.393068	3.800587
32	6	0	1.617658	-0.586957	2.503460
33	6	0	1.966267	1.518081	1.354853
34	6	0	2.128674	2.124608	2.615964
35	6	0	1.818727	0.020386	3.740901
36	1	0	1.378401	-1.645179	2.463183
37	1	0	2.340606	3.189631	2.655251
38	1	0	1.757406	-0.570164	4.649989
39	1	0	2.202622	1.890991	4.755499
40	6	0	2.144614	2.410960	0.163787
41	6	0	2.395043	4.252168	-1.968050
42	6	0	1.242145	3.473978	0.001731
43	6	0	3.213938	2.291469	-0.758919
44	6	0	3.306581	3.208739	-1.823121
45	6	0	1.361823	4.390746	-1.041378
46	1	0	0.416409	3.563722	0.700279
47	1	0	4.139031	3.132014	-2.516646
48	1	0	0.644646	5.200375	-1.133213
49	1	0	2.503545	4.957671	-2.785974
50	6	0	4.313191	1.296773	-0.625163
51	6	0	6.502312	-0.437785	-0.442818
52	6	0	4.770117	0.587022	-1.749581
53	6	0	4.985501	1.100743	0.596986
54	6	0	6.075724	0.239171	0.698149
55	6	0	5.862132	-0.276112	-1.667523
56	1	0	4.254647	0.695268	-2.697472
57	1	0	4.662247	1.639903	1.479138
58	1	0	6.575968	0.123927	1.654961
59	1	0	6.190274	-0.817312	-2.552820
60	7	0	7.678469	-1.354014	-0.377457
61	6	0	8.970881	-0.632376	-0.070231
62	1	0	9.796061	-1.342328	-0.144718
63	1	0	9.090439	0.177682	-0.788947
64	1	0	8.910992	-0.228623	0.939500
65	6	0	7.464524	-2.533834	0.541647
66	1	0	6.544120	-3.036329	0.246419
67	1	0	8.319110	-3.206479	0.453972
68	1	0	7.377887	-2.167523	1.563557
69	6	0	-2.344358	-2.456704	-0.079238
70	6	0	-3.443484	-2.196271	-0.937323
71	6	0	-1.481180	-3.518305	-0.399462
72	6	0	-3.596412	-2.981897	-2.096123
73	6	0	-1.660694	-4.299939	-1.539213
74	1	0	-0.642055	-3.718989	0.259905
75	6	0	-2.722004	-4.022904	-2.401115
76	1	0	-4.451307	-2.800667	-2.740376
77	1	0	-0.975782	-5.115696	-1.751009
78	1	0	-2.884793	-4.623934	-3.290779
79	6	0	-4.502294	-1.184868	-0.656234
80	6	0	-4.955763	-0.337690	-1.684948
81	6	0	-5.129260	-1.101136	0.601070
82	6	0	-5.987050	0.571804	-1.472521
83	1	0	-4.478815	-0.376018	-2.658859
84	6	0	-6.162330	-0.196670	0.831729

85	1	0	-4.819088	-1.759860	1.403543
86	6	0	-6.574718	0.634523	-0.209658
87	1	0	-6.331788	1.231260	-2.259426
88	1	0	-6.653674	-0.134857	1.794986
89	1	0	-2.231481	-2.551011	4.539033
90	7	0	-7.656365	1.603321	0.030246
91	8	0	-8.159096	1.635894	1.154902
92	8	0	-7.992538	2.331511	-0.905982
93	1	0	7.778561	-1.736942	-1.322189

Complete Reference 58

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2. S. M. Mathew and C. S. Hartley, *Macromolecules*, 2011, **44**, 8425-8432.
3. We often dope MALDI samples with CuI to promote ionization. While this was not done explicitly for these samples, our MALDI target retains enough residual copper impurities that we often observe prominent Cu^+ adducts in the spectra.