Electronic Supplementary Information to:

Thienopyrazine Polymers as Stable N-type Materials for Organic Supercapacitors

*Bryony T. McAllister, Tyler B. Schon, P.M. DiCarmine, Dwight S. Seferos**

B. T. McAllister, T. B. Schon, P.M. DiCarmine and D. S. Seferos
Department of Chemistry, University of Toronto, 80 St. George Street, Toronto, Ontario, M5S 3H6 Canada
E-mail: dseferos@chem.utoronto.ca

Table of Contents:

Part 4: Continued

Figure S23: Charge discharge behaviour of 1.4 µm potentiostatically polymerized PPTP film at 1.5 V over 200 cycles

Figure S24: Equivalent circuit used to fit impedance data for PPTP film

Geometry coordinates for TP, DMTP, NTP, PATP, PTP, *t*BuPTP and hexamers

Part 5: References

Part 1: NMR

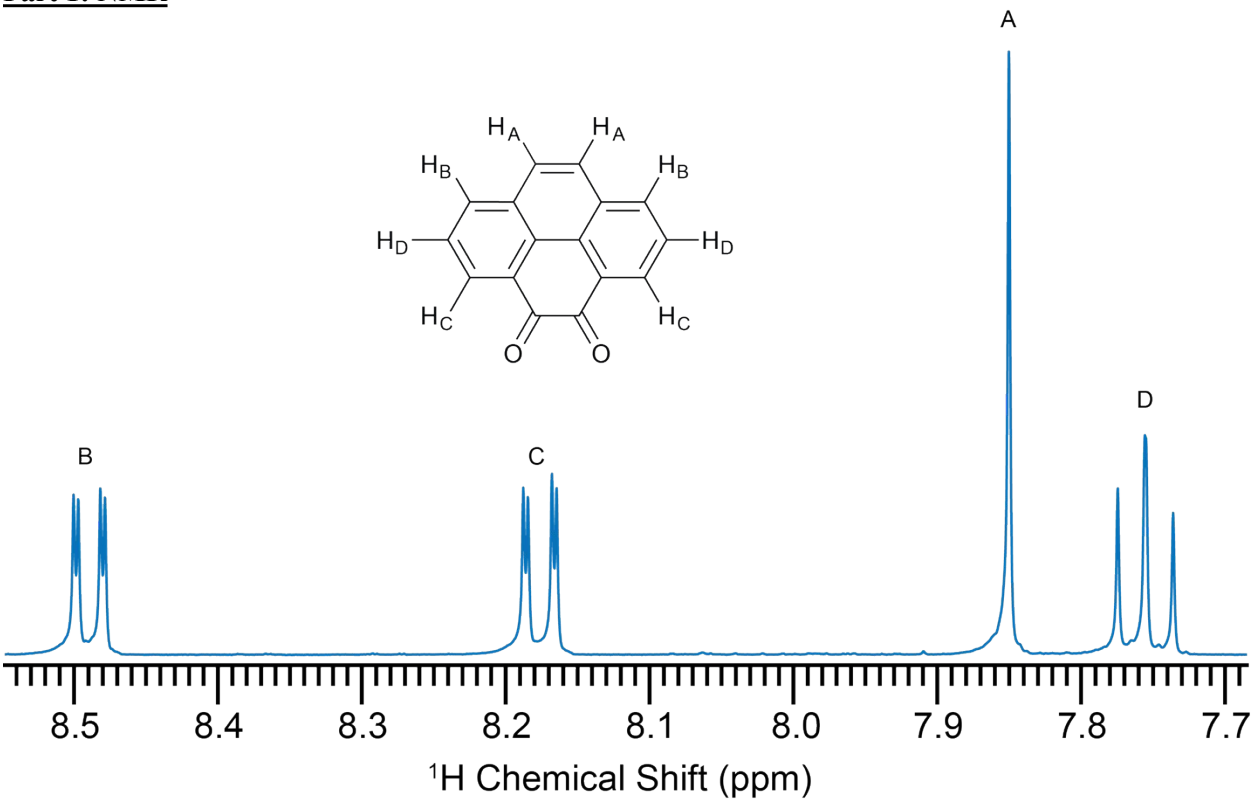

Figure S1: ^{1}H NMR spectrum of pyrene-4,5-dione

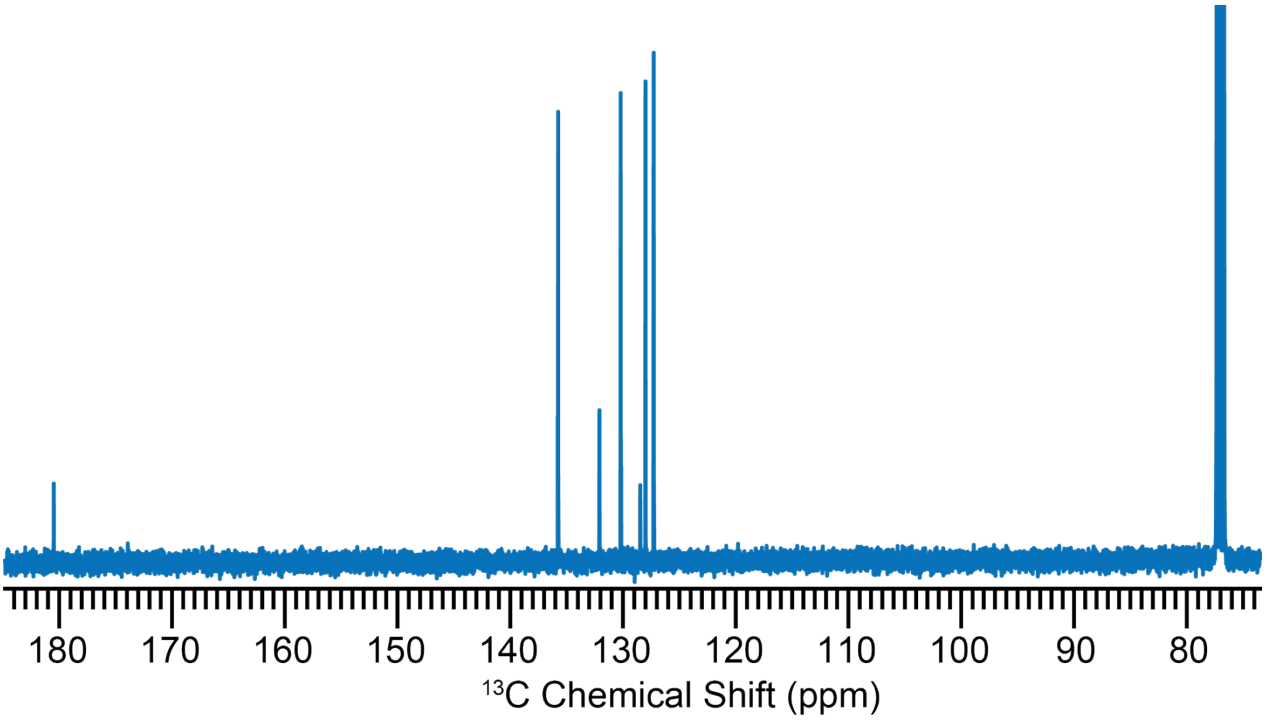

Figure S2: ^{13}C NMR spectrum of pyrene-4,5-dione

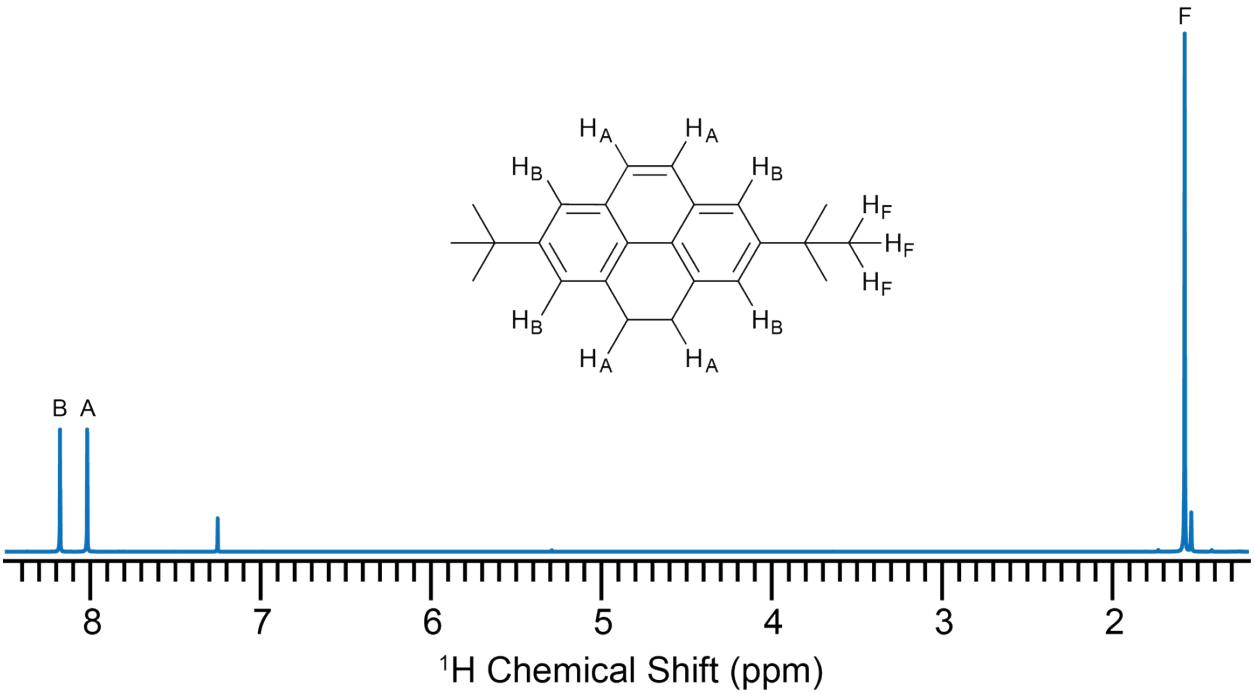

Figure S3: ^{1}H NMR spectrum of 2,7-di-*tert*-butylpyrene

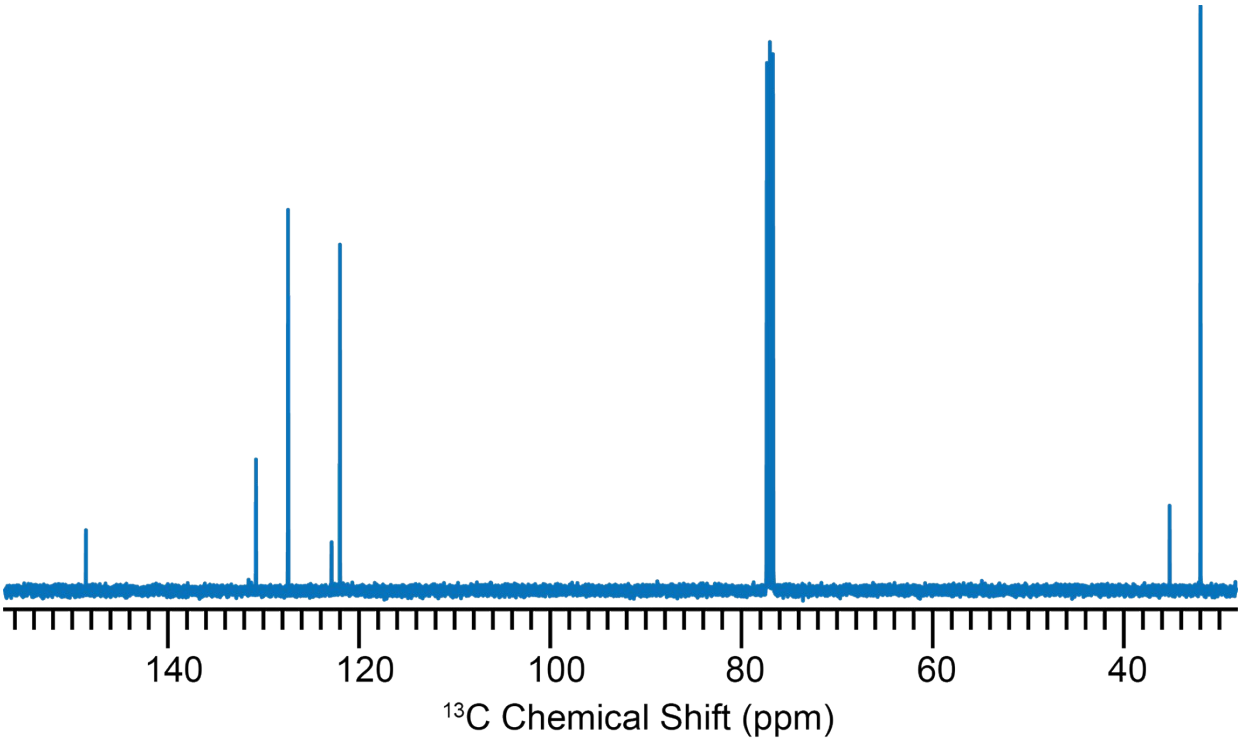

Figure S4: ^{13}C NMR spectrum of 2,7-di-*tert*-butylpyrene

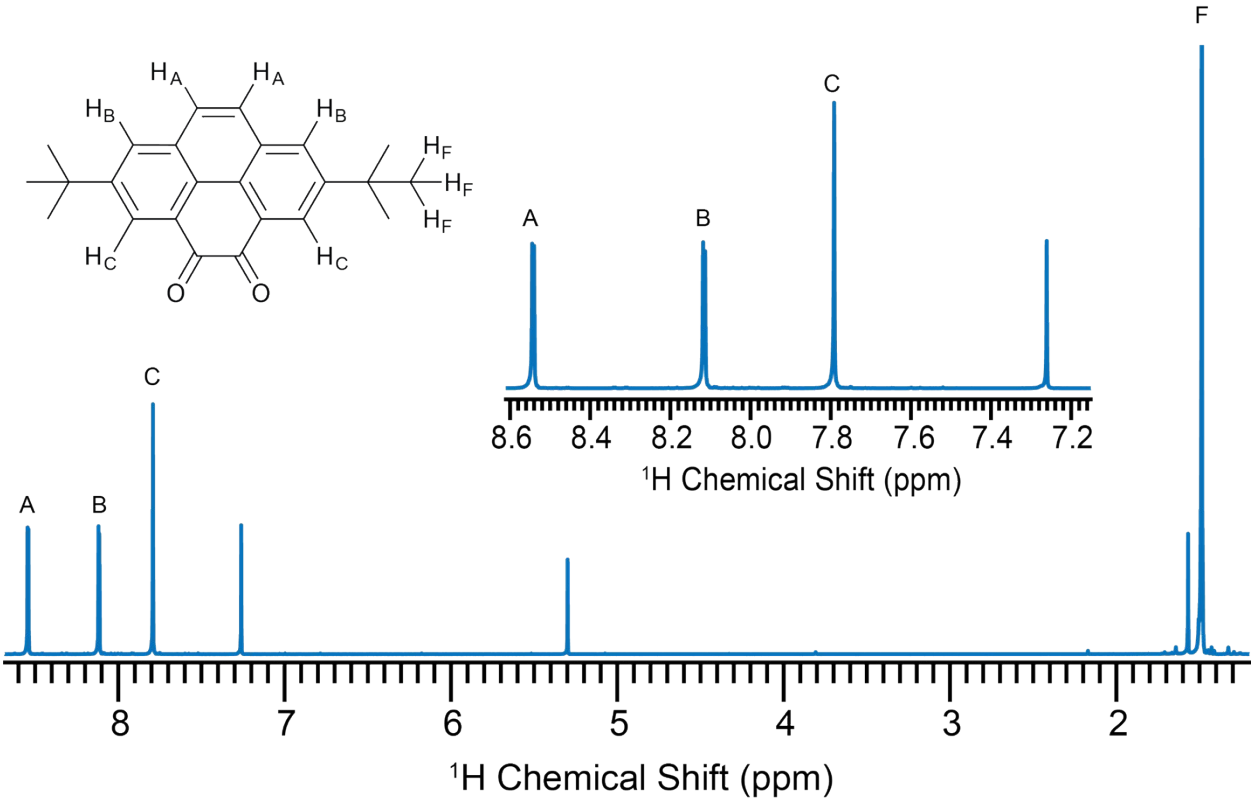

Figure S5: ^{1}H NMR spectrum of 2,7-di-tert-butylpyrene-4,5-dione

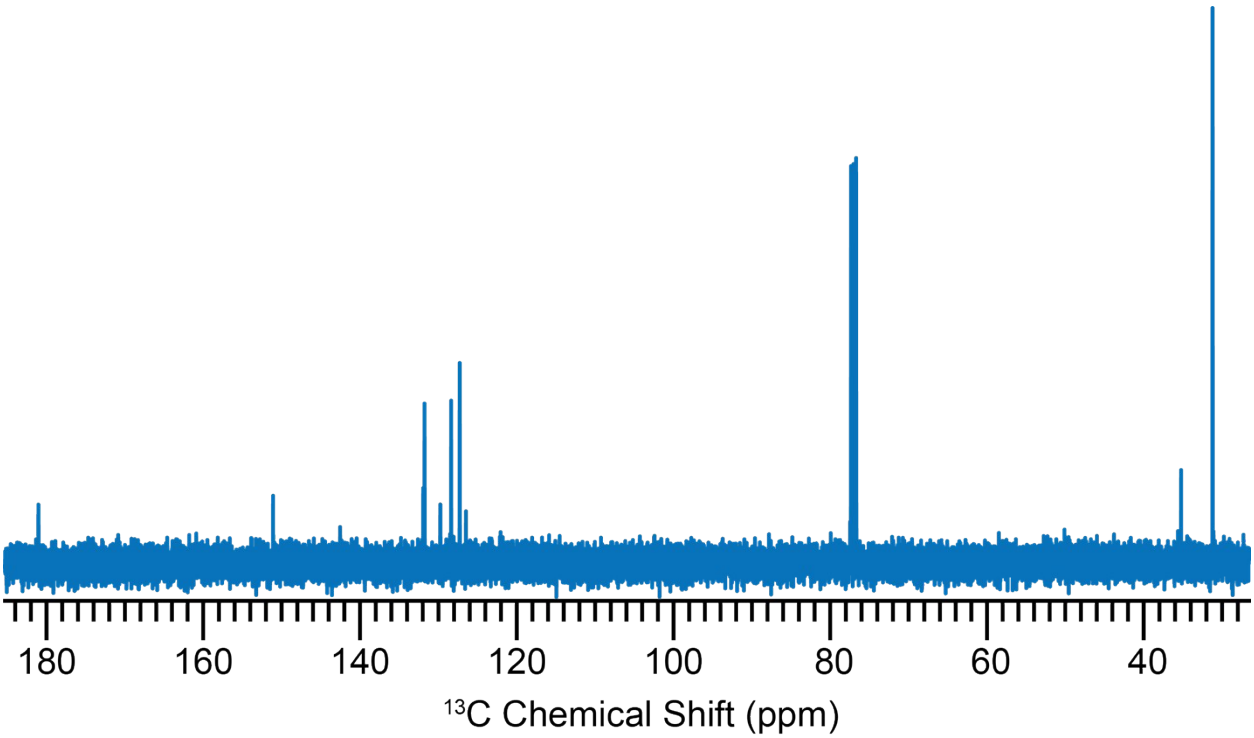

Figure S6: ^{13}C NMR spectrum of 2,7-di-tert-butylpyrene-4,5-dione

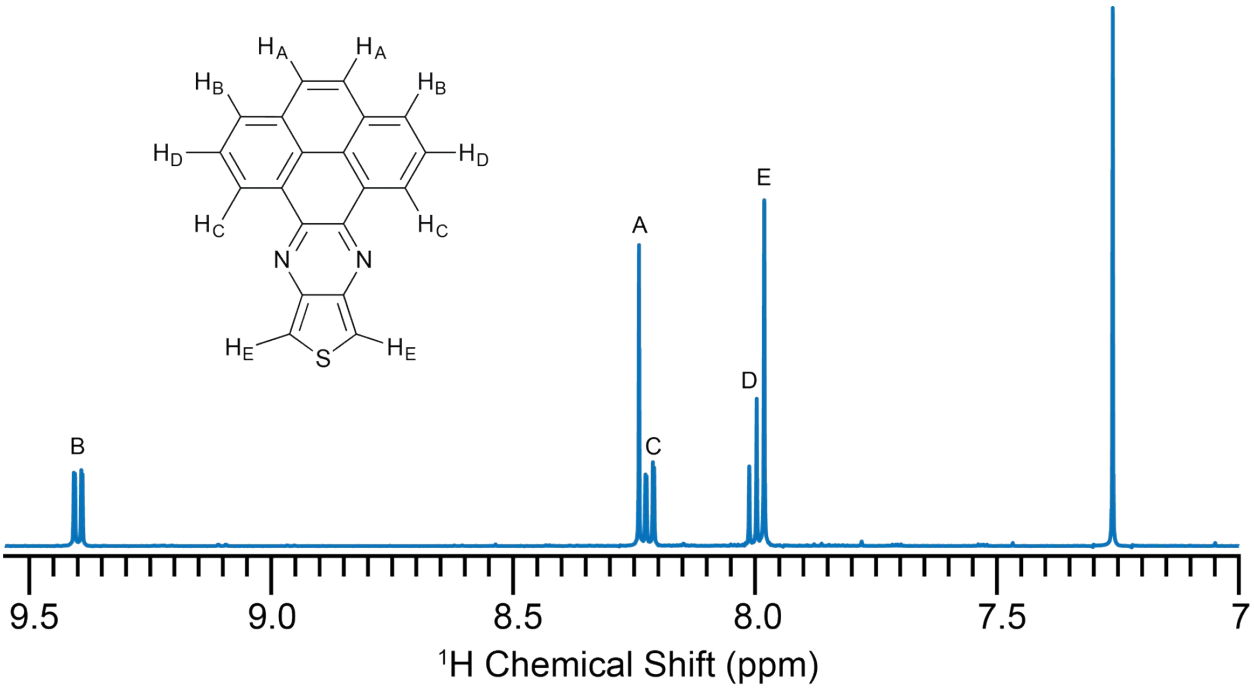

Figure S7: ^{1}H NMR spectrum of PTP

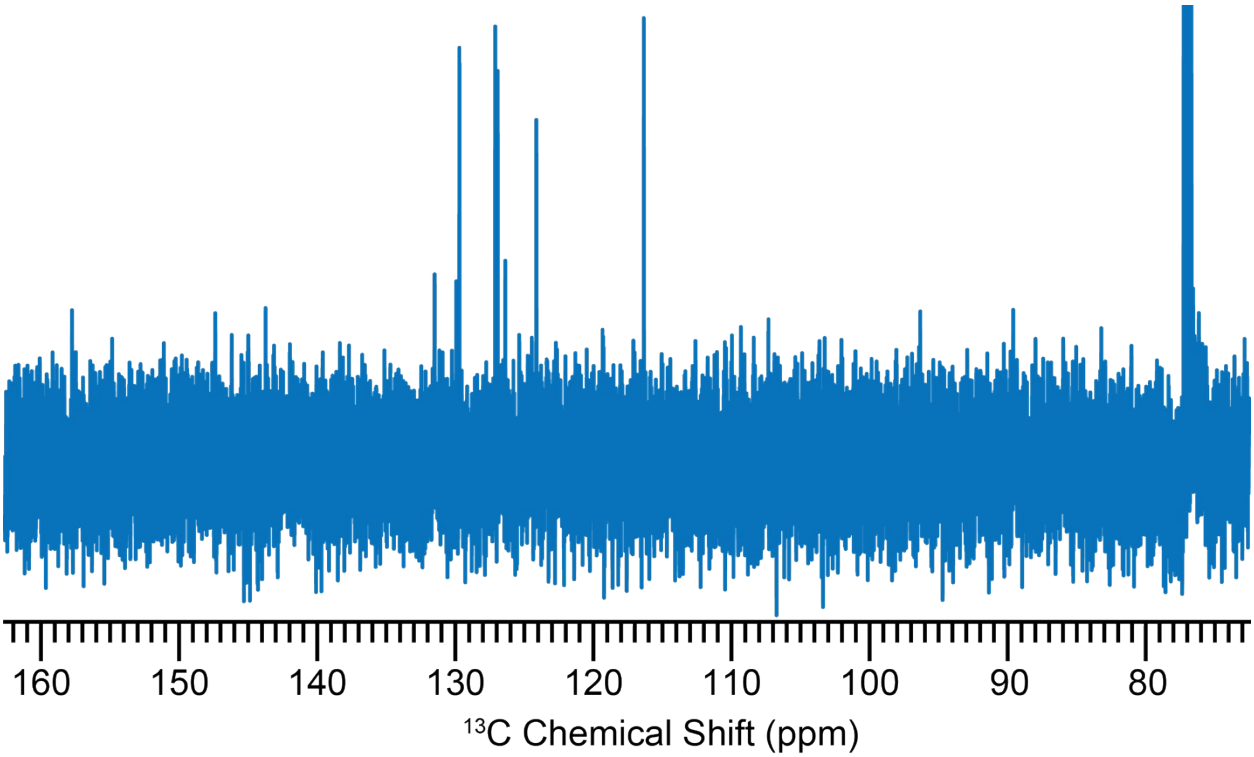

Figure S8: ^{13}C NMR spectrum of PTP (note: peak intensity is low due to insolubility of PTP)

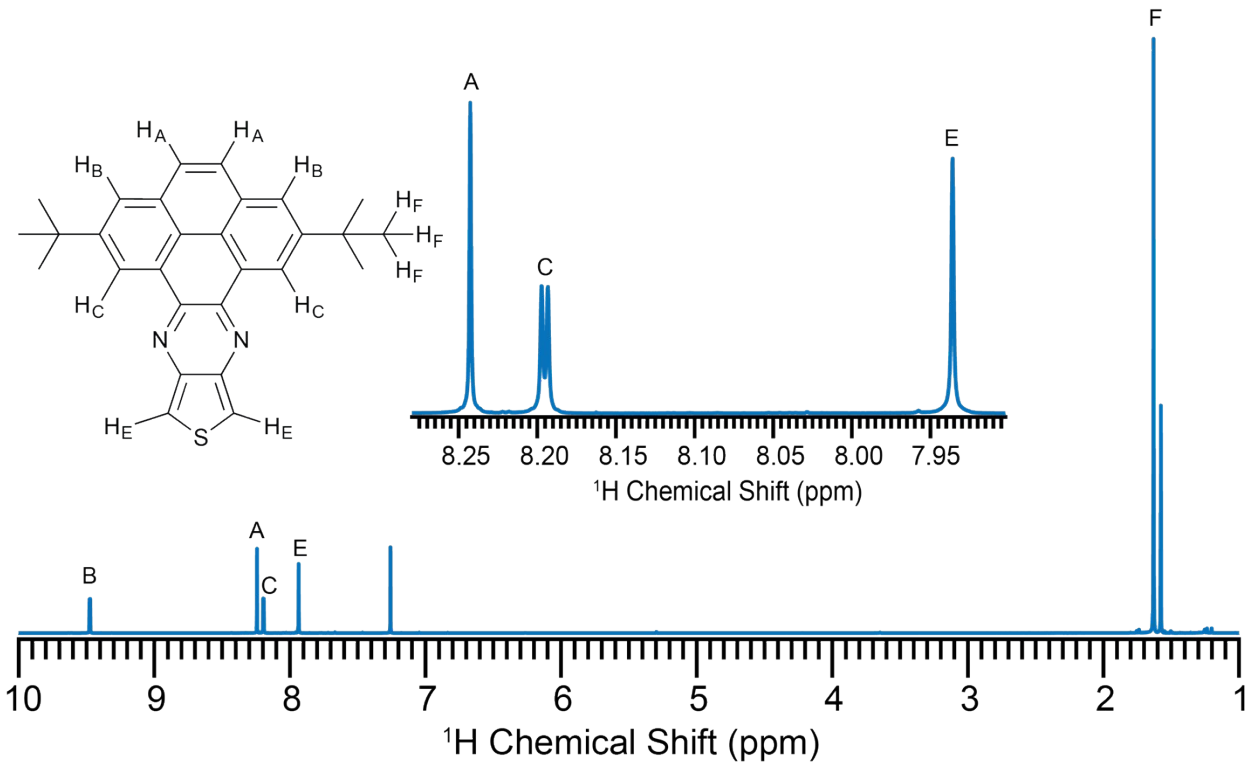

Figure S9: ^{1}H NMR spectrum of *t*BuPTP

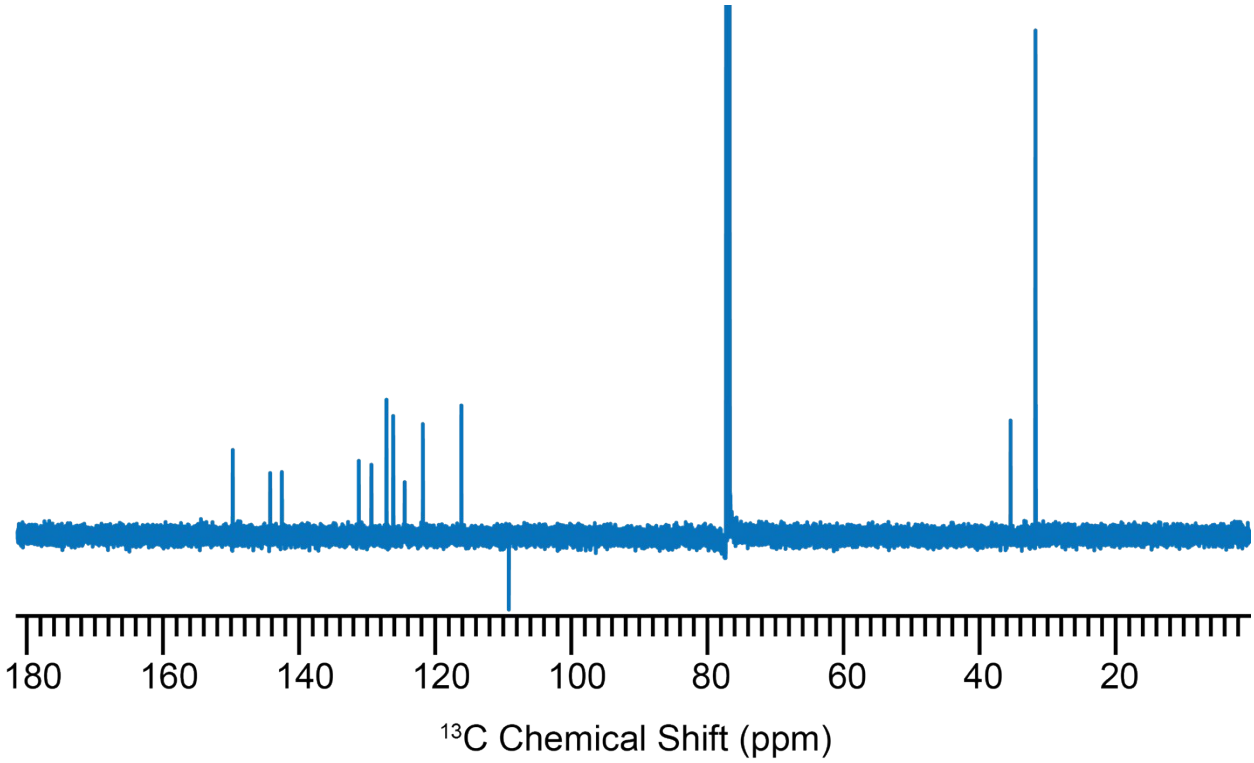

Figure S10: ^{13}C NMR spectrum of *t*BuPTP

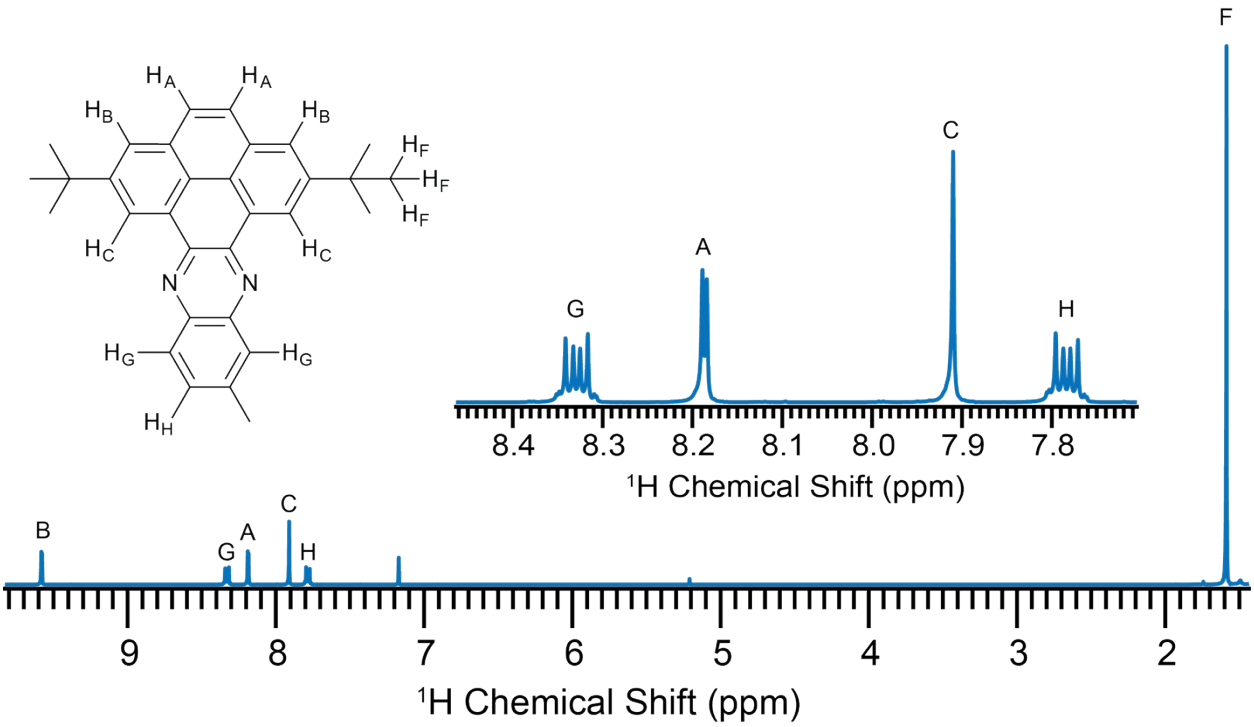

Figure S11: ^{1}H NMR spectrum of *t*BuPP

Part 2: Monomer Properties

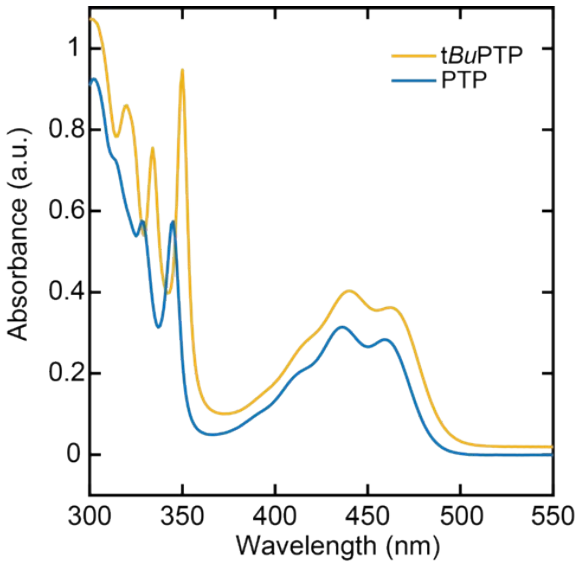

Figure S12: UV-Vis spectra of TP monomers in CH_2Cl_2 solution

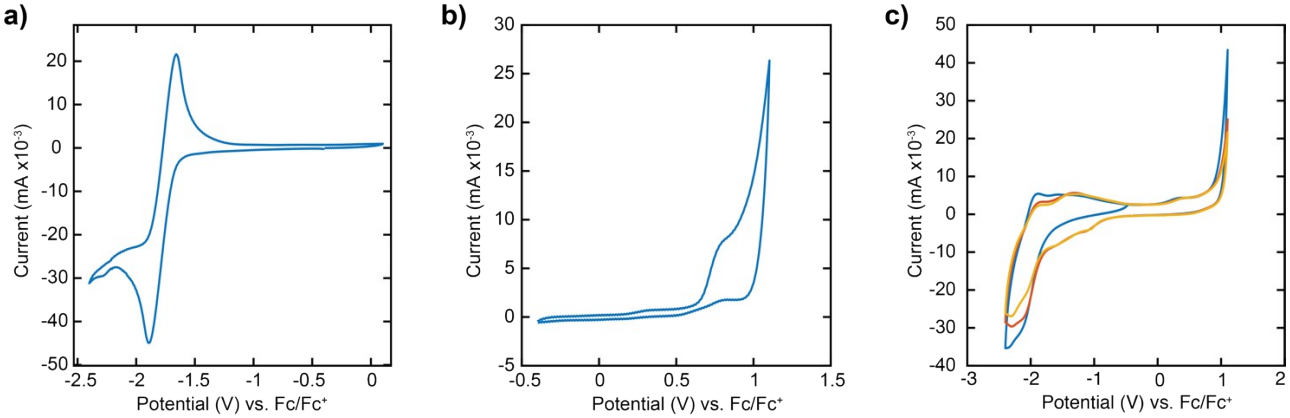

Figure S13: Electrochemical behaviour of *t*BuPTP (1.5 mM) in 0.1 M $TBAPF_6$ in DCM on a platinum button working electrode in a 3-electrode cell with a platinum mesh counter electrode and silver wire pseudoreference referenced to ferrocene, performed at 100 mV s^{-1}. (a) Reversible reduction of *t*BuPTP; (b) Irreversible oxidation of *t*BuPTP; (c) Electrochemical behaviour of P*t*BuPTP polymerized on Pt button electrode in 18 CV scans. The blue, red and yellow traces represent the first, second and third scans, respectively.

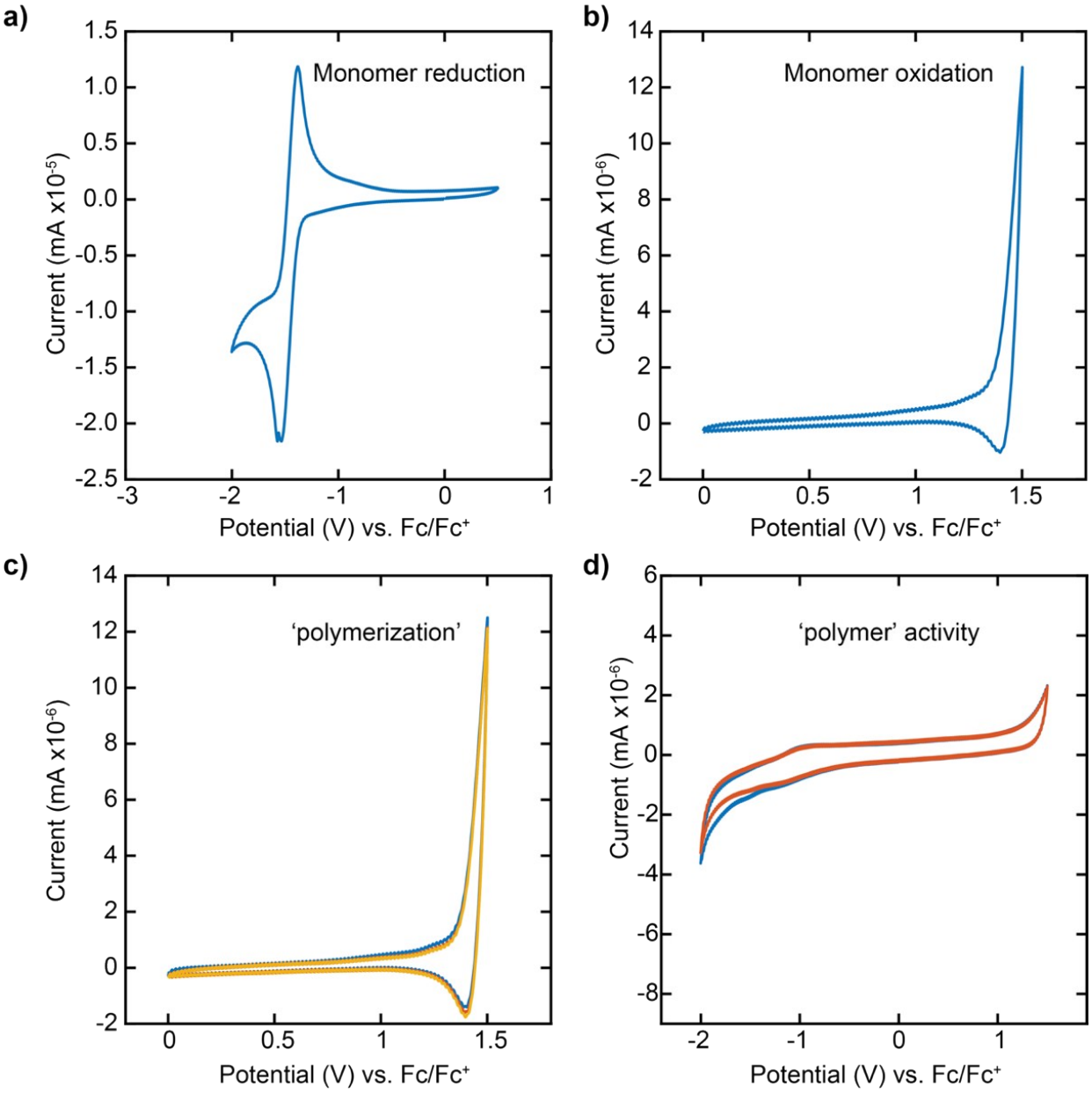

Figure S14: Electrochemical activity of *t*BuPP modified monomer demonstrating (a) reversible reduction; (b) irreversible oxidation; (c) CV of monomer solution over 18 cycles; and (d) electrode after oxidizing monomer solution for 18 cycles.

Part 3: Computational Analysis of Hexamers

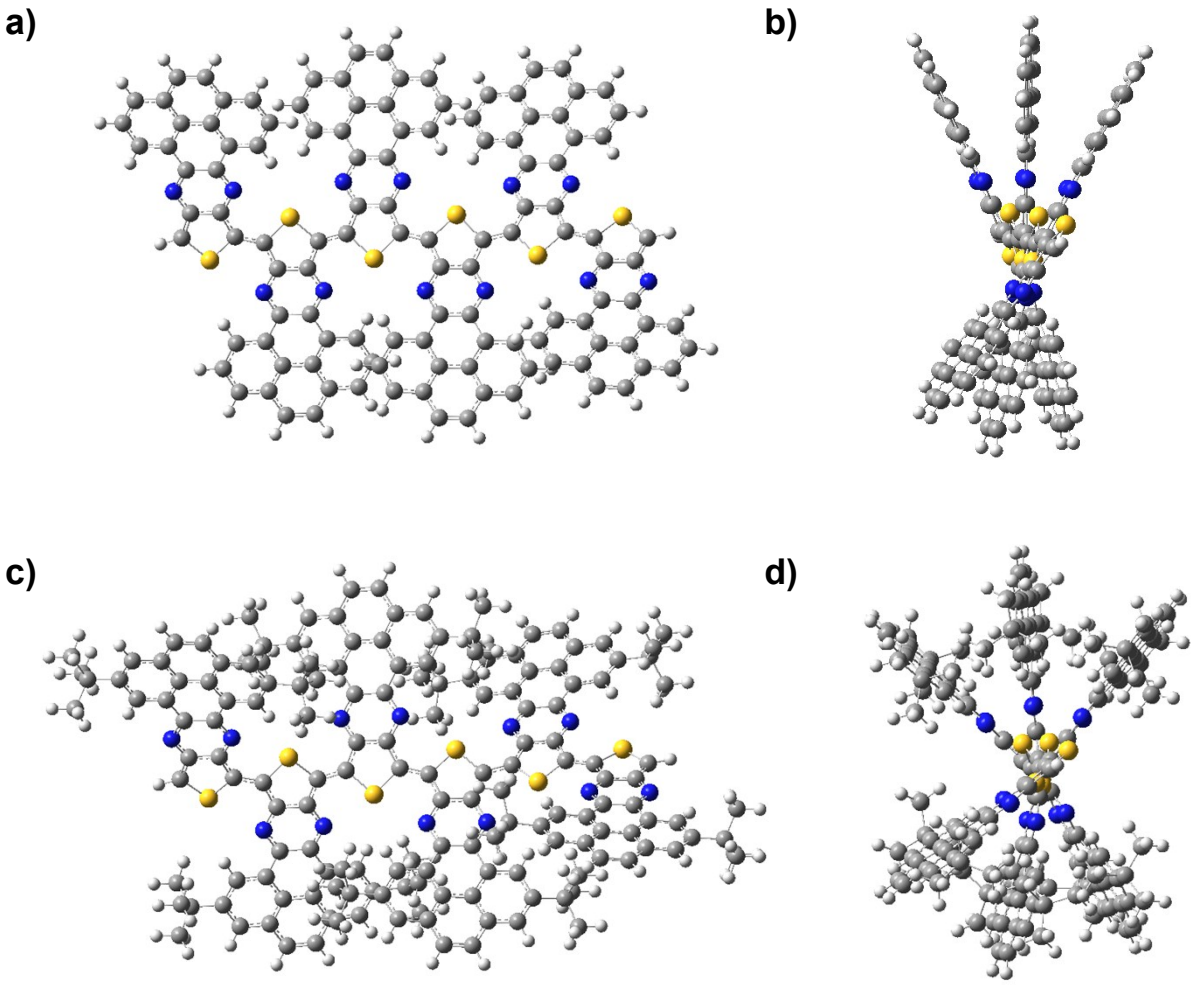

Figure S15: Optimized geometry of (a, b) PTP hexamer and (c, d) *t*BuPTP hexamer. Hexamer geometries were optimized using the B3LYP function and 6-31g(d) basis set. Grey, white, blue and yellow spheres correspond to carbon, hydrogen, nitrogen and sulfur atoms, respectively.

Part 4: PPTP Polymer Characterization

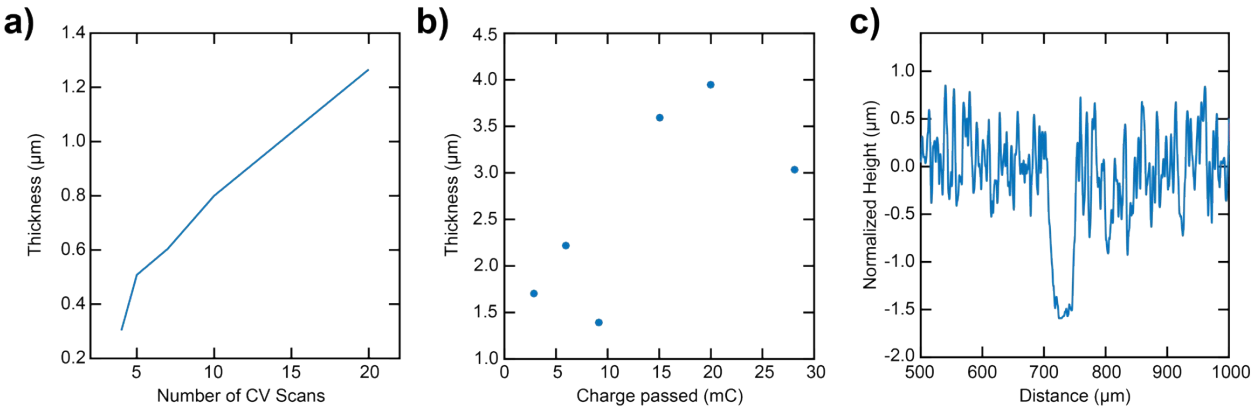

Figure S16: Determination of PPTP polymer film thicknesses via profilometry. (a) Thicknesses of CV polymerized films as a function of number of CV cycles; (b) Thickness of potentiostatically polymerized films as a function of charge passed; (c) Representative histogram of film height for 1.4 µm film.

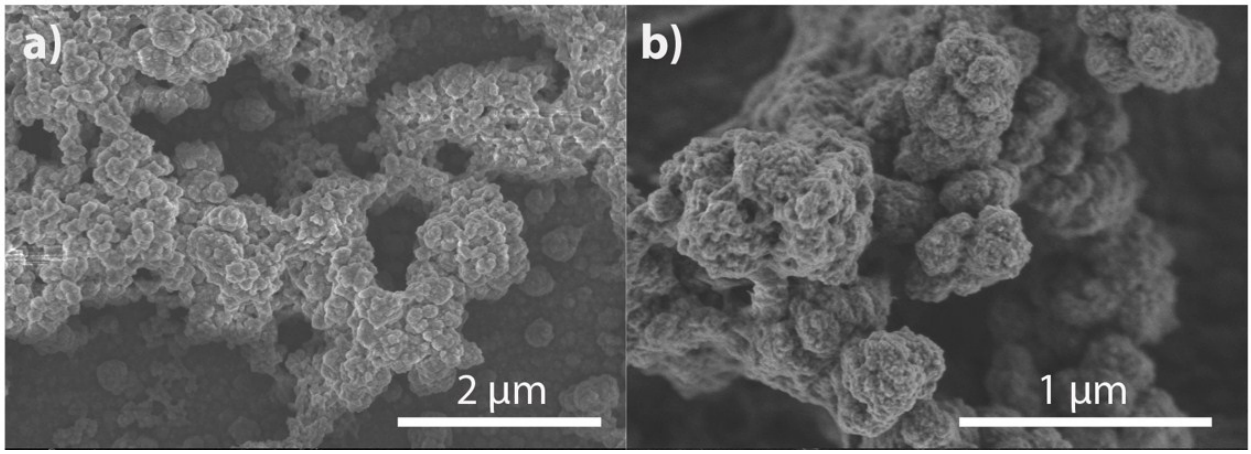

Figure S17: Examination of morphology and chemical composition of PPTP polymer films on gold Kapton using SEM. (a, b) SEM image of 1.4 µm potentiostatically polymerized film obtained at 0.5 kV in deceleration mode

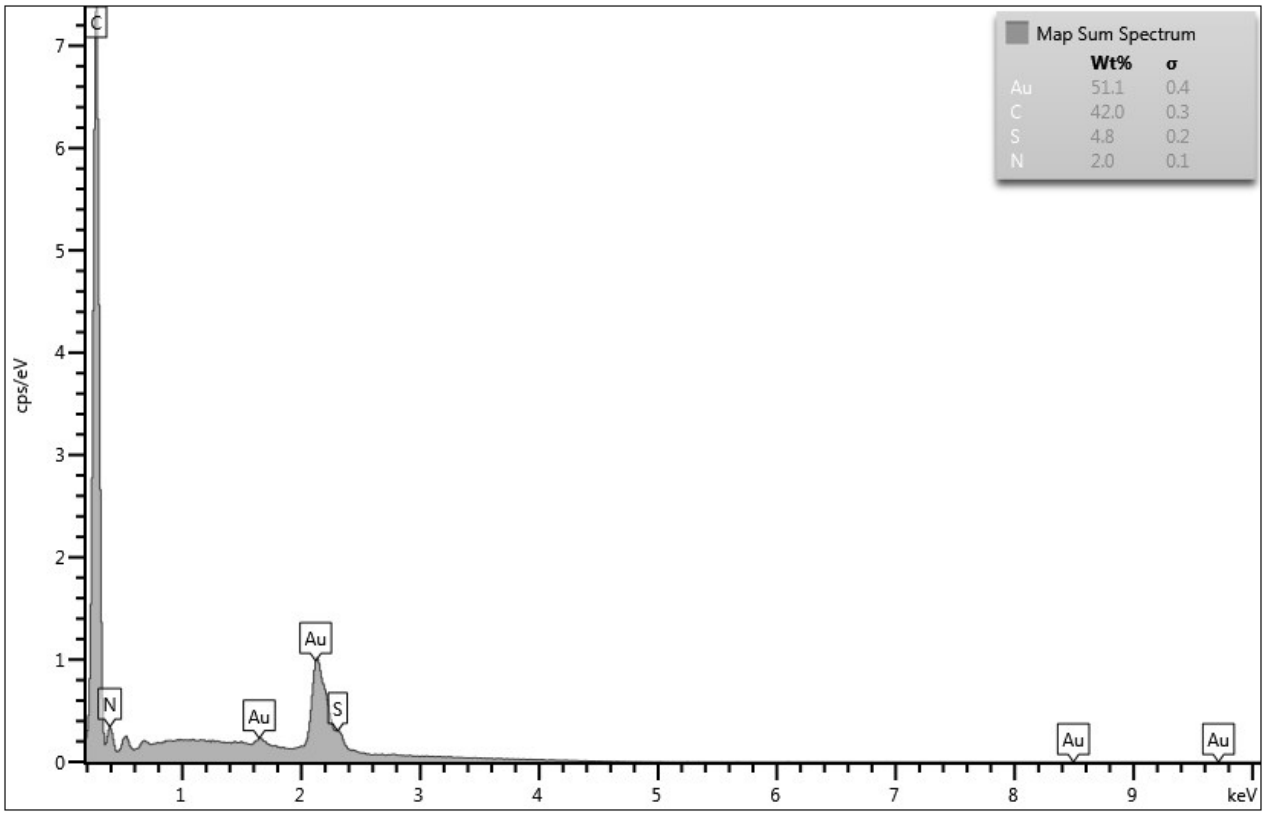

Figure S18: EDX Spectrum of 1.4µm potentiostatically polymerized film

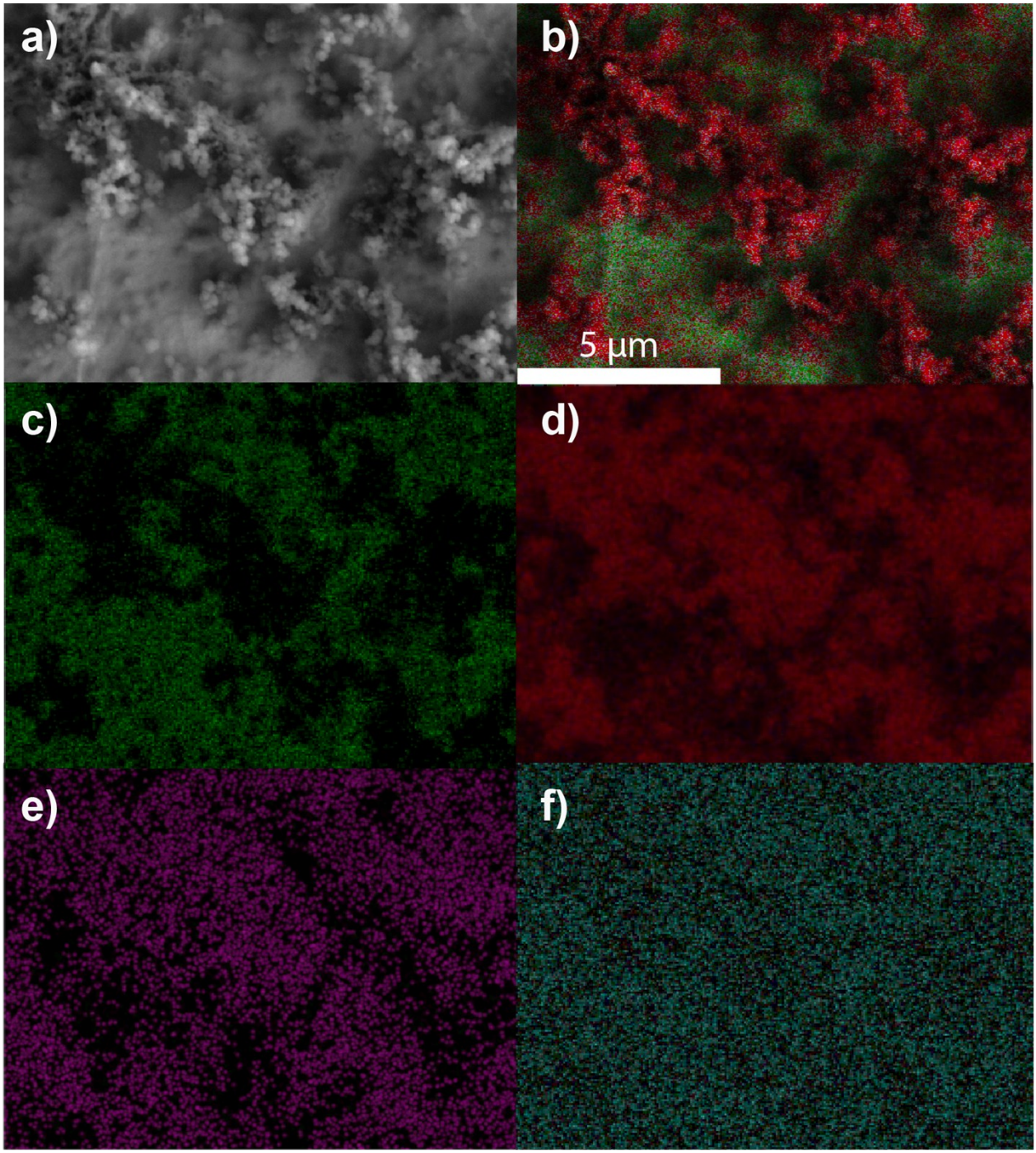

Figure S19: (a) SEM image of PPTP film region used to collect elemental contrast map, (b) elemental map showing distribution of all elements, (c) distribution of gold, (d) distribution of carbon, (e) distribution of nitrogen, and (f) distribution of sulfur.

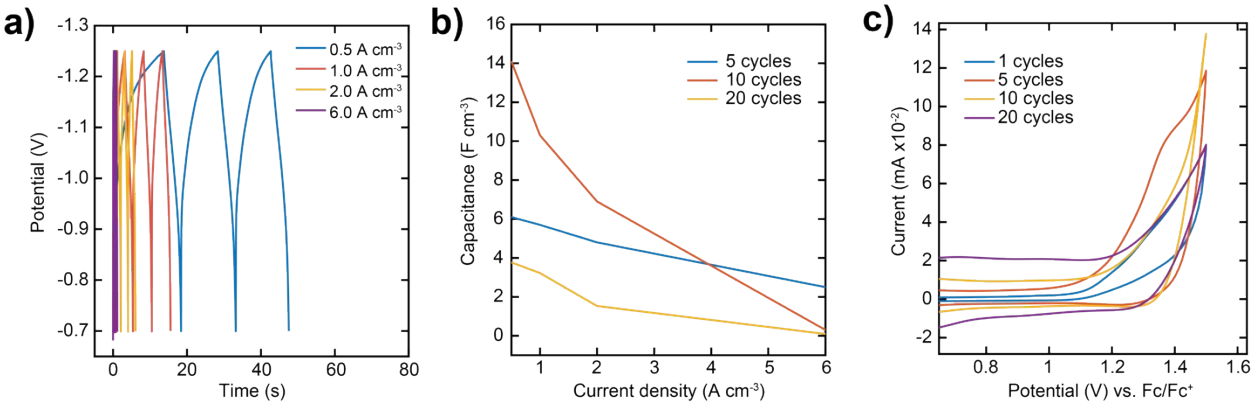

Figure S20: (a) Representative charge-discharge behaviour for 0.8 µm CV polymerized PPTP film; (b) Rate capability of PPTP films polymerized in 5, 10 and 20 CV cycles; (c) Representative CV of polymerization showing increase of oxidative peak up to 10 cycles, followed by subsequent decrease in current.

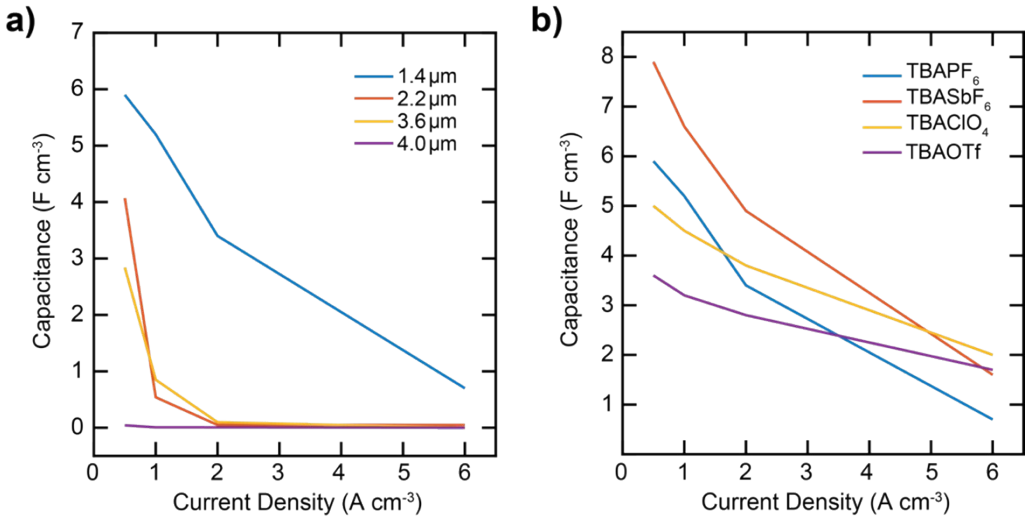

Figure S21: Performance of potentiostatically polymerized PPTP films. (a) Trend in capacitance and rate capability with increasing film thickness; (b) Trend in capacitance and rate capability with different electrolytes.

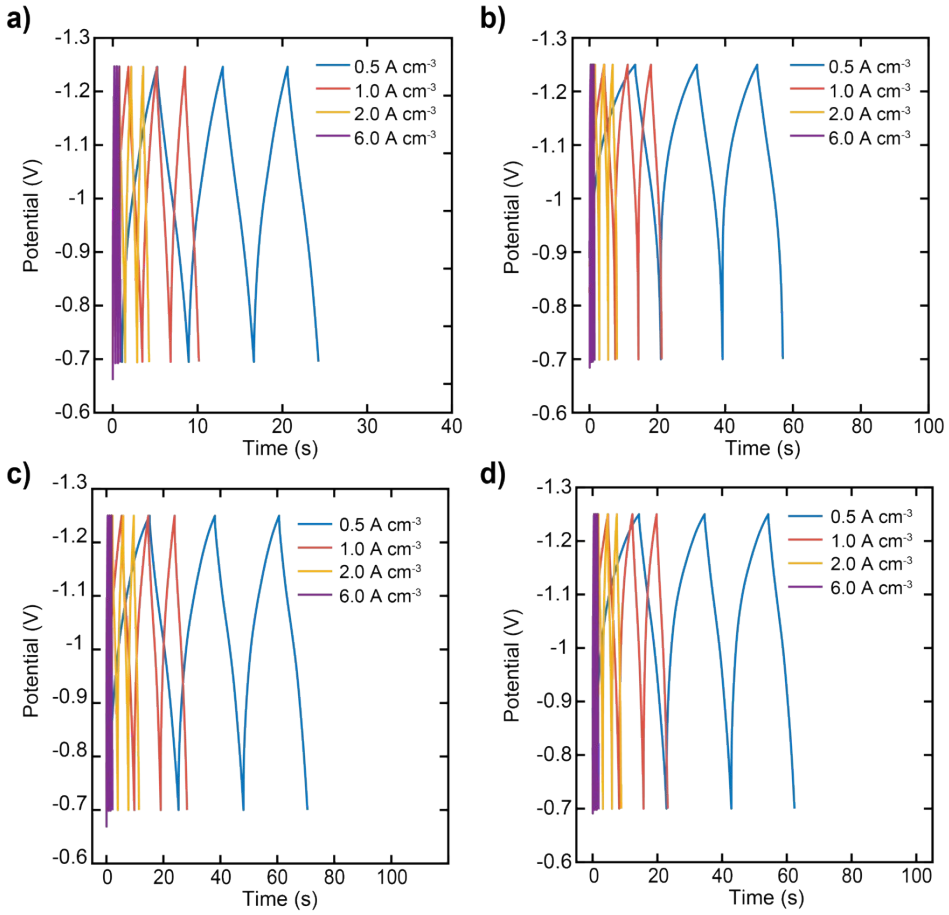

Figure S22: The effect of electrolyte concentration on capacitance of 1.4 µm PPTP films polymerized potentiostatically at 1.5 V. (a) 0.1 M $TBAPF_6$ in polymerization solution and testing solution (b) 0.1M $TBAPF_6$ in polymerization solution and 0.5 M in testing solution (c) 0.5 M $TBAPF_6$ in polymerization solution and 0.1 M in testing solution (d) 0.5 M $TBAPF_6$ in polymerization solution and testing solution.

Table S1: Effect of electrolyte concentration on capacitance of 1.4 µm PPTP films polymerized potentiostatically at 1.5 V

Concentration of $TBAPF_6$ in polymerization solution (M)	Concentration of $TBAPF_6$ in testing solution (M)	Capacitance at 0.5 A cm^{-3}	Capacitance at 1.0 A cm^{-3}	Capacitance at 2.0 A cm^{-3}	Capacitance at 6.0 A cm^{-3}
0.1	0.1	5.9	5.2	3.4	0.7
0.1	0.5	8.8	7.6	6.0	2.6
0.5	0.1	9.8	8.9	7.3	2.9
0.5	0.5	8.5	7.2	5.7	3.2

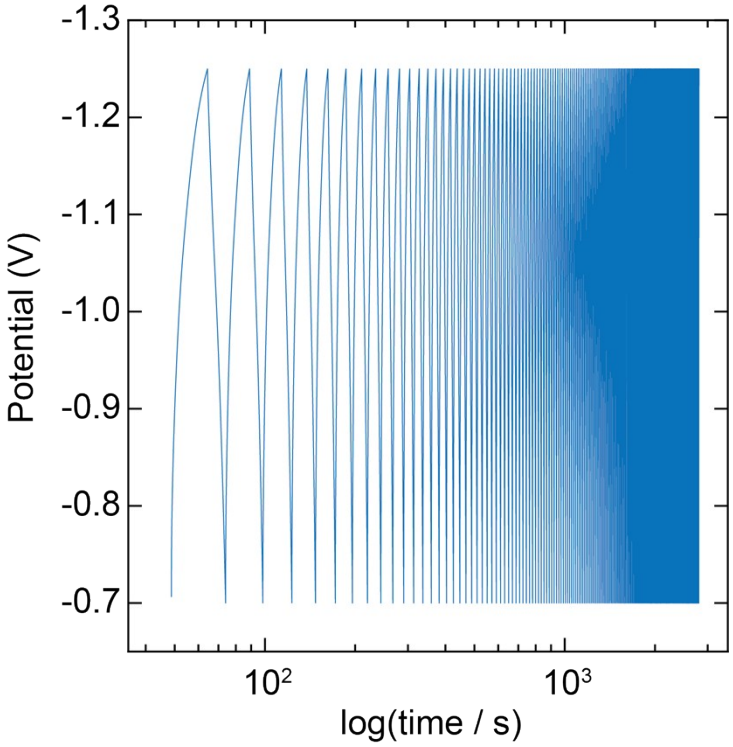

Figure S23: Charge discharge behaviour of 1.4 µm potentiostatically polymerized PPTP film at 1.5 V over 200 cycles. PPTP film was polymerized and tested in 0.1 M $TBAPF_6$

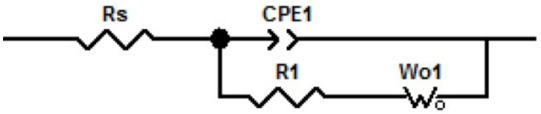

Figure S24: Equivalent circuit used to fit impedance data for PPTP film

Geometry Coordinates for TP

C	-4.02017	1.4121	0.
C	-2.62501	1.4121	0.
C	-2.62513	3.82836	-0.0012
C	-4.01995	3.82829	-0.00168
H	-2.07493	4.78051	-0.00126
H	-4.57008	4.78057	-0.00263
N	-4.71755	2.62008	-0.00068
N	-1.92747	2.61985	0.
C	-2.16951	-0.12918	0.00176
C	-4.79011	0.07839	0.00063
S	-3.66331	-1.11541	0.00137
H	-1.19581	-0.12757	0.00176
H	-5.76381	0.08027	0.00063

Geometry Coordinates for DMTP

C	-4.13738	1.48715	0.00009
C	-2.7351	1.55466	-0.00005
C	-2.60235	3.68049	-0.00112
C	-4.04145	3.73868	-0.00128
N	-4.80748	2.68205	-0.00067
N	-1.92426	2.5654	-0.00037
C	-2.16611	0.00587	0.0016
C	-4.71696	0.2334	0.00042
S	-3.51208	-0.98749	0.00186
H	-1.13908	-0.32455	0.00221
H	-5.76742	-0.0126	-0.00008
C	-1.79915	4.99444	-0.002
H	-2.04313	5.56102	-0.87627
H	-2.04385	5.56263	0.87103
H	-0.7524	4.7726	-0.00136
C	-4.7358	5.11326	-0.00236
H	-4.44649	5.65968	0.87093
H	-4.44629	5.6584	-0.87638
H	-5.79706	4.97677	-0.00238

Geometry Coordinates for NTP

C	-4.02017	1.4121	0.
C	-2.62501	1.4121	0.
C	-2.62513	3.82836	-0.0012
C	-4.01995	3.82829	-0.00168
N	-4.71755	2.62008	-0.00068
N	-1.92747	2.61985	0.
C	-2.16951	-0.12918	0.00176
C	-4.79011	0.07839	0.00063
S	-3.66331	-1.11541	0.00137
H	-1.19581	-0.12757	0.00176
H	-5.76381	0.08027	0.00063

C	-1.85462	5.16175	-0.00128
C	-4.36364	5.39343	-0.00291
C	-2.98392	6.14261	-0.00259
C	-5.67801	5.8796	-0.00303
H	-6.4999	5.19447	-0.0024
C	-2.51631	7.59045	0.00141
C	-5.52247	7.15792	-0.00309
H	-6.59243	7.14918	-0.00324
C	-3.86684	8.13018	-0.00119
H	-3.33149	9.05663	0.00072
C	-0.81203	7.47269	0.0029
C	-0.56786	5.38453	-0.01002
H	0.3079	4.76976	-0.01174
C	0.09427	6.47832	0.02057
H	-0.31984	8.31282	-0.00294
H	1.06796	6.47602	0.02247

Geometry Coordinates for PATP

C	-11.85833	5.67426	-0.77758
C	-11.83867	4.96168	0.40392
C	-12.4528	5.47976	1.56672
C	-13.09672	6.73977	1.52264
C	-13.10189	7.44794	0.29842
C	-12.49529	6.92676	-0.82773
C	-12.42657	4.73324	2.79207
C	-13.72197	7.25631	2.71985
C	-13.67549	6.49119	3.91004
C	-13.01244	5.21848	3.9159
C	-14.28255	6.98322	5.08783
H	-14.23661	6.37488	6.00375
C	-14.92254	8.20569	5.08992
C	-14.97233	8.97045	3.91106
C	-14.38438	8.50554	2.75094
H	-11.37961	5.27109	-1.68182
H	-11.34363	3.98023	0.45665
H	-13.59402	8.42938	0.23354
H	-12.50717	7.48992	-1.7727
H	-15.39484	8.58807	6.0065
H	-15.48423	9.94418	3.9197
H	-14.43689	9.12217	1.84175
N	-12.98931	4.45987	5.17482
N	-11.74608	3.43023	2.78963
C	-12.24946	3.23768	5.08436
C	-11.30319	3.00553	4.05137
C	-10.30959	2.01967	3.9825
C	-11.79028	2.33575	6.15245
H	-12.34528	2.68285	6.99885
S	-9.97938	1.59859	5.60644
H	-10.03474	1.6601	3.12037

Geometry Coordinates for PTP

C	-6.68891	-4.72037	-0.00045
C	-5.29607	-4.72037	-0.00045
C	-4.5876	-3.51188	-0.00045
C	-5.30472	-2.28727	-0.00041
C	-6.72385	-2.29661	-0.00038
C	-7.40066	-3.52303	-0.00048
C	-3.14855	-3.4698	-0.00038
C	-4.59593	-1.04147	-0.00019
C	-3.17684	-1.03214	-0.00016
C	-2.47772	-2.29066	-0.0003
C	-2.5	0.19435	0.
H	-1.39982	0.20721	-0.00003
C	-3.21172	1.39162	0.00015
C	-4.60464	1.39162	0.00018
C	-5.31306	0.18318	-0.00003
C	-6.75215	0.14105	-0.00024
C	-7.42297	-1.03807	-0.0004
H	-8.52353	-1.06612	-0.00092
H	-7.29046	1.1014	-0.00016
H	-7.23313	-5.67685	-0.00071
H	-4.74501	-5.67265	-0.00054
H	-8.50082	-3.53586	-0.00086
H	-2.6676	2.34818	0.00013
H	-5.15562	2.34398	0.0002
N	-1.0082	-2.25335	-0.00068
N	-2.42996	-4.75219	-0.00078
C	-1.09634	-4.77156	-0.10344
C	-0.31016	-3.39448	0.00118
C	1.11223	-3.87785	-0.05473
H	1.62533	-2.9414	0.01378
C	-0.4059	-5.99106	-0.09694
H	-0.94211	-6.90661	0.04139
S	1.1798	-5.50597	-0.23979

Geometry Coordinates for *t*BuPTP

C	-5.87619	-4.22567	-0.00045
C	-4.48335	-4.22567	-0.00045
C	-3.77488	-3.01718	-0.00045
C	-4.492	-1.79257	-0.00041
C	-5.91113	-1.80191	-0.00038
C	-6.58794	-3.02833	-0.00048
C	-2.33583	-2.9751	-0.00038
C	-3.78321	-0.54677	-0.00019
C	-2.36412	-0.53744	-0.00016
C	-1.665	-1.79597	-0.0003
C	-1.68728	0.68905	0.
H	-0.5871	0.70191	-0.00003
C	-2.399	1.88632	0.00015

C	-3.79192	1.88632	0.00018
C	-4.50034	0.67788	-0.00003
C	-5.93943	0.63575	-0.00024
C	-6.61025	-0.54337	-0.0004
H	-7.71081	-0.57142	-0.00092
H	-6.47774	1.5961	-0.00016
H	-3.93229	-5.17795	-0.00054
H	-7.6881	-3.04116	-0.00086
H	-4.3429	2.83868	0.0002
C	-1.63757	3.22491	0.00012
C	-6.63777	-5.56417	-0.00082
C	-2.47407	4.29132	0.73129
H	-1.86883	5.154	0.91672
H	-3.31081	4.56655	0.12382
H	-2.82378	3.89438	1.66137
C	-1.38903	3.67406	-1.45181
H	-0.87249	4.61112	-1.45181
H	-0.79585	2.93981	-1.95571
H	-2.32606	3.78332	-1.95671
C	-0.28818	3.04792	0.72083
H	-0.44955	2.58286	1.67087
H	0.35522	2.43265	0.12722
H	0.16735	4.00529	0.86516
C	-7.98249	-5.38987	0.72922
H	-8.64543	-4.80967	0.12195
H	-8.4159	-6.3508	0.91271
H	-7.82046	-4.88803	1.66024
C	-6.89568	-6.00764	-1.45286
H	-5.96101	-6.1424	-1.95598
H	-7.43718	-6.9305	-1.4531
H	-7.46804	-5.25813	-1.95837
C	-5.79673	-6.63351	0.72082
H	-4.93809	-6.87161	0.12841
H	-5.48101	-6.25732	1.67145
H	-6.38674	-7.51459	0.86398
N	-0.19548	-1.75865	-0.00068
N	-1.61724	-4.25749	-0.00078
C	0.50256	-2.8997	-0.01478
C	-0.27965	-4.27467	-0.00106
C	1.92693	-3.35843	-0.01927
H	2.44025	-2.41993	0.00545
C	0.41025	-5.49442	0.01192
H	-0.13478	-6.41514	0.0226
S	2.00657	-5.02637	0.00398

Geometry Coordinates for PTP hexamer

C	-0.53968	-1.58025	-0.24627
C	-8.27795	-2.08225	-0.65071
C	-6.89121	-2.20751	-0.55265

C	-6.07345	-1.07894	-0.55887
C	-6.65494	0.21129	-0.6636
C	-8.07069	0.33306	-0.75865
C	-8.86111	-0.83053	-0.75221
C	-4.61515	-1.20799	-0.45733
C	-5.83683	1.39381	-0.66573
C	-4.42077	1.30527	-0.58054
C	-3.78619	-0.01084	-0.5012
C	-3.65755	2.47313	-0.56624
H	-2.58084	2.39073	-0.49325
C	-4.26847	3.7255	-0.6432
C	-5.64585	3.82687	-0.73701
C	-6.45282	2.67436	-0.75035
C	-7.88217	2.75704	-0.84616
C	-8.65384	1.64056	-0.85272
H	-9.7345	1.71999	-0.92484
H	-8.33831	3.7403	-0.91304
H	-8.89929	-2.9719	-0.64577
H	-6.42527	-3.18139	-0.47036
H	-9.9404	-0.73432	-0.82543
H	-3.65633	4.62072	-0.63638
H	-6.1187	4.80236	-0.80082
N	-4.0962	-2.41213	-0.32983
N	-2.46504	-0.08509	-0.45922
C	-2.74511	-2.49189	-0.25192
C	-1.92057	-1.30957	-0.33725
C	-1.99978	-3.6445	-0.08721
H	-2.36143	-4.65594	0.0183
S	-0.31807	-3.30123	-0.03233
C	0.55057	-0.66726	-0.31054
C	1.90345	-0.91564	-0.00974
S	0.36779	0.99074	-0.83541
N	2.39913	-2.08859	0.4241
C	2.75195	0.22636	-0.19701
C	2.06597	1.36745	-0.65413
C	3.69895	-2.14827	0.66945
N	4.07354	0.16039	0.04638
C	4.55956	-0.9982	0.46433
C	4.27056	-3.40232	1.16265
C	5.99668	-1.11449	0.71749
C	5.66688	-3.48049	1.4104
C	3.4654	-4.51751	1.3943
C	6.85419	-0.03538	0.50346
C	6.52308	-2.34771	1.18582
C	6.22472	-4.70111	1.88681
H	2.40256	-4.43851	1.20507
C	4.01797	-5.70965	1.86348
C	8.22258	-0.15363	0.74902
H	6.43688	0.89493	0.14
C	7.92036	-2.46082	1.43667
C	5.37838	-5.80268	2.10592

C	7.63685	-4.77574	2.13031
H	3.37582	-6.5666	2.03868
C	8.75013	-1.34814	1.21049
H	8.87442	0.69645	0.57612
C	8.44569	-3.70772	1.91442
H	5.80652	-6.73179	2.47031
H	8.04902	-5.7127	2.49279
H	9.81534	-1.43764	1.40189
H	9.51274	-3.77974	2.10247
C	2.59759	2.6637	-0.90662
C	1.99045	3.75099	-1.5678
S	4.19139	3.14821	-0.3762
N	0.78155	3.72381	-2.15857
C	2.8139	4.9369	-1.59918
C	4.03806	4.74615	-0.98589
C	0.37713	4.8309	-2.76124
N	2.37512	6.08047	-2.18043
C	1.18427	6.04351	-2.74245
C	-0.9018	4.82521	-3.47245
C	0.66175	7.26634	-3.36309
C	-1.36938	6.02314	-4.0781
C	-1.6624	3.6599	-3.57421
C	1.38898	8.45452	-3.32031
C	-0.59939	7.23595	-4.01302
C	-2.61755	6.01912	-4.76254
H	-1.28806	2.75231	-3.11851
C	-2.88103	3.66106	-4.25433
C	0.8884	9.617	-3.909
H	2.34914	8.45401	-2.81989
C	-1.10173	8.42332	-4.61801
C	-3.35557	4.82345	-4.83743
C	-3.09088	7.23501	-5.35982
H	-3.45919	2.74567	-4.31837
C	-0.33908	9.60341	-4.5495
H	1.46713	10.53383	-3.86394
C	-2.3701	8.38277	-5.28735
H	-4.30626	4.82241	-5.36232
H	-4.04619	7.21787	-5.87596
H	-0.72573	10.50782	-5.00999
H	-2.74215	9.29509	-5.74403
C	5.1878	5.76031	-0.8403
C	6.41203	5.56975	-0.22705
S	5.05747	7.33919	-1.50298
N	6.8358	4.43859	0.3884
C	7.25384	6.74062	-0.30077
C	6.6492	7.82582	-0.96796
C	8.05544	4.45281	0.88618
N	8.50077	6.73791	0.20507
C	7.1751	9.12713	-1.20528
C	8.54779	3.25281	1.57263
C	8.9209	5.6194	0.7753

C	6.65525	10.12778	-2.04844
S	8.61425	9.72607	-0.41285
C	7.73241	2.13259	1.72334
C	9.87021	3.23542	2.08712
C	10.28863	5.55645	1.29152
N	5.55332	10.00509	-2.8103
C	7.4258	11.33833	-2.04509
C	8.54432	11.29037	-1.19173
C	8.20254	0.99287	2.37783
H	6.72769	2.16837	1.3214
C	10.3459	2.06804	2.74981
C	10.73639	4.3738	1.94051
C	11.16079	6.63616	1.1495
C	5.20728	11.04423	-3.55443
N	7.06744	12.39496	-2.79696
C	9.52672	12.29899	-0.98149
C	9.49074	0.95928	2.88438
H	7.55339	0.13023	2.48742
C	11.68758	2.05188	3.25783
C	12.06477	4.3162	2.44894
H	10.80862	7.52738	0.64638
C	12.46382	6.57051	1.64484
C	5.97714	12.27404	-3.53848
C	4.02563	10.94007	-4.41204
C	10.51895	12.36709	0.01792
S	9.67902	13.69706	-2.01999
H	9.8563	0.07079	3.39077
C	12.5079	3.12325	3.11193
H	12.03832	1.15586	3.76129
C	12.91047	5.42913	2.28827
H	13.12381	7.42327	1.52904
C	5.54324	13.41093	-4.35221
C	3.63666	12.05648	-5.19914
C	3.27987	9.7627	-4.46879
N	10.66678	11.4886	1.02668
C	11.37891	13.52082	-0.10377
C	11.03181	14.32793	-1.17108
H	13.52275	3.09442	3.49742
H	13.92357	5.38189	2.67642
C	6.24606	14.61568	-4.33741
C	4.38653	13.28258	-5.16635
C	2.48512	11.95757	-6.03115
H	3.59378	8.92006	-3.8662
C	2.15413	9.67163	-5.28797
C	11.63737	11.72255	1.89596
N	12.39837	13.73068	0.76501
H	11.49401	15.25413	-1.47682
C	5.82718	15.69407	-5.11741
H	7.12146	14.69807	-3.70605
C	3.96589	14.38642	-5.96179
C	1.75988	10.75299	-6.05829

C	2.09394	13.09048	-6.82012
H	1.58675	8.74724	-5.31979
C	12.53997	12.85524	1.73913
C	11.79181	10.82929	3.04476
C	4.70404	15.58272	-5.92008
H	6.38618	16.62376	-5.09252
C	2.79939	14.24922	-6.78607
H	0.88286	10.68022	-6.69458
H	1.21355	13.00154	-7.44955
C	13.64498	13.03259	2.68836
C	12.86279	11.04111	3.95504
C	10.89774	9.78108	3.26544
H	4.38038	16.42299	-6.52711
H	2.49047	15.09842	-7.38821
C	14.55345	14.07875	2.53771
C	13.78826	12.12631	3.77091
C	13.01755	10.16675	5.06767
H	10.07995	9.63924	2.57073
C	11.05032	8.93306	4.36326
C	15.60534	14.24354	3.4404
H	14.42404	14.75852	1.70494
C	14.85921	12.30369	4.69276
C	12.09648	9.11885	5.2506
C	14.10894	10.3772	5.97527
H	10.34697	8.12146	4.51458
C	15.75742	13.3697	4.50361
H	16.30475	15.06231	3.30629
C	14.98987	11.39373	5.79428
H	12.21527	8.45475	6.10159
H	14.21648	9.7005	6.81778
H	16.57435	13.50117	5.20705
H	15.81112	11.53959	6.48967

Geometry Coordinates for *t*BuPTP hexamer

C	0.44277	-1.56936	-0.52714
C	-6.53351	-3.69913	2.07686
C	-5.22497	-3.50598	1.5967
C	-4.54967	-2.29823	1.74368
C	-5.18898	-1.21093	2.3938
C	-6.49833	-1.39465	2.90695
C	-7.14136	-2.63645	2.73456
C	-3.19318	-2.11794	1.21925
C	-4.5407	0.06059	2.53046
C	-3.24871	0.28848	1.99389
C	-2.5593	-0.80484	1.2957
C	-2.65403	1.53716	2.13233
H	-1.66851	1.66431	1.70281
C	-3.28873	2.60178	2.79839
C	-4.55588	2.37105	3.32003
C	-5.20096	1.12441	3.19786

C	-6.51672	0.8998	3.72363
C	-7.13743	-0.30071	3.58048
H	-8.13764	-0.45076	3.97635
H	-7.01585	1.71696	4.23629
H	-4.70616	-4.30544	1.08372
H	-8.14574	-2.73805	3.12862
H	-5.08835	3.15959	3.83892
N	-2.57571	-3.14891	0.66848
N	-1.3813	-0.56835	0.75703
C	-1.36255	-2.92438	0.12578
C	-0.76743	-1.60938	0.1405
C	-0.58089	-3.88523	-0.54347
S	0.85388	-3.10868	-1.16732
C	-7.23204	-5.05045	1.84847
C	-2.56831	3.95596	2.91681
C	-8.65826	-5.07806	2.42472
H	-8.66718	-4.92192	3.50708
H	-9.30265	-4.32344	1.96485
H	-9.11338	-6.05363	2.23483
C	-7.32167	-5.32639	0.32991
H	-6.33555	-5.3692	-0.13745
H	-7.81497	-6.28567	0.14579
H	-7.89722	-4.548	-0.17895
C	-6.41619	-6.17413	2.52463
H	-5.40132	-6.24114	2.1282
H	-6.3394	-6.01285	3.60295
H	-6.89788	-7.14344	2.36321
C	-2.28795	4.51126	1.50187
H	-1.77192	5.47439	1.56431
H	-1.66006	3.83716	0.91523
H	-3.21842	4.66338	0.9479
C	-3.4005	4.99757	3.68444
H	-4.35126	5.21041	3.18795
H	-3.61424	4.67792	4.70813
H	-2.84848	5.93922	3.74587
C	-1.22999	3.76266	3.66504
H	-1.39621	3.37492	4.67392
H	-0.56836	3.06497	3.14699
H	-0.70059	4.71644	3.75355
C	-0.9488	-5.22664	-0.85825
C	-0.91559	-5.86512	-2.11065
S	-1.47943	-6.36239	0.35783
N	-0.56033	-5.28242	-3.27202
C	-1.32575	-7.24005	-2.06356
C	-1.66624	-7.68059	-0.77203
C	-0.60304	-6.0259	-4.36501
N	-1.35356	-7.99824	-3.17645
C	-0.993	-7.42616	-4.31311
C	-0.25941	-5.41652	-5.65312
C	-0.98377	-8.22742	-5.54042
C	-0.28467	-6.21743	-6.82349

C	0.08237	-4.07162	-5.74574
C	-1.30722	-9.57993	-5.52077
C	-0.6355	-7.60591	-6.76691
C	0.04811	-5.62157	-8.06749
H	0.08307	-3.49688	-4.82888
C	0.41121	-3.4623	-6.97004
C	-1.31043	-10.36886	-6.68521
H	-1.55774	-10.01519	-4.56222
C	-0.63912	-8.38405	-7.95339
C	0.38781	-4.25511	-8.11155
C	0.02963	-6.43414	-9.2499
C	0.77741	-1.96815	-6.99542
C	-0.97759	-9.74979	-7.88438
C	-1.67356	-11.86078	-6.58506
C	-0.296	-7.75238	-9.19514
H	0.63347	-3.83222	-9.07861
H	0.28546	-5.97215	-10.19896
C	2.01973	-1.72993	-6.10712
C	1.09911	-1.46692	-8.41373
C	-0.40748	-1.1393	-6.44989
H	-0.96887	-10.31417	-8.8094
C	-1.63503	-12.56739	-7.95109
C	-0.66993	-12.56967	-5.64748
C	-3.10078	-12.0053	-6.00991
H	-0.30268	-8.3529	-10.10008
H	2.29277	-0.67013	-6.10949
H	1.84304	-2.02358	-5.06999
H	2.87918	-2.2999	-6.47067
H	1.95366	-1.99053	-8.8512
H	0.24764	-1.57792	-9.09083
H	1.35208	-0.40392	-8.38137
H	-1.30338	-1.28541	-7.05949
H	-0.65907	-1.40922	-5.42195
H	-0.16323	-0.07257	-6.46069
H	-2.34899	-12.13476	-8.65747
H	-0.64087	-12.53097	-8.40508
H	-1.89733	-13.62159	-7.82855
H	-0.68044	-12.14659	-4.6407
H	-0.91356	-13.63312	-5.56212
H	0.35097	-12.48785	-6.03045
H	-3.18745	-11.56397	-5.01458
H	-3.83624	-11.51643	-6.65464
H	-3.37343	-13.06214	-5.92857
C	-2.14298	-8.96557	-0.37798
C	-2.17453	-9.53795	0.90838
S	-2.83091	-10.09855	-1.51598
N	-1.6629	-8.97882	2.02327
C	-2.77489	-10.85047	0.9368
C	-3.17759	-11.27573	-0.31562
C	-1.73803	-9.67969	3.14215
N	-2.89742	-11.54105	2.09772

H	-3.63172	-12.21878	-0.57897
C	-2.40468	-10.97844	3.18122
C	-1.12031	-9.14753	4.36051
C	-2.53463	-11.68513	4.46248
C	-1.24561	-9.8754	5.57276
C	-0.40056	-7.95644	4.34455
C	-3.21195	-12.89596	4.54652
C	-1.95509	-11.1201	5.62564
C	-0.6486	-9.35404	6.74897
H	-0.32017	-7.43765	3.39806
C	0.21312	-7.43275	5.49762
C	-3.35076	-13.59649	5.75883
H	-3.63552	-13.28783	3.63069
C	-2.0754	-11.81653	6.85609
C	0.06859	-8.14351	6.68301
C	-0.78811	-10.08163	7.97782
C	1.01382	-6.12255	5.40436
C	-2.77438	-13.03931	6.89393
C	-4.12082	-14.92818	5.77762
C	-1.47225	-11.25461	8.03018
H	0.51723	-7.77852	7.59927
H	-0.33179	-9.67323	8.87482
C	0.09031	-4.98701	4.91131
C	1.608	-5.70227	6.75989
C	2.17785	-6.30581	4.40377
H	-2.84796	-13.54231	7.85105
C	-4.17014	-15.55779	7.18035
C	-5.57283	-14.68662	5.30659
C	-3.4341	-15.93144	4.82321
H	-1.56828	-11.79161	8.96938
H	0.64742	-4.04762	4.8424
H	-0.32698	-5.19444	3.92425
H	-0.74642	-4.83141	5.59716
H	0.83221	-5.52683	7.51046
H	2.3035	-6.44837	7.15455
H	2.16427	-4.76833	6.64485
H	2.85588	-7.10011	4.72842
H	1.8208	-6.56191	3.40395
H	2.75674	-5.38093	4.32034
H	-3.17165	-15.78652	7.56313
H	-4.67258	-14.90959	7.90369
H	-4.72746	-16.49759	7.14417
H	-5.61155	-14.27724	4.29479
H	-6.13543	-15.62539	5.30565
H	-6.08892	-13.98538	5.96821
H	-3.41203	-15.56733	3.79384
H	-2.40186	-16.12216	5.12941
H	-3.9683	-16.88666	4.82471
C	1.42081	-0.38003	-0.55025
C	2.8025	-0.42028	-0.5854
S	0.84242	1.23651	-0.57509

N	3.57555	-1.53521	-0.582
C	3.39191	0.89656	-0.63186
C	2.4425	1.93595	-0.61178
C	4.87738	-1.3585	-0.67026
N	4.72539	1.06242	-0.73671
C	2.66356	3.34481	-0.60407
C	5.46939	-0.02904	-0.78849
C	5.75319	-2.53768	-0.64636
C	1.7587	4.36768	-0.9391
S	4.17577	4.05297	-0.09212
C	6.91492	0.10408	-0.98932
C	7.15198	-2.36356	-0.79516
C	5.23	-3.81498	-0.48262
N	0.50057	4.17943	-1.38203
C	2.30399	5.68699	-0.78746
C	3.6306	5.69607	-0.32046
C	7.50098	1.34692	-1.20881
C	7.72381	-1.06176	-0.97965
C	7.98907	-3.50899	-0.77669
H	4.15585	-3.89802	-0.3768
C	6.04428	-4.96213	-0.45265
C	-0.21164	5.25601	-1.67004
N	1.57052	6.78141	-1.06746
C	4.47573	6.82214	-0.09357
C	8.88377	1.49941	-1.42036
H	6.84663	2.20898	-1.22099
C	9.12316	-0.9252	-1.1657
C	7.41433	-4.78335	-0.60102
C	9.40282	-3.33473	-0.94714
C	5.39581	-6.34442	-0.26401
C	0.3318	6.59321	-1.49104
C	-1.57204	5.09017	-2.19012
C	5.65731	6.89837	0.66892
S	4.15827	8.38845	-0.79913
C	9.67079	0.3546	-1.38362
C	9.4583	2.90038	-1.69126
C	9.94314	-2.10234	-1.13753
H	8.0841	-5.63529	-0.58851
H	10.03888	-4.21496	-0.92892
C	4.41312	-6.61102	-1.42688
C	6.43292	-7.48052	-0.2427
C	4.62399	-6.37189	1.07459
C	-0.506	7.76094	-1.77895
C	-2.34483	6.24367	-2.48011
C	-2.11097	3.82686	-2.40865
N	6.17035	5.89873	1.41382
C	6.27798	8.20127	0.6349
C	5.56619	9.10703	-0.12965
H	10.74197	0.42081	-1.53387
C	10.9804	2.87693	-1.91394
C	8.79579	3.48519	-2.95983

C	9.16042	3.822	-0.48819
H	11.01466	-1.98932	-1.27445
H	3.93789	-7.58986	-1.30923
H	3.61991	-5.86162	-1.47166
H	4.93179	-6.60235	-2.38953
H	6.99399	-7.54201	-1.17927
H	7.14818	-7.36739	0.5767
H	5.92741	-8.43984	-0.10359
H	5.29504	-6.19142	1.91895
H	3.8373	-5.61505	1.10919
H	4.1508	-7.34756	1.22276
C	-0.03482	9.05374	-1.57653
C	-1.8213	7.56135	-2.27087
C	-3.66065	6.0766	-2.9841
H	-1.4843	2.97502	-2.17926
C	-3.4114	3.64119	-2.91135
C	7.26595	6.15997	2.10676
N	7.43143	8.44675	1.30493
H	5.79373	10.1476	-0.30386
H	11.51808	2.50318	-1.03806
H	11.26098	2.26376	-2.77502
H	11.34019	3.89113	-2.10597
H	7.71287	3.57603	-2.85149
H	9.19045	4.48409	-3.16936
H	8.99094	2.85554	-3.83249
H	8.08954	3.92062	-0.30089
H	9.62167	3.44	0.42614
H	9.55698	4.82551	-0.6708
C	-0.81726	10.19017	-1.84977
H	0.97094	9.15949	-1.19143
C	-2.62366	8.69574	-2.55828
C	-4.1634	4.77671	-3.18922
C	-4.44452	7.24384	-3.27015
C	-3.93974	2.21271	-3.12938
C	7.9285	7.45842	2.01867
C	7.81101	5.12937	2.99556
C	-2.10144	9.98594	-2.34088
C	-0.23024	11.58961	-1.59543
C	-3.95068	8.49315	-3.06491
H	-5.17089	4.68619	-3.57804
H	-5.45096	7.10924	-3.65557
C	-3.94218	1.45602	-1.78157
C	-5.37177	2.19613	-3.69093
C	-3.02268	1.47265	-4.12933
C	9.18719	7.67747	2.74368
C	9.01542	5.39143	3.69968
C	7.1606	3.912	3.17433
H	-2.74201	10.82946	-2.56983
C	-1.21634	12.71424	-1.95549
C	0.1328	11.72785	-0.09944
C	1.04369	11.7762	-2.45036

H	-4.55908	9.36552	-3.28495
H	-4.31145	0.43487	-1.91811
H	-2.9419	1.39069	-1.34766
H	-4.58766	1.95278	-1.052
H	-6.08428	2.67736	-3.01524
H	-5.43643	2.69091	-4.66396
H	-5.70254	1.16338	-3.82895
H	-3.00102	1.9838	-5.09568
H	-1.99405	1.4023	-3.76909
H	-3.38458	0.45332	-4.2957
C	9.87396	8.88125	2.63782
C	9.70133	6.64311	3.56454
C	9.53969	4.38939	4.55568
H	6.23994	3.75598	2.62707
C	7.65651	2.913	4.03252
H	-1.49184	12.69561	-3.01362
H	-2.13384	12.6621	-1.36284
H	-0.75632	13.68581	-1.75653
H	0.87001	10.98543	0.21371
H	0.55432	12.7177	0.10078
H	-0.75088	11.60411	0.53255
H	1.80925	11.0348	-2.21111
H	0.81841	11.68802	-3.51668
H	1.47637	12.76663	-2.27801
C	11.08012	9.12062	3.32163
H	9.44039	9.64111	2.00036
C	10.91134	6.86897	4.2705
C	8.84599	3.17231	4.70268
C	10.76526	4.64788	5.25573
C	6.87461	1.59903	4.20156
C	11.57478	8.10395	4.12959
C	11.78922	10.47512	3.15058
C	11.42216	5.82934	5.11681
H	9.27183	2.43244	5.36998
H	11.16229	3.8736	5.90572
C	6.74145	0.89756	2.83202
C	7.56714	0.62687	5.17236
C	5.46549	1.91118	4.75533
H	12.49712	8.24049	4.682
C	13.08693	10.56594	3.97167
C	12.14602	10.6817	1.6611
C	10.84659	11.60964	3.61245
H	12.34916	6.00747	5.65406
H	6.18842	-0.04074	2.93836
H	6.20845	1.51219	2.10429
H	7.72227	0.66309	2.41043
H	8.56336	0.34031	4.82389
H	7.66388	1.04676	6.17758
H	6.97816	-0.28997	5.25854
H	5.52474	2.40322	5.73024
H	4.89939	2.56412	4.08757

H	4.89179	0.98739	4.87773
H	12.90238	10.46054	5.04435
H	13.8147	9.8058	3.6744
H	13.5547	11.54182	3.81674
H	11.25963	10.67068	1.02312
H	12.64511	11.64513	1.51778
H	12.82007	9.89717	1.30615
H	9.92218	11.63542	3.03153
H	10.57354	11.49035	4.66453
H	11.33561	12.58218	3.49911

References

[1] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, 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, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.